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

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

Carsten Beta
Biologische Physik
Institut für Physik und Astronomie
Universität Potsdam
Karl-Liebknecht-Str. 24/25
D-14476 Potsdam
beta@uni-potsdam.de

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

The Dynamics and Statistical Physics Division covers theoretical and experimental activities in all areas of statistical physics, quantum dynamics and many-body systems, nonlinear dynamics and pattern formation, data analysis and machine learning as well as active matter, fluid physics , soft matter and complex fluids. The DY section has strong links and joint sessions with the sections of Biological Physics (BP), Chemical Physics and Polymers (CPP), Socio- and Econophysics (SOE), and Low Temperatures (TT).

Overview of Invited Talks and Sessions

(Lecture halls MOL213, ZEU147, ZEU160, and ZEU250; Poster P1)

Invited Talks

DY 2.1	Mon	9:30–10:00	HSZ 03	**Enhanced variational Monte Carlo for Rydberg atom arrays** — •Stefanie Czischek
DY 2.2	Mon	10:00–10:30	HSZ 03	**Data mining the output of quantum simulators – from critical behavior to algorithmic complexity** — •Marcello Dalmonte
DY 2.3	Mon	10:30–11:00	HSZ 03	**Reinforcement learning for quantum technologies** — •Florian Marquardt
DY 2.4	Mon	11:00–11:30	HSZ 03	**Machine learning of phase transition** — •Christof Weitenberg
DY 5.1	Mon	9:30–10:00	MOL 213	**Extreme events, entropies and instantons for turbulence and water waves** — •Joachim Peinke, André Fuchs, Matthias Wächter
DY 8.1	Mon	12:30–13:00	ZEU 250	**Novel phenomena and analysis methods in oscillator networks: higher-order interactions, higher-order averaging, and inference** — •Hiroshi Kori
DY 10.6	Mon	16:30–17:00	ZEU 160	**Long-range communications enable the hierarchical self-organization of active matter** — •Igor Aronson, Alexander Ziepke, Ivan Maryshev, Erwin Frey
DY 11.1	Mon	15:00–15:30	ZEU 250	**The challenge of structured disorder in statistical physics** — •Marc Mezard
DY 11.2	Mon	15:30–16:00	ZEU 250	**The emergence of concepts in shallow neural-networks** — •Elena Agliari
DY 11.3	Mon	16:00–16:30	ZEU 250	**Adaptive Kernel Approaches to Feature Learning in Deep Neural Networks** — •Zohar Ringel
DY 11.5	Mon	17:00–17:30	ZEU 250	**Analysing the dynamics of message passing algorithms** — •Manfred Opper, Burak Cakmak
DY 11.6	Mon	17:30–18:00	ZEU 250	**Deep Learning Theory Beyond the Kernel Limit** — •Cengiz Pehlevan
DY 14.1	Tue	9:30–10:00	MOL 213	**Unraveling structural and dynamical features in glassy fluids using machine learning** — •Laura Filion, Frank Smallenburg, Rinske Alkemade
DY 25.1	Wed	9:30–10:00	MOL 213	**Many-body localization from Hilbert- and real-space points of view** — •Ivan Khaymovich, Giuseppe De Tomasi, Frank Pollmann, Simone Warzel
DY 26.1	Wed	9:30–10:00	ZEU 160	**More is different: High-throughput 3D tracking reveals bacterial navigation strategies** — •Katja Taute

DY 26.2	Wed	10:00–10:30	ZEU 160	**Variability and heterogeneity in natural swarms** — •Gil Ariel
DY 26.5	Wed	11:15–11:45	ZEU 160	**Superstatistical Analysis and Modelling of Complex Dynamical Systems** — •Claus Metzner, Christoph Mark, Ben Fabry, Patrick Krauss, Achim Schilling, Maximilian Traxdorf, Holger Schulze
DY 27.1	Wed	9:30–10:00	ZEU 250	**Evolution in changing environments and driven disordered systems** — •Joachim Krug, Suman Das, Muhittin Mungan
DY 37.6	Thu	11:00–11:30	MOL 213	**Power law error growth rates – a dynamical mechanism for a strictly finite prediction horizon in weather forecasts** — Hynek Bednar, Jonathan Brisch, Burak Budanur, •Holger Kantz
DY 38.1	Thu	9:30–10:00	ZEU 160	**Acoustically propelled nano- and microparticles: From fundamentals to applications** — •Raphael Wittkowski
DY 56.5	Fri	10:30–11:00	ZEU 160	**Transport and self-organization in living fluids** — •Matthias Weiss

Invited Talks of the joint Symposium Dynamics of Opinion Formation – From Quorum Sensing to Polarization (SYOF)

See SYOF for the full program of the symposium.

SYOF 1.1	Mon	9:30–10:00	HSZ 01	**Towards understanding of the social hysteresis – insights from statistical physics** — •Katarzyna Sznajd-Weron
SYOF 1.2	Mon	10:00–10:30	HSZ 01	**Polarization in attitude distributions from surveys and models of continuous opinion dynamics** — •Jan Lorenz, Martin Gestefeld
SYOF 1.3	Mon	10:30–11:00	HSZ 01	**Collective patterns and stable misunderstandings in networks striving for consensus without a common value system** — •Johannes Falk, Edwin Eichler, Katja Windt, Marc-Thorsten Hütt
SYOF 1.4	Mon	11:15–11:45	HSZ 01	**A yet undetected cognitive bias, revealed by opinion dynamics simulations** — •Guillaume Deffuant
SYOF 1.5	Mon	11:45–12:15	HSZ 01	**Extreme switches in kinetic exchange models of opinion.** — •Parongama Sen, Kathakali Biswas

Invited Talks of the joint Symposium SKM Dissertation Prize 2023 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ 04	**Diffusion of antibodies in solution: from individual proteins to phase separation domains** — •Anita Girelli
SYSD 1.2	Mon	10:00–10:30	HSZ 04	**Intermediate Filament Mechanics Across Scales** — •Anna V. Schepers
SYSD 1.3	Mon	10:30–11:00	HSZ 04	**Ultrafast Probing and Coherent Vibrational Control of a Surface Structural Phase Transition** — •Jan Gerrit Horstmann
SYSD 1.4	Mon	11:00–11:30	HSZ 04	**Electro-active metasurfaces employing metal-to-insulator phase transitions** — •Julian Karst
SYSD 1.5	Mon	11:30–12:00	HSZ 04	**The role of unconventional symmetries in the dynamics of many-body systems** — •Pablo Sala

Invited Talks of the joint Symposium Physics of Fluctuating Paths (SYFP)

See SYFP for the full program of the symposium.

SYFP 1.1	Tue	9:30–10:00	HSZ 01	**Time at which a stochastic process achieves its maximum** — •Satya Majumdar
SYFP 1.2	Tue	10:00–10:30	HSZ 01	**Fluctuations and molecule-spanning dynamics of single Hsp90 proteins on timescales from nanoseconds to days** — •Thorsten Hugel
SYFP 1.3	Tue	10:30–11:00	HSZ 01	**Path reweighting for Langevin dynamics** — •Bettina Keller
SYFP 1.4	Tue	11:15–11:45	HSZ 01	**Out-of-equilibrium dynamics of trapped Brownian particles** — •Raul A. Rica
SYFP 1.5	Tue	11:45–12:15	HSZ 01	**Thermodynamics of Clocks** — •Patrick Pietzonka

Invited Talks of the joint Symposium Topology in Quantum and Classical Physics – From Topological Insulators to Active Matter (SYQC)

See SYQC for the full program of the symposium.

SYQC 1.1	Wed	15:00–15:30	HSZ 01	**Topological magnetic whirls for computing** — •Karin Everschor-Sitte
SYQC 1.2	Wed	15:30–16:00	HSZ 01	**Topological waves from solids to geo/astrophysical flows** — •Pierre Delplace, Antoine Venaille, Nicolas Perez, Guillaume Laibe, Armand Leclerc, Manolis Perrot, Brad Marston
SYQC 1.3	Wed	16:00–16:30	HSZ 01	**Topological Phase Transitions in Population Dynamics** — •Erwin Frey
SYQC 1.4	Wed	16:45–17:15	HSZ 01	**Topological invariants protect robust chiral currents in active matter** — •Evelyn Tang
SYQC 1.5	Wed	17:15–17:45	HSZ 01	**Topological defects in biological active matter** — •Amin Doostmohammadi

Sessions

DY 1.1–1.3	Sun	16:00–18:15	HSZ 01	**Tutorial: Physics Meets Machine Learning (joint session DY/TUT/TT)**
DY 2.1–2.9	Mon	9:30–13:00	HSZ 03	**Focus Session: Physics Meets ML I – Machine Learning for Complex Quantum Systems (joint session TT/DY)**
DY 3.1–3.12	Mon	9:30–13:00	TOE 317	**Active Matter I (joint session BP/CPP/DY)**
DY 4.1–4.11	Mon	9:30–12:30	ZEU 250	**Pattern Formation, Delay and Nonlinear Stochastic Systems**
DY 5.1–5.9	Mon	9:30–12:15	MOL 213	**Fluid Physics: Turbulence and Convection**
DY 6.1–6.11	Mon	10:00–13:00	ZEU 160	**Statistical Physics: General I**
DY 7.1–7.10	Mon	10:00–12:45	ZEU 147	**Granular Matter and Contact Dynamics**
DY 8.1–8.1	Mon	12:30–13:00	ZEU 250	**Invited Talk: Dynamics of Networks (joint session DY/SOE)**
DY 9.1–9.12	Mon	14:00–17:15	MOL 213	**Quantum Dynamics, Decoherence and Quantum Information**
DY 10.1–10.11	Mon	15:00–18:15	ZEU 160	**Active Matter II (joint session DY/BP/CPP)**
DY 11.1–11.8	Mon	15:00–18:30	ZEU 250	**Focus Session: Physics Meets ML II – Understanding Machine Learning as Complex Interacting Systems (joint session DY/TT)**
DY 12.1–12.13	Tue	9:30–13:15	HSZ 204	**Nonequilibrium Quantum Many-Body Systems I (joint session TT/DY)**
DY 13.1–13.11	Tue	9:30–12:30	TOE 317	**Active Matter III (joint session BP/CPP/DY)**
DY 14.1–14.1	Tue	9:30–10:00	MOL 213	**Invited Talk: Machine Learning and Complex Fluids**
DY 15.1–15.1	Tue	9:30–10:00	ZEU 260	**Physics of Contagion Processes I (joint session SOE/DY)**
DY 16.1–16.11	Tue	10:00–13:00	MOL 213	**Complex Fluids and Soft Matter (joint session DY/CPP)**
DY 17.1–17.10	Tue	10:00–12:45	ZEU 160	**Machine Learning in Dynamics and Statistical Physics I**
DY 18.1–18.8	Tue	10:00–12:15	ZEU 147	**Nonlinear Dynamics, Synchronization and Chaos**
DY 19.1–19.3	Tue	10:00–10:45	ZEU 260	**Physics of Contagion Processes II (joint session SOE/DY)**
DY 20.1–20.5	Tue	11:00–12:15	ZEU 260	**Networks: From Topology to Dynamics I (joint session SOE/DY)**
DY 21.1–21.5	Tue	14:00–15:15	MOL 213	**Quantum Chaos and Coherent Dynamics**
DY 22.1–22.5	Tue	14:00–15:15	ZEU 160	**Machine Learning in Dynamics and Statistical Physics II**
DY 23.1–23.5	Tue	14:00–15:15	ZEU 250	**Statistical Physics: General II**
DY 24.1–24.4	Tue	14:00–15:00	ZEU 147	**Glasses and Glass Transition (joint session DY/CPP)**
DY 25.1–25.12	Wed	9:30–13:00	MOL 213	**Many-Body Quantum Dynamics (joint session DY/TT)**
DY 26.1–26.10	Wed	9:30–13:00	ZEU 160	**Focus Session: From Inter-individual Variability to Heterogeneous Group Dynamics and Disorder in Active Matter (joint session DY/BP/CPP)**
DY 27.1–27.12	Wed	9:30–13:00	ZEU 250	**Statistical Physics: Far From Equilibrium I**
DY 28.1–28.5	Wed	9:30–11:45	ZEU 260	**Focus Session: Critical Transitions in Society, Economy, and Nature (joint session SOE/DY)**
DY 29.1–29.11	Wed	10:00–13:00	ZEU 147	**Wetting, Droplets and Microfluidics (joint session DY/CPP)**
DY 30.1–30.13	Wed	15:00–18:30	HSZ 204	**Nonequilibrium Quantum Many-Body Systems II (joint session TT/DY)**
DY 31.1–31.12	Wed	15:00–18:15	MOL 213	**Microswimmers and Fluid Physics of Life (joint session DY/CPP)**

DY 32.1–32.12	Wed	15:00–18:15	ZEU 160	**Focus Session: Physics of Fluctuating Paths (joint session DY/CPP)**
DY 33.1–33.6	Wed	15:00–16:30	ZEU 250	**Biologically Inspired Statistical Physics (joint session DY/BP)**
DY 34.1–34.6	Wed	16:45–18:15	ZEU 250	**Statistical Physics: Far From Equilibrium II**
DY 35.1–35.12	Thu	9:30–13:00	TOE 317	**Statistical Physics of Biological Systems I (joint session BP/DY)**
DY 36.1–36.13	Thu	9:30–13:00	MER 02	**Wetting, Fluidics and Liquids at Interfaces and Surfaces I (joint session CPP/DY)**
DY 37.1–37.8	Thu	9:30–12:00	MOL 213	**Data Analytics of Complex Dynamical Systems (joint session DY/SOE)**
DY 38.1–38.12	Thu	9:30–13:00	ZEU 160	**Active Matter IV (joint session DY/BP/CPP)**
DY 39.1–39.1	Thu	9:30–10:00	ZEU 260	**Networks: From Topology to Dynamics II (joint session SOE/DY)**
DY 40.1–40.9	Thu	10:00–12:30	ZEU 250	**Stochastic Thermodynamics**
DY 41.1–41.3	Thu	10:00–10:45	ZEU 260	**Networks: From Topology to Dynamics III (joint session SOE/DY)**
DY 42.1–42.17	Thu	13:00–16:00	P1	**Poster: Active Matter, Soft Matter, Fluids**
DY 43.1–43.22	Thu	13:00–16:00	P1	**Poster: Quantum Dynamics and Many-Body Systems**
DY 44.1–44.22	Thu	13:00–16:00	P1	**Poster: Statistical Physics**
DY 45.1–45.16	Thu	13:00–16:00	P1	**Poster: Nonlinear Dynamics, Pattern Formation and Networks**
DY 46.1–46.10	Thu	13:00–16:00	P1	**Poster: Machine Learning and Data Analytics**
DY 47.1–47.5	Thu	15:00–16:15	MER 02	**Wetting, Fluidics and Liquids at Interfaces and Surfaces II (joint session CPP/DY)**
DY 48.1–48.9	Thu	15:00–17:30	MOL 213	**Dynamics and Chaos in Many-Body Systems I (joint session DY/TT)**
DY 49.1–49.10	Thu	15:00–17:45	ZEU 160	**Critical Phenomena and Phase Transitions**
DY 50.1–50.2	Thu	15:00–15:30	ZEU 260	**Evolutionary Game Theory (joint session SOE/DY)**
DY 51	Thu	18:00–19:00	ZEU 160	**Members' Assembly**
DY 52.1–52.9	Fri	9:30–12:00	BAR Schö	**Statistical Physics of Biological Systems II (joint session BP/DY)**
DY 53.1–53.8	Fri	9:30–12:00	TOE 317	**Active Matter V (joint session BP/CPP/DY)**
DY 54.1–54.12	Fri	9:30–13:00	MER 02	**Complex Fluids and Colloids, Micelles and Vesicles (joint session CPP/DY)**
DY 55.1–55.11	Fri	9:30–12:30	MOL 213	**Dynamics and Chaos in Many-Body Systems II (joint session DY/TT)**
DY 56.1–56.11	Fri	9:30–12:45	ZEU 160	**Brownian Motion and Anomalous Diffusion**
DY 57.1–57.8	Fri	9:30–11:45	ZEU 250	**Networks: From Topology to Dynamics IV (joint session DY/SOE)**

Members' Assembly of the Dynamics and Statistical Physics Division

Thursday 18:00–19:00 ZEU 160

- Report
- Elections
- Future activities of DY
- Any other business

DY 1: Tutorial: Physics Meets Machine Learning (joint session DY/TUT/TT)

Machine learning has revolutionized many application fields such as computer vision and natural language processing. In physics there is a growing interest in using machine learning to enhance the analysis of experimental data and to devise and optimize experiments or numerical simulations. On the other hand physicists use their intuition and methods from statistical physics and complex systems theory to better understand the working principles of modern machine learning methods. This tutorial session introduces some subfields within this area and the basic methods involved.

Organized by Sabine Andergassen (Tübingen), Martin Gärttner (Heidelberg), Moritz Helias (Jülich), and Markus Schmitt (Cologne)

Time: Sunday 16:00–18:15 Location: HSZ 01

Tutorial DY 1.1 Sun 16:00 HSZ 01

Machine Learning for Quantum Technologies — •Florian Marquardt — Max Planck Institute for the Science of Light and Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany

Machine learning is revolutionizing science and technology. In the past few years, it has become clear that it promises significant benefits as well for the development of quantum technologies. In this tutorial I will first give a brief introduction to neural networks. I will then discuss a number of areas and examples in which machine learning is being successfully applied in this context. These include measurement data analysis and quantum state representation, approximate quantum dynamics, parameter estimation, discovering strategies for hardware-level quantum control, the optimization of quantum circuits, and the discovery of quantum experiments, discrete quantum feedback strategies, and quantum error correction protocols.

Reference: "Artificial intelligence and machine learning for quantum technologies", M. Krenn, J. Landgraf, T. Foesel, and F. Marquardt, Phys. Rev. A 107, 010101 (2023).

Tutorial DY 1.2 Sun 16:45 HSZ 01

The Unreasonable Effectiveness of Gaussians in the Theory of Deep Neural Networks — •Zohar Ringel — Racah Institute of Physics, Hebrew University in Jerusalem

Physical Sciences are in many ways the success story of explaining fundamental phenomena using simple math [1]. The fact that physical phenomena could be arranged in that manner is remarkable. Yet this simplicity does not necessarily carry over to life sciences or data sciences. Indeed prominent authors have argued against our desire to rely on neat mathematical structures when analyzing big data [2].

In the past half-decade several results have emerged which balance mathematical simplicity with data-induced complexity. These could be seen as a middle ground between the above juxtaposing views. The common divider here is the use of Gaussian distributions as approximants of various different quantities in deep neural networks (DNNs). Specifically these Gaussians emerge when describing outputs of DNNs with random weights, outputs of trained DNNs at random times, outputs of fixed DNNs over random input data, and fluctuations of hidden DNN pre-activations. In this tutorial I will present these quantities, provide arguments supporting their Gaussianity, and outline several theoretical implications.

[1] The Unreasonable Effectiveness of Mathematics in the Natural Sciences. Wigner (1960)

[2] The Unreasonable Effectiveness of Data. Halevy, Norvig, Pereira (2009)

Tutorial DY 1.3 Sun 17:30 HSZ 01

Computing learning curves for large machine learning models using the replica approach — •Manfred Opper — Inst. für Softwaretechnik und Theor. Informatik, TU Berlin — Centre for Systems Modelling and Quantitative Biomedicine, University of Birmingham, UK

Methods of statistical physics have been used for a long time to mathematically analyse the typical performance of machine learning models in the limit where both the number of data and the number of parameters (such as network weights) is large. By defining Boltzmann-Gibbs probability distributions over parameters where the cost function of the machine learning problem plays the role of a hamiltoninan, one can derive analytical expressions for training errors and generalisation errors using the corresponding partition functions and free energies in terms of a usually small number of order parameters.

Since the models depend on a set of random data to be learnt, additional appropriate statistical (so-called quenched) averages of free energies over this 'disorder' have to be performed. The replica approach is a prominent analytical tool from the statistical physics of disordered systems to solve this nontrivial technical challenge.

In this tutorial I will give an introduction to this approach. Starting with an explicit calculation for simple single layer perceptrons, I will then argue how the method can be applied to more complex problems such as kernel machines (support vector machines and Gaussian processes) and multilayer networks.

DY 2: Focus Session: Physics Meets ML I – Machine Learning for Complex Quantum Systems (joint session TT/DY)

Modern machine learning methods open new perspectives on the high-dimensional data arising naturally in complex quantum systems. The applications range from the analysis of experimental observations over optimal control to the enhancement of numerical simulations in and out of equilibrium. This focus session brings together experts in the field to discuss recent progress and promising directions for future research.

Organizers: Markus Schmitt (University of Cologne), Martin Gärttner (University of Heidelberg)

Time: Monday 9:30–13:00 Location: HSZ 03

Invited Talk DY 2.1 Mon 9:30 HSZ 03

Enhanced variational Monte Carlo for Rydberg atom arrays — •Stefanie Czischek — Department of Physics, University of Ottawa, Ottawa, Canada, K1N 6N6

Rydberg atom arrays are promising candidates for high-quality quantum computation and quantum simulation. However, long state preparation times limit the amount of measurement data that can be generated at reasonable timescales. This restriction directly affects the estimation of operator expectation values, as well as the reconstruction and characterization of quantum states.

Over the last years, neural networks have been explored as a powerful and systematically tuneable ansatz to represent quantum wave functions. Via tomographical state reconstruction, such numerical models can significantly reduce the amount of necessary measurements to accurately reconstruct operator expectation values. At the same time, neural networks can find ground state wave functions of given Hamiltonians via variational energy minimization.

While both approaches experience individual limitations, a combination of the two leads to a significant enhancement in the variational ground state search by naturally finding an improved network initialization from a limited amount of measurement data. Additional specific modifications of the neural network model and its implementation can further optimize the performance of variational Monte Carlo simulations for Rydberg atom arrays and provide significant insights into their behaviour.

Invited Talk DY 2.2 Mon 10:00 HSZ 03

Data mining the output of quantum simulators – from critical behavior to algorithmic complexity — •Marcello Dalmonte — Abdus Salam International Centre for Theoretical Physics, Trieste (I)

Recent experiments with quantum simulators and noisy intermediate-scale quantum devices have demonstrated unparalleled capabilities of probing many-body wave functions, via directly probing them at the single quantum level via projective measurements. However, very little is known about to interpret and analyse such huge datasets. In this talk, I will show how it is possible to provide such characterisation of many-body quantum hardware via a direct and assumption-free data mining. The core idea of this programme is the fact that the output of quantum simualtors and computers can be construed as a very high-dimensional manifold. Such manifold can be characterised via basic topological concepts, in particular, by their intrinsic dimension. Exploiting state of the art tools in non-parametric learning, I will discuss theoretical results for both classical and quantum many-body spin systems that illustrate how data structures undergo structural transitions whenever the underlying physical system does, and display universal (critical) behavior in both classical and quantum mechanical cases. I will conclude with remarks on the applicability of our theoretical framework to synthetic quantum systems (quantum simulators and quantum computers), and emphasize its potential to provide a direct, scalable measure of Kolmogorov complexity of output states.

Invited Talk DY 2.3 Mon 10:30 HSZ 03

Reinforcement learning for quantum technologies — •Florian Marquardt — Max Planck Institute for the Science of Light and Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany

Complex quantum devices require sophisticated control. Discovering such control strategies from scratch with the help of machine learning will enable us to keep pace with the ever-increasing demands encountered when scaling up quantum computers. In this talk, I will describe how the field of reinforcement learning can deliver on this promise. I will present examples ranging from the optimization of quantum circuits to the model-based discovery of better quantum feedback strategies. Moreover, in a recent collaboration with our experimental colleagues, we could show how to train a novel latency-optimized neural network by reinforcement learning in an experiment, acting on a superconducting qubit in cycles of less than one microsecond.

Invited Talk DY 2.4 Mon 11:00 HSZ 03

Machine learning of phase transition — •Christof Weitenberg — Universität Hamburg, Institut für Laserphysik, Hamburg, Germany

Machine learning is emerging as vital tool in many sciences. In quantum physics, notable examples are neural networks for the efficient representation of quantum many-body states and reinforcement learning of preparation and read-out routines. In this talk, I will present our results on machine learning of quantum phase transitions using classification techniques. This approach works very well even on noisy experimental data both with supervised and unsupervised machine learning, as we demonstrate for quantum simulators based on ultracold atoms. Next to the practical advantages, such techniques might in the future reveal phase transitions, for which conventional order parameters are not known.

15 min. break

DY 2.5 Mon 11:45 HSZ 03

Machine learning optimization of Majorana hybrid nanowires — •Matthias Thamm and Bernd Rosenow — Institut für Theoretische Physik, Universität Leipzig

As the complexity of quantum systems such as quantum bit arrays increases, efforts to automate expensive tuning are increasingly worthwhile. We investigate machine learning based tuning of gate arrays using the CMA-ES algorithm for the case study of Majorana wires with strong disorder. We find that the algorithm is able to efficiently improve the topological signatures, learn intrinsic disorder profiles, and completely eliminate disorder effects. For example, with only 20 gates, it is possible to fully recover Majorana zero modes destroyed by disorder by optimizing gate voltages.

DY 2.6 Mon 12:00 HSZ 03

Model-independent learning of quantum phases of matter with quantum convolutional neural networks — •Yu-Jie Liu[1], Adam Smith[2], Michael Knap[1], and Frank Pollmann[1] — [1]Technical University of Munich, 85748 Garching, Germany — [2]University of Nottingham, Nottingham, NG7 2RD, UK

Quantum convolutional neural networks (QCNNs) have been introduced as classifiers for gapped quantum phases of matter. Here, we propose a model-independent protocol for training QCNNs to discover order parameters that are unchanged under phase-preserving perturbations. We initiate the training sequence with the fixed-point wavefunctions of the quantum phase and then add translation-invariant noise that respects the symmetries of the system to mask the fixed-point structure on short length scales. Without the translational invariance or other additional symmetries, we prove that a phase-classifying QCNN cannot exist. We illustrate this approach by training the QCNN on phases protected by time-reversal symmetry in one dimension, and test it on several time-reversal symmetric models exhibiting trivial, symmetry-breaking, and symmetry-protected topological order. The QCNN discovers a set of order parameters that identifies all three phases and accurately predicts the location of the phase boundary. The

proposed protocol paves the way towards hardware-efficient training of quantum phase classifiers on a programmable quantum processor.

DY 2.7 Mon 12:15 HSZ 03

Simulating spectral functions of two-dimensional systems with neural quantum states — •Tiago Mendes Santos[1], Markus Schmitt[2], and Markus Heyl[1] — [1]University of Augsburg, Augsburg, Germany — [2]Forschungszentrum Jülich, Jülich, Germany

Spectral functions are key tools to characterize and probe condensed matter systems. Simulating such quantities in interacting two-dimensional quantum matter is, however, still an outstanding challenge. This work presents a numerical approach to simulate spectral functions using Neural Quantum States. As the key aspect, our scheme leverage the flexibility of artificial-neural-network wave functions to access spectral properties by simulating the dynamics of localized excitations with the time-dependent variational Monte Carlo. For demonstration, we study the dynamical structure factor (DSF) of models describing two-dimensional quantum phase transitions, namely, the quantum Ising and a square-lattice Rydberg Atom Arrays model in a regime of parameters relevant to quantum simulators. When combined with deep network architectures whose number of variational parameters increase at a mild polynomial expense with the number of spins, we showcase that our approach reliably describes the DSF for unprecedented system sizes and time scales.

DY 2.8 Mon 12:30 HSZ 03

Efficient optimization of deep neural quantum states toward machine precision — •Ao Chen and Markus Heyl — Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany

Neural quantum states (NQSs) have emerged as a novel promising numerical method to solve the quantum many-body problem. However, it has remained a central challenge to train modern large-scale deep network architectures, which would be key to utilize the full power of NQSs and to make them competitive or superior to conventional numerical approaches. Here, we propose a minimum-step stochastic reconfiguration (MinSR) method that reduces the optimization complexity by orders of magnitude while keeping similar accuracy as compared to conventional stochastic reconfiguration. In this talk, I will show MinSR allows for an accurate training on unprecedentedly deep NQS with up to 64 layers and more than 10^5 parameters in the spin-1/2 Heisenberg J_1-J_2 models on the square lattice. With limited numerical resources, partly obtained on single workstations, we find that this approach yields better variational energies as compared to existing NQS results and we further observe that the accuracy of our ground state calculations approaches different levels of machine precision on modern GPU and TPU hardware.

DY 2.9 Mon 12:45 HSZ 03

Time-dependent variational principle for quantum and classical dynamics — •Moritz Reh[1], Markus Schmitt[2], and Martin Gärttner[1,3,4] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, 50937 Köln, Germany — [3]Physikalisches Institut, Universität Heidelberg, Im Neuenheimer Feld 226, 69120 Heidelberg, Germany — [4]Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 16, 69120 Heidelberg, Germany

The solution of many-body quantum dynamics is a challenging feat due to the curse of dimensionality, hindering the exploration of dynamics beyond a mediocre number of qubits. Neural Networks can variationally approximate the state of interest and therefore present a promising tool as they allow to efficiently represent the quantum state at the expense of truncating the Hilbert space.

We present such a scheme that is aimed at solving dissipative quantum dynamics using a probabilistic framework, i.e. the so-called POVM-formalism and demonstrate it for spin chains of up to 40 spins. We then show that the generality of the approach allows us to translate this formalism directly to the case of partial differential equations in high dimensions, defeating the exponential growth of grid cells when adding dimensions.

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

Time: Monday 9:30–13:00 Location: TOE 317

Invited Talk DY 3.1 Mon 9:30 TOE 317

Emergent properties in motile active matter — •Roland G. Winkler — Theoretical Physics of Living Matter (IBI-5/IAS-2), Forschungszentrum Jülich, Jülich

Motile active matter systems, ranging from assemblies of bacteria, self-organized bio-polymers such as the cytoskeleton of living cells, to schools of fish and flocks of birds, exhibit intriguing emerging structural and dynamical out-of-equilibrium properties, even with reminiscence to classical turbulence. Their spatiotemporal dynamics is controlled by the propulsion of the active agents in combination with various direct interactions. The latter are typically anisotropic and emerge from different sources, such as elongated agent shapes, intrinsic flexibility and constraints, microswimmer flow fields etc. By analytical theory and mesoscale simulations, we study the physical aspects of motile active matter, ranging from propulsion of bacteria and linear filaments to large-scale collective properties of active agents, and unravel its generic features. Studies on individual polymers reveal fundamental differences in their dynamical and conformational properties depending on their propulsion mechanism, which is illustrated for polymers either tangentially driven or composed of active Brownian particles. In the latter case, hydrodynamic interactions additionally affect the conformational properties, in contrasts to passive polymers. Moreover, hydrodynamic interactions determine the activity-induced phase behavior. For spherical microswimmers (squirmers), hydrodynamics suppresses motility-induced phase separation, but enhances collective turbulent-like large-scale flows.

DY 3.2 Mon 10:00 TOE 317

High-resolution mapping of odd fluctuations and oscillations in living chiral crystals — •Jinghui Liu[1,2], Lisa Lin[1], Yuchao Chen[1], Yu-Chen Chao[1], and Nikta Fakhri[1] — [1]Department of Physics, Massachusetts Institute of Technology — [2]Center for Systems Biology Dresden

It has been shown that active crystals formed by self-assembling clusters of swimming starfish embryos exhibit signatures of odd mechanics, such as self-sustained chiral waves. How are these observed chiral waves and oscillations are actuated and how their dynamics couple to the formation and dissolution of the living chiral crystal? Here, we report the use of vibrational mode decomposition to dissect various non-equilibrium phases of the crystal dynamics. By analyzing embryo cluster trajectories over the time course of crystal formation and dissolution, we identify the spatial modes responsible for the collective actuation of an oscillatory active crystal both in spontaneous and mechanically excited conditions. We also report a direct extraction of dispersion relation from fluctuations of confined crystals to infer odd elastic moduli. Taken together, our results unveil the complex spatiotemporal origin of mechanical waves in non-reciprocal materials and provide insight on the design principles of collective phases of active metamaterials.

DY 3.3 Mon 10:15 TOE 317

Self-organized chemotaxis of coupled cell populations — •Mehmet Can Ucar and Edouard Hannezo — Institute of Science and Technology Austria, Am Campus 1, 3400 Klosterneuburg, Austria

Many processes in development and disease such as tissue morphogenesis, cancer invasion and immune response rely on collective directional movement of cells. In a wide array of systems this collective motility is driven locally by self-generated chemokine or stiffness gradients, as opposed to pre-patterned, global guidance cues. While recent studies have explored migration mechanisms of a single species of cells, the role of self-generated gradients navigating multiple cell types remains largely untested. Here we address this issue by introducing a theoretical framework for self-organized guidance of chemotactically coupled cell populations. Combining analytical theory and simulations with experiments on immune cell populations, we discover a diverse spectrum of collective migration patterns controlled by single-cell proper-

ties. We find that differential chemotactic sensitivity leads to efficient colocalization of distinct cell types, and show that this coupling also depends on the geometry and initial configuration of the dynamical system. We finally outline conditions for robust, sustained multicellular interactions relevant for physiological settings such as during immune response.

DY 3.4 Mon 10:30 TOE 317

Geometry-induced patterns in collective cell migration — •David Brückner — Institute of Science and Technology, Am Campus 1, 3400 Klosterneuburg, Austria

The coordinated migration of cell collectives is increasingly well understood at the level of large two-dimensional confluent monolayers. However, many physiological migration processes rely on small polarized cell clusters and their responses to external confining geometries, such as 2D channels and 3D curved environments. How active motion and cell-cell interactions interplay with such external boundaries remains poorly understood. I will discuss how external geometries can induce patterns in collective cell migration, using two examples. First, we show that the migration efficiency of 2D confined cell clusters is determined by the contact geometry of cell-cell contacts that are either parallel or perpendicular to the direction of migration. Our minimal active matter model reveals how cell-cell interactions determine a geometry-dependent supracellular stress field that controls this response to external boundaries. Secondly, we show how the interplay of curvature and active flocking dynamics of 3D cell spheroids induces a collective mode of cell migration manifesting as a propagating velocity wave. Together, these approaches provide a conceptual framework to understand how cell-cell interactions interplay with 2D and 3D geometries to determine the emergent dynamics of collective cell migration.

DY 3.5 Mon 10:45 TOE 317

Shape primed AC-electrophoretic microrobots — •Florian Katzmeier and Friedrich C. Simmel — Technical University of Munich, Munich, Germany

Second-order electrokinetic flow around colloidal particles caused by concentration polarization electro-osmosis can be utilized to controllably move asymmetric particle dimers in AC electrical fields. To demonstrate this actuation mechanism, we created particle dimers from micron-sized silica spheres with sizes 1.01 μm and 2.12 μm by connecting them with DNA linker molecules. The dimers can be steered along arbitrarily chosen paths within a 2D plane by controlling the direction of the AC electric field in a fluidic chamber with the joystick of a gamepad. Further utilizing induced dipole-dipole interactions, we demonstrate that particle dimers can be used to controllably pick up monomeric particles and release them at any desired position, and also to assemble several particles into groups. Systematic experiments exploring the dependence of the movement direction and velocity on buffer composition, frequency, and field strength further elucidate the underlying physical mechanism, and provide operational parameter ranges for our micro robotic swimmers which we termed 'SPACE-bots'.

15 min. break

DY 3.6 Mon 11:15 TOE 317

Rodrolls: self-rolling rods powered by light and chemical gradients — •Ann Rosna George[1], Martin Wittmann[2], Antonio Stocco[1], Igor M. Kulić[1], and Juliane Simmchen[2] — [1]CNRS, Institute Charles Sadron, Strasbourg, France — [2]Physical chemistry, TU Dresden, Germany

The self-rolling motion upon spontaneous symmetry breaking is demonstrated by certain rod-shaped microorganisms like viruses. Hence it is imperative that we understand the mechanism of this symmetry breaking triggering the active rolling motion. This behaviour has also been demonstrated on the macroscopic scale by rod-like objects. It is very interesting to try and replicate this on a microscopic scale. The main aim of the project is to create a new class of active rods that exhibit rolling activity under chemical and optical gradients. To achieve this, it is important to understand the mechanism of activity of rod-like objects under chemical and optical stimuli.

Experiments conducted using silica Janus rods with a Platinum layer in an aqueous solution of H2O2 give interesting results and exhibit different kinds of activity when parameters like concentration of H2O2 and aspect ratio of rods are changed. Under specific conditions, particles are capable of switching their direction of motion. Experiments done using rods covered in gold nanoparticles under an optical gradient also reveal promising results of being able to make the rods roll upon providing sufficient energy to break the symmetry and fine-tuning certain parameters.

DY 3.7 Mon 11:30 TOE 317

Active Nematic Multipoles: Flow Responses and the Dynamics of Defects and Colloids — •Alexander J. H. Houston[1,2] and Gareth P. Alexander[1,3] — [1]Department of Physics, Gibbet Hill Road, University of Warwick, Coventry, CV4 7AL, United Kingdom — [2]Department of Physics, University of York, Heslington, York YO10 5DD, United Kingdom — [3]Centre for Complexity Science, Zeeman Building, University of Warwick, Coventry, CV4 7AL, United Kingdom

Two fundamental questions in active nematics are how to extract useful work from their non-equilibrium dynamics and how to extend the topological defect-based description of dynamics that has proved useful in two dimensions to three dimensions, in which the defects form geometrically-complex loops. We introduce a general description of localised distortions in active nematics using the framework of 'active nematic multipoles'. We give the Stokesian flows for arbitrary multipoles in terms of differentiation of a fundamental flow response and describe them explicitly up to quadrupole order. This allows the identification of the dipolar and quadrupolar distortions that generate self-propulsion and self-rotation respectively and serves as a guide for the design of arbitrary flow responses. Our results can be applied to both defect loops in three-dimensional active nematics and to systems with colloidal inclusions. They reveal the geometry-dependence of the self-dynamics of defect loops and provide insights into how colloids might be designed to achieve propulsive or rotational dynamics, and more generally for the extraction of work from active nematics.

DY 3.8 Mon 11:45 TOE 317

Structure and Dynamics of Active Polymer — •Sunil Pratap Singh — Indian Institute of Science Education and Research Bhopal, India, 462066

In this talk we are going to present structural and dynamical properties of a self-propelled filament using coarse-grained Brownian dynamics simulations. We consider two kinds of self-propulsion force on polymers, in case one force is applied tangent to the filament and in another model direction of active force is considered to be random. Case one shows that chain's stiffness and radius of gyration monotonically decrease. Moreover, the radius of gyration of the filament shows universal scaling for various bending rigidities with flexure number. In the latter model, where monomers are assumed to be active Brownian particle (ABP), displays a non-monotonic behaviour of end-to-end distance with activity strength. We will discuss here the role of many-body interactions on its structure and relaxation behavior. Additional we talk about the rheological behavior of chain under linear shear-flow. Our simulations reveal that active polymer's zero-shear viscosity varies in non-monotonic fashion with the active noise. More-importantly the viscosity decreases in the intermediate regime, that is followed by an increase in the more extensive Pe regime. We attribute the decrease of the zero-shear viscosity in the intermediate regime is due to many-body interactions among chain monomers.

DY 3.9 Mon 12:00 TOE 317

Pumping, Mixing, and Signal Transmission in Active Pores — •Goncalo Antunes[1,2,3], Paolo Malgaretti[1,2,3], Siegfried Dietrich[2,3], and Jens Harting[1,4] — [1]Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien (IEK–11), Forschungszentrum Jülich, Cauer Str. 1, 91058 Erlangen, Germany — [2]Max–Planck–Institut für Intelligente Systeme, Heisenbergstr. 3, 70569 Stuttgart, ,Germany — [3]IV. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [4]Department Chemie- und Bioingenieurwesen und Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Fürther Straße 248, 90429 Nürnberg, Germany

Much attention is currently being given to the problem of manipulating fluids at the microscale, with successful applications to fields such as 3D fabrication and biomedical research. An intriguing technique to manipulate fluid flows in a pore is diffusioosmosis. We show both numerically and analytically that a corrugated catalytic pore can act as a micropump even when it is fore-aft symmetric. This phenomenology is possible due to a spontaneous symmetry breaking which occurs when advection rather than diffusion is the dominant mechanism of solute

transport. Relaxing the condition of Stokes flow leads to unsteady flow, and persistent oscillations with a tunable frequency appear. We further include the inverse chemical reaction that consumes solute and introduces an additional timescale. Finally, we find that the flow may lose its axial symmetry and hence promote mixing in the low Reynolds number regime.

DY 3.10 Mon 12:15 TOE 317

Interacting particles in an activity landscape — •Adam Wysocki[1], Anil Kumar Dasanna[1,2], and Heiko Rieger[1,2] — [1]Department of Theoretical Physics and Center for Biophysics, Saarland University, Saarbrücken, Germany — [2]INM-Leibniz Institute for New Materials, Saarbrücken, Germany

We study interacting active Brownian particles (ABPs) with a space-dependent swim velocity. We find that, although an equation of state exists, a mechanical equilibrium does not apply to ABPs in activity landscapes. The pressure imbalance originates in the flux of polar order across the interface between regions of different activity. An active-passive patch system is mainly controlled by the smallest global density for which the passive patch can be close packed. Below this density a critical point does not exist and the system splits continuously into a dense passive and a dilute active phase with increasing activity. Above this density and for sufficiently high activity the active phase may start to phase separate into a gas and a liquid phase caused by the same mechanism as motility-induced phase separation of ABPs with a homogeneous swim velocity.

DY 3.11 Mon 12:30 TOE 317

Active phase fluctuations of Chlamydomonas axonemes — •Abhimanyu Sharma[1], Benjamin M. Friedrich[2], and Veikko F. Geyer[1] — [1]B CUBE - Center for Molecular Bioengineering, TU Dresden, Dresden, Germany — [2]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany

Cilia and eukaryotic flagella generate periodic beat patterns by the activity of dynein motors. Earlier studies revealed active fluctuations in the ciliary beat arising presumably from small number fluctuations in the collective dynamics of the molecular motors that drive the beat. A theoretical model of the beating cilium as a system of coupled motors predicts that the fluctuations measured in terms of the quality factor of the oscillations scale with the number of beat-generating-motors.

To measure those fluctuations experimentally, we use in situ reactivated axonemes, the mechanical core of motile cilia isolated from the green alga Chlamydomonas. To modulate the number of motors in beating axonemes, we make use of motor mutants or partially extract molecular motors biochemically.

Using shape mode analysis and limit-cycle reconstruction, we characterize the phase fluctuations in the beat and report for the first time the relation between beat parameters and the motor number in Chlamydomonas axonemes. We experimentally infer scaling relations for the beat frequency, mean beat amplitude, and the quality factor. Further, using mass spectrometry, we identify specific dynein motors and infer their role in regulating the beat fluctuations.

DY 3.12 Mon 12:45 TOE 317

Lattice dynamics of pulsating active particles — •Alessandro Manacorda and Étienne Fodor — University of Luxembourg

Cells in epithelial tissues can drastically deform their shapes and volume giving rise to collective behavior such as size oscillation and wave propagation. These phenomena have a strinking impact in many biological contexts such as embryonic development, cardiac arrhythmias and uterine contraction.

The theoretical models describing the emergence of contractile waves so far consider the cells as motile particles, where activity is represented by self-propulsion; however this ingredient is questionable in dense systems where particles barely move. We therefore introduce a novel class of active matter where the activity is the ability to change an internal degree of freedom at the single-particle level e.g. particles' size. The collective behavior of active particles is investigated in a lattice model, where the interplay between pulsation and synchronization gives rise to emergent behavior such as wave propagation. Fluctuating hydrodynamic equations can be obtained from microscopic dynamics and their predictive power is shown in comparison with numerical simulations.

We highlight the minimal ingredients needed for the complex behavior above-mentioned and point out future directions in the growing field of pulsating active matter.

DY 4: Pattern Formation, Delay and Nonlinear Stochastic Systems

Time: Monday 9:30–12:30 Location: ZEU 250

DY 4.1 Mon 9:30 ZEU 250

Spiral waves within a bistability parameter region of an excitable medium — •Vladimir Zykov and Eberhard Bodenschatz — Max Plank Institute for Dynamics and Self-Organization, D-37077, Goettingen, Germany

Spiral waves are a well-known and intensively studied dynamic phenomenon in excitable media of various types. Most studies have considered an excitable medium with a single stable resting state. However, spiral waves can be maintained in an excitable medium with bistability. Our calculations, performed using the widely used Barkley model, clearly show that spiral waves in the bistability region exhibit unique properties. For example, a spiral wave can either rotate around a core that is in an unexcited state, or the tip of the spiral wave describes a circular trajectory located inside an excited region. The boundaries of the parameter regions with positive and negative cores have been defined numerically and analytically evaluated. It is also shown that the creation of a positive or *negative* core may depend on the initial conditions, which leads to hysteresis of spiral waves.

DY 4.2 Mon 9:45 ZEU 250

Band Pattern Formation in a Suspension of Red Blood Cells During Centrifugation in a Percoll Density Gradient — •Felix Maurer, Thomas John, Christian Wagner, and Alexis Darras — Dynamics of Fluids, Experimental Physics, Saarland University, 66123 Saarbrücken, Germany

Percoll is a suspension of silica nanoparticles often used to establish density gradients and separate biological matter in centrifugation protocols. When red blood cells (RBCs) sediment in a Percoll medium, they form patterns of discrete bands. While this is a popular approach for RBC age separation, the mechanisms involved in band formation were unknown. In a series of experiments we could show that the formation of those patterns could be explained by cell aggregation. We developed a new continuum model to describe the volumetric RBC density under the influence of attractive pair interaction. Our numerical solutions are characterized by pattern formation and transitions between the equilibrium states depending on aggregation energy and initial volumetric RBC concentration.

DY 4.3 Mon 10:00 ZEU 250

A missing amplitude equation — •Tobias Frohoff-Hülsmann[1] and Uwe Thiele[1,2] — [1]Institute of Theoretical Physics, WWU Münster — [2]Center for Nonlinear Science (CeNoS), WWU Münster

Amplitude (or envelope) equations describe the spatiotemporal dynamics of the essential linear mode(s) in the vicinity of a stability threshold and represent universal equations for spatially extended systems [3]. They are determined by the type of linear instability, the symmetries and whether or not conservation laws are present [5, 6]. For systems without conservation laws these equations are well studied, e.g. the complex Ginzburg-Landau equation [1]. However, the presence of conservation laws is highly relevant for a wide spectrum of pattern forming systems, e.g. for certain reaction diffusion (RD) systems [2, 4]. Here, we review the basic types of linear instabilities in the presence of conservation laws and show that there are relevant cases for which the amplitude equation is still unknown. We focus on such a missing case and derive an amplitude equation relevant for practically important RD systems.

[1] I. S. Aranson and L. Kramer. Rev. Mod. Phys., 74:99-143, 2002.
[2] C. Beta, N. S. Gov, and A. Yochelis. Cells, 9:1533, 2020.
[3] M. C. Cross and P. C. Hohenberg. Rev. Mod. Phys., 65:851-1112, 1993.
[4] J. Halatek and E. Frey. Nature Phys., 14:507-514, 2018.
[5] P. C. Matthews and S. M. Cox. Nonlinearity, 13:1293-1320, 2000.
[6] F. Bergmann, L. Rapp, and W. Zimmermann. Phys. Rev. E,

98:020603, 2018.

DY 4.4 Mon 10:15 ZEU 250

The universal CHEOPS, the path to it, and applications — Andre Förtsch and •Walter Zimmermann — Theoretische Physik, Universität Bayreuth

Solutions to fundamental questions in the field of nonequilibrium phase transitions are presented. What are the 'generic transport equations for oscillatory phase separation' (GTOPS) in systems described by conserved fields? GTOPS cover both classical and oscillatory phase separation. But what is the universal equation for oscillatory phase separation, i.e., the counterpart of the famous universal complex Ginzburg-Landau equation (cGLE) for an unconserved order parameter [1]? It is the 'Cahn-Hilliard model extended to oscillatory phase separation' (CHEOPS) that includes the model in [2] as a special case. By generalizing methods from [3-6] CHEOPS is derived from GTOPS or even from a chemotaxis model for two species. Examples of surprising solutions of GTOPS and CHEOPS (patterns) are presented and some of them are also illustrated by a so-called minimal model (MIMO).

[1] I. Aranson, L. Kramer, Rev. Mod. Phys. 74, 99 (2002)
[2] W. Zimmermann, Physica A 237, 575 (1997)
[3] F. Bergmann et al., Phys. Rev. E 98, 020603(R) (2018)
[4] L. Rapp et al., Eur. Phys. J E 42, 57 (2019)
[5] F. Bergmann, W. Zimmermann, PLoS ONE 14, e0218328 (2019)
[6] F. J. Thomsen, L. Rapp, F. Bergmann, W. Zimmermann, New J. Phys. (FT) 23, 042002 (2021)

DY 4.5 Mon 10:30 ZEU 250

Quasi-steady interface flows in simple reaction-diffusion systems — •Tobias Alexander Roth, Henrik Weyer, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, München, Germany

Intracellular protein patterns are essential features of living systems. A well-studied framework for describing simple protein systems are 2-component reaction-diffusion systems that preserve mass (2cMCRD). These genuine non-equilibrium systems can not be written in terms of a variational approach: there is neither a free energy nor a classical surface tension. Interestingly, it was found that the long-term evolution of these reaction-diffusion systems, however, is phenomenologically similar to the interface dynamics of phase-separating thermodynamic systems.

Here we show that an interface line in 2cMCRD systems obeys a flow, that interpolates between two paradigmatic limits: the two-sided Mullins-Sekerka flow and the area-preserving geodesic curvature flow. This generalised flow conserves area and minimises the interface length. One can tune its character by the time scale of diffusive mass redistribution compared to reactive turnover.

15 min. break

DY 4.6 Mon 11:00 ZEU 250

Amplitude expansion of the phase-field crystal model on deformable surfaces — •Lucas Benoit–Maréchal, Marco Salvalaglio, Ingo Nitschke, and Axel Voigt — Institute of Scientific Computing, TU Dresden, Dresden, Germany

The Phase Field Crystal (PFC) model describes lattices at diffusive timescales but atomic lengthscales, thus requiring subatomic resolution meshes. To remedy this restriction, the complex amplitude expansion (APFC) was developed, whereby the amplitude of the density fluctuations is modeled instead of the density itself, enabling simulations at mesoscales that retain atomistic features.

We extend the two-dimensional APFC model to include out-of-plane displacements in order to study the coupling between crystal defects and surface deformation, paving the way for applications such as the topological tuning of mechanical properties of crystalline sheets.

To validate our model, we compare representative settings with atomistic simulations from the PFC model and Molecular Dynamics and find, within certain limits that we discuss, excellent agreement between all models.

DY 4.7 Mon 11:15 ZEU 250

Laminar chaos in systems with quasiperiodic delay — •David Müller-Bender[1] and Günter Radons[1,2] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]ICM - Institute for Mechanical and Industrial Engineering, 09117 Chemnitz, Germany

A new type of chaos called laminar chaos was found in singularly perturbed dynamical systems with periodic time-varying delay [Phys. Rev. Lett. 120, 084102 (2018)]. It is characterized by nearly constant laminar phases, which are periodically interrupted by irregular bursts, where the intensity levels of the laminar phases vary chaotically from phase to phase. In this paper, we demonstrate that laminar chaos can also be observed in systems with quasiperiodic delay, where we generalize the concept of conservative and dissipative delays to such systems. It turns out that the durations of the laminar phases vary quasiperiodically and follow the dynamics of a torus map in contrast to the periodic variation observed for periodic delay. Theoretical and numerical results indicate that introducing a quasiperiodic delay modulation into a time-delay system can lead to a giant reduction of the dimension of the chaotic attractors. By varying the mean delay and keeping other parameters fixed, we found that the Kaplan-Yorke dimension is modulated quasiperiodically over several orders of magnitudes, where the dynamics switches quasiperiodically between different types of high- and low-dimensional types of chaos.

Details can be found in the preprint [arXiv:2210.04706 (2022)].

DY 4.8 Mon 11:30 ZEU 250

Pulse generation in opto-electronic neurons with time-delayed feedback — •Jonas Mayer Martins[1], Svetlana V. Gurevich[1], and Julien Javaloyes[2] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9 and Center for Nonlinear Science (CeNoS), University of Münster, Corrensstrasse 2, 48149 Münster, Germany — [2]Departament de Física and IAC-3, Universitat de les Illes Balears, C/ Valldemossa km 7.5, 07122 Mallorca, Spain

We study a neuromorphic circuit composed of a nano resonant tunneling diode (RTD) operated in the excitable regime, where the diode generates, when triggered, an all-or-nothing electrical response pulse. This pulse is fed into a nano laser diode (LD), which in turn emits an optical pulse that is re-injected with time delay back into the RTD. Our theoretical analysis of this time-delayed opto-electronic nonlinear system describes how such neuron-like excitability can lead to sustained periodic pulsations due to the time-delayed feedback. We derive a bifurcation diagram through numerical continuation, unveiling the rich dynamics of the system. Furthermore, direct numerical simulations of the RTD-LD reveal emerging solitons that may serve as memory for information. Opto-electronic neurons like the RTD-LD are particularly interesting because they allow for fast computations at very low energy consumption and are therefore promising candidates for new computational architectures that mimic the brain.

DY 4.9 Mon 11:45 ZEU 250

Spontaneous vortex formation by microswimmers with retarded attractions — Xiangzun Wang[1], •Pin-Chuan Chen[2], Klaus Kroy[2], Viktor Holubec[3], and Frank Cichos[1] — [1]Peter Debye Institute for Soft Matter Physics, Leipzig University, 04103 Leipzig, Germany — [2]Institute for Theoretical Physics, Leipzig University, Postfach 100 920, 04009 Leipzig, Germany — [3]Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University, 18000 Prague, Czech Republic

In recent experiments done in the Molecular Nanophotonics Group in the Peter Debye Institute, thermophoretic microswimmers are observed to self-assemble into bi-stable orbital modes due to retarded attractive interactions.

A single agent which is attracted to an immobilized target with a time delay can be described by a time-local overdamped Langevin equation with a potential determined by time delay, and the transition in between the two stable modes is well predicted by Kramers' escape rate. Simulations of multiple agents attracted to one target also show that the collective behavior can be reduced to a one-agent description; however, the experiments (with up to 16 agents) show otherwise. The discrepancy between the results are attributed to additional effects in experiments.

We further show results of extended simulations with larger number of agents, which demonstrate two transitions depending solely on the time delay.

DY 4.10 Mon 12:00 ZEU 250

Stochastic pH oscillator confined to lipid vesicles — •Arthur Straube[1], Stefanie Winkelmann[1], and Felix Höfling[2,1] — [1]Zuse Institute Berlin — [2]Institut für Mathematik, Freie Universität Berlin

We study an urea-urease-based pH oscillator confined to lipid vesicles serving as an open reactor [1,2]. In contrast to conventional pH oscillators in closed reactors, the exchange with the vesicle exterior periodically resets the pH clock that switches the system from acid to basic, resulting in self-sustained oscillations. Stochastic simulations for microscopically small vesicles predict a significant statistical variation of the oscillation period. Although the mean period remains remarkably robust for vesicle sizes down to nearly 200 nm, the periodicity of the rhythm is gradually destroyed for smaller vesicles [1]. We analyze the structure of the limit cycle, which controls the dynamics for giant vesicles and dominates the strongly stochastic oscillations in small vesicles of submicrometer size. We derive reduced two-variable models, amenable to analytic treatments, and show that the accuracy of predictions, including the period of oscillations, is highly sensitive to the choice of the reduction scheme [2]. The accurate description of a single pH oscillator is crucial for rationalizing experiments and understanding communication of vesicles and synchronization of rhythms.

[1] A. Straube, S. Winkelmann, C. Schütte, F. Höfling, J. Phys. Chem. Lett. **12**, 9888 (2021). [2] A. Straube, S. Winkelmann, F. Höfling, ZIB Report 22-21 (2022), preprint (DOI: 10.12752/8817).

DY 4.11 Mon 12:15 ZEU 250

Sampling from the rule 150 fractal though an iterated stochastic process — •Jens Christian Claussen — University of Birmingham, UK

A widely known, but surprising way of sampling points from the Sierpinski fractal is through an iterated stochastic process where in each time step one of three operators is applied, which can be interpreted from their number representation, or as a geometric operation. While the Sierpinski fractal can also be generated by the rule 90 elementary cellular automaton (ECA), the ECA rule 150 generates a fractal pattern with a 2-step self-simularity resembling a generalization of a Fibonacci iteration [1]. Here we show that the rule 150 fractal can be generated without a 2-step iteration. We introduce a set of 6 operators, which allow to generate the rule 150 fractal from a stochastic process. We show that these 6 operators can be reduced to 4 operators, by adding one operator to the 3 operators from the rule 90 case. The operators for the rule 150 can be interpreted both from their number representation and geometrically. Further each point of the rule 150 fractal can be represented by a any base-6 number, or by a 4-letter symbolic sequence with a grammar restriction.

[1] Jens Christian Claussen, J. Math. Phys 49, 062701 (2008)

DY 5: Fluid Physics: Turbulence and Convection

Time: Monday 9:30–12:15 Location: MOL 213

Invited Talk DY 5.1 Mon 9:30 MOL 213

Extreme events, entropies and instantons for turbulence and water waves — •Joachim Peinke, André Fuchs, and Matthias Wächter — Inst. of Physics, University of Oldenburg, Germany

Complex systems like turbulence and ocean waves can produce extreme events like large changes in wind speed or monster waves. It has long been debated whether coherent structures or special statistical properties are essential for the understanding. Here we show a comprehensive stochastic approach for Lagrangian and Eulerian turbulence, as well as, for waves, leading to a joint multi-point statistic. We consider cascade trajectories through scales as realizations of a stochastic Langevin process that can be deduced from data. Knowledge of the stochastic equations allows determination of the entropy production of each cascade trajectory. Trajectories with negative entropies are linked to large fluctuations like extreme wind speeds or monster waves. Thus entropy seems to select different structures. Furthermore, negative and positive entropy values are balanced by rigorous fluctuation theorems, so that extreme and normal fluctuations are mutually dependent. In this way the entropy concept links statistics with the coherent structure approach. Finally, trajectories concentrate around an optimal path, called instanton, which is the minimum of an effective action given by the estimated stochastic equations. Entropons, defined as instantons conditioned on fixed entropy values, pinpoint the trajectories responsible for the emergence of non-Gaussian statistics at small scales. Ann. Rev. Cond. Matt. Phys. 10, 107-132 (2019), EPL 137, 53001 (2022), Phys. Rev. Lett. 129, 034502 (2022)

DY 5.2 Mon 10:00 MOL 213

Discrete and Continuous Symmetry Reduction for Minimal Parametrizations of Chaotic Fluid Flows — •Simon Kneer and Nazmi Burak Budanur — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Mathematical laws that govern fluid motion preserve their shape under translation, rotation, and reflection of coordinates. Consequently, most hydrodynamic systems of interest exhibit a set of symmetries, the action of which on the fluid states commutes with the dynamics. In complex flows, typical non-laminar fluid states are not invariant under these symmetries. Thus, each solution of the system has many dynamically equivalent symmetry copies. For data-driven model reduction methods, such as undercomplete Autoencoders, this multiplicity is not desired since it results in an artificial inflation of the training data which does not yield any physical insight. We consider this problem in the sinusoidally-driven Navier-Stokes equations in two dimensions, i.e. Kolmogorov flow, which is symmetric under continuous translations as well as discrete rotations and reflections. We formulate a symmetry reduction that combines first Fourier mode slicing with invariant polynomials that yields a fully invariant formulation of the corresponding dynamical system. Through this symmetry reduction, we are able to find a minimal approximation to the inertial manifold of this system as well as ordinary differential equations on this manifold that describe the dynamics.

DY 5.3 Mon 10:15 MOL 213

Spontaneous symmetry breaking for extreme vorticity and strain in the three-dimensional Navier-Stokes equations — •Timo Schorlepp[1], Tobias Grafke[2], Sandra May[3], and Rainer Grauer[1] — [1]Institute for Theoretical Physics I, Ruhr-University Bochum, Germany — [2]Mathematics Institute, University of Warwick, United Kingdom — [3]Department of Mathematics, TU Dortmund University, Germany

We investigate the spatio-temporal structure of the most likely configurations realizing extremely high vorticity or strain in the stochastically forced three-dimensional incompressible Navier-Stokes equations. Most likely configurations are computed by numerically finding the highest probability velocity field realizing an extreme constraint as solution of a large optimization problem. High-vorticity configurations are identified as pinched vortex filaments with swirl, while high-strain configurations correspond to counter-rotating vortex rings. We additionally observe that the most likely configurations for vorticity and strain spontaneously break their rotational symmetry for extremely high observable values. Instanton calculus and large deviation theory allow us to show that these maximum likelihood realizations determine the tail probabilities of the observed quantities. In particular, we are able to demonstrate that artificially enforcing rotational symmetry for large strain configurations leads to a severe underestimate of their probability, as it is dominated in likelihood by an exponentially more likely symmetry-broken vortex-sheet configuration.

DY 5.4 Mon 10:30 MOL 213

Delayed onset in spanwise rotating compressible convection — •Kevin Lüdemann and Andreas Tilgner — Institute for Astrophysics and Geophysics, Göttingen, Germany

We are investigating compressible convection with spanwise rotation in direct numerical simulations meaning that the direction of gravity and the axis of rotation are perpendicular to each other. This is a model for the equatorial region of gas planets like Jupiter or Earth's outer core. Both consist of compressible liquids ranging many orders of magnitude in density variations for Jupiter to about 20 percent of density changes for earth outer core. We are more interested in moderate density changes since those are realizable in laboratory experiment like the one performed in Lyon. From a parameter study in the number of density scale heights controlling the compressibility and the Ekman number controlling the global rate of rotation, we find that the onset of convection is delayed by compressibility and rotation. Additionally, a horizontal drift of the many slender convection rolls has been found at the onset for high rotation rates. An extensive study is presented

highlighting these unforeseen results.

DY 5.5 Mon 10:45 MOL 213

Offshore wind: Evidence for two-dimensional turbulence and role of sea horizon — •So-Kumneth Sim[1], Joachim Peinke[2], and Philipp Maass[1] — [1]Fachbereich Physik, Universität Osnabrück, Germany — [2]Insitut für Physik & ForWind, Universität Oldenburg, Germany

We analyze offshore wind speeds with a time resolution of one second over a period of 20 months [1]. Wind speed power spectra show a scaling behavior that is governed by three- and two-dimensional turbulence [2]. The latter is observed for frequencies lower than a crossover frequency f_{2D}. An analysis of the third moment (third-order structure function) of wind speed fluctuations provides strong evidence of this transition to two-dimensional turbulence [3]. We argue that $f_{2D} \sim \bar{v}/d$, where $\bar{v}$ is the mean wind speed and d the distance between the measurement device and the sea horizon. For the regime of two-dimensional turbulence, two scaling regimes are predicted, which originate from an inverse energy and an enstrophy cascade. Our results indicate that the scaling due to the inverse energy cascade occurs at low frequencies and is followed by the scaling of the enstrophy cascade at higher frequencies. This in agreement with the theoretical prediction but contrary to earlier observations.

[1] S.-K. Sim, J. Peinke, P. Maass, arXiv:2203.07685 (2022).
[2] X. Larsén, S. Larsen, E. Petersen, Boundary-Layer Meteorol. 159, 349 (2016).
[3] R. Cerbus, P. Chakraborty, Phys. Fluids 299, 111110 (2017).

15 min. break

DY 5.6 Mon 11:15 MOL 213

Convective turbulent superstructures in Rayleigh-Benard convection — •Hiufai Yik[1], Stephan Weiss[1,2], and Eberhard Bodenschatz[1] — [1]Max Planck Institute for Dynamics and Self-Organization — [2]Max Planck Center for Complex Fluid Dynamics

We report experimental results on turbulent superstructures in high-turbulence thermal convection. The 0.7 m high, 3.5 m wide and 0.35 m deep rectangular cell was installed in the Göttingen U-Boot and filled with sulphur hexafluoride at pressures up to 19 bar. Convection in this installation can be investigated up to Rayleigh numbers Ra = 10^13 at Prandtl numbers of about 0.8. More than 200 thermistors were distributed in the upper and lower plates for temperature and heat flux measurements, and 20 additional thermistors in the centre of the cell to measure the fluid temperature along the longitudinal axis. We report the results on turbulent superstructures and their dependence on heat transport and boundary conditions. For this purpose, the upper and lower plates of the convection cell were each divided into 4 sections, with an independent temperature control allowing both homogeneous and inhomogeneous temperature boundary conditions and the selection of different turbulent superstructures.

DY 5.7 Mon 11:30 MOL 213

Statistical field theory for a stochastic linear advection-stretching model for turbulence — Lukas Bentkamp, Maurizio Carbone, and •Michael Wilczek — Theoretical Physics I, University of Bayreuth, 95440 Bayreuth

A major obstacle in developing a statistical field theory of turbulence is the analysis of the functional equations that govern the complete statistics of the flow field. Simplified models of turbulence may help to develop such a statistical framework. In this contribution, we discuss the stochastic linear advection and stretching of an incompressible passive vector field as a model for small-scale turbulence. The model encompasses non-Gaussian statistics due to an intermittent energy flux from large scales to small scales, thereby displaying hallmark features of turbulence. We explore this model using the Hopf functional formalism, which naturally leads to a decomposition of the complex non-Gaussian statistics into Gaussian sub-ensembles based on different realizations of advection and stretching.

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 101001081).

DY 5.8 Mon 11:45 MOL 213

Description of laminar-turbulent transition of an airfoil boundary layer measured by differential image thermography using directed percolation theory — •Tom T. B. Wester, Joachim Peinke, and Gerd Gülker — ForWind, University of Oldenburg, Institute of Physics, Oldenburg, Germany

Transition from laminar to turbulent flow is still a challenging problem. Recent studies indicate a good agreement when describing this phase transition with the directed percolation theory. This study presents a new experimental approach by means of differential image thermography (DIT) enabling to investigate this transition on the suction side of a heated airfoil. The results extend the applicability of the directed percolation theory to describe the transition on curves surfaces. The experimental effort allows for the first time an agreement between all three universal exponents of the (1+1)D directed percolation for such airfoil application. Furthermore, this study proves that the theory holds for a wide range of flows, as shown by the various conditions tested. Such a large parameter space was not covered in any examination so far. The findings underline the significance of percolation models in fluid mechanics and show that this theory can be used as a high precision tool for the problem of transition to turbulence.

DY 5.9 Mon 12:00 MOL 213

How to generate turbulence with highest Reynolds numbers in the wind tunnel — •Lars Neuhaus, Michael Hölling, and Joachim Peinke — ForWind, University of Oldenburg, Institute of Physics, Oldenburg, Germany

In order to study objects like buildings, vehicles or wind turbines under the influence of wind fluctuations, the generation of laboratory flows that resemble atmospheric turbulence is of prime importance. This is where active grids come into play, allowing to excite the wind tunnel flow in a user-defined way. With a blockage induced flow design, it is possible to recreate atmospheric flows through their time series or to create single coherent structures such as gusts defined by industrial standards. In addition, it is possible to generate turbulence with large integral length scales through a random driving that follows a stochastic process. Velocity fluctuations with correlation lengths and thus integral scales much larger than the transverse dimensions of the wind tunnel can be generated. By combining active grid excitation with fan speed modulation, it is additionally possible to generate a flow characterized by an inertial range of four decades and an integral Reynolds number of $2 * 10^7$. By a newly developed active grid it is furthermore possible to vary the turbulent properties over height to mimic height dependencies found in the atmosphere and also to generate a turbulent non-turbulent interface.

DY 6: Statistical Physics: General I

Time: Monday 10:00–13:00 Location: ZEU 160

DY 6.1 Mon 10:00 ZEU 160

Noether's theorem in statistical mechanics — •Sophie Hermann and Matthias Schmidt — Universität Bayreuth, Bayreuth, Deutschland

Noether's Theorem is familiar to most physicists due its fundamental role in linking the existence of conservation laws to the underlying symmetries of a physical system. Typically the systems are described in the particle-based context of classical mechanics or on the basis of field theory. We apply Noether's calculus of invariant variations to thermal systems, where fluctuations are paramount and one aims for a statistical mechanical description, both in and out of equilibrium. Generating functionals, such as the free energy, yield mechanical laws under continuous translational and rotational symmetry operations. The resulting global theorems express vanishing of total internal and total external forces and torques. Local sum rules interrelate density correlators, as well as static and time direct correlation functions via infinite hierarchies, including memory. We demonstrate that this approach is consistent with the earlier work in equilibrium, and that it enables one to go, with relative ease, beyond the sum rules that these authors formulated. For anisotropic particles, systematic coupling of orbital and spin motion is identified. The theory allows to shed new light on the spatio-temporal coupling of correlations in complex systems. We present novel exact and nontrivial identities that apply to time-dependent problems and driven and active fluids.

DY 6.2 Mon 10:15 ZEU 160

Mean-field brittle yielding of amorphous solids — •Jack T. Parley[1] and Peter Sollich[1,2] — [1]Institut für Theoretische Physik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Department of Mathematics, King's College London, London WC2R 2LS, UK

We study the brittle yielding of athermal amorphous solids within the celebrated Hébraud-Lequeux mean-field elastoplastic model, which incorporates the sign-varying nature of Eshelby interactions as a Gaussian mechanical noise. As in finite-dimensional particle simulations, we find a critical value of the initial disorder, below which yielding in the limit of quasistatic shear becomes a discontinuous non-equilibrium transition. We find evidence that in this limit yielding cannot be described as a spinodal instability, in contrast to the behaviour found in driven random magnets or depinning-like models. At small but finite shear rates, we show that the tail exponents characterising the decay of the plastic yield rate function on either side of its peak at the transition are related to the athermal aging exponents. We finally derive analytically the scaling with shear rate of the peak susceptibility at the random critical point, and discuss the connection to avalanches in finite-size systems.

DY 6.3 Mon 10:30 ZEU 160

Bringing the power of Monte Carlo methods to long-range-interacting molecular systems — •Philipp Höllmer[1], A. C. Maggs[2], and Werner Krauth[3] — [1]University of Bonn, Germany — [2]ESPCI Paris, France — [3]École normale supérieure de Paris, France

Molecular simulations are widespread in molecular sciences to study, e.g., protein folding. Here, chemical systems are modeled empirically by a set of atomic positions with parameterized interaction potentials. Nowadays, molecular-dynamics (MD) simulations are predominantly used to study long-range-interacting molecular systems because of their superior computational complexities and Newtonian dynamics when compared to traditional Markov-chain Monte Carlo (MCMC) simulations. We argue that both disadvantages of traditional reversible MCMC are overcome by event-chain Monte Carlo (ECMC), which is a family of non-reversible MCMC methods.

In this talk, we will explore how ECMC samples the equilibrium Boltzmann distribution exactly, although it uses non-equilibrium dynamics and never computes the total system potential. We will discuss how ECMC's sole restriction of the global-balance condition yields a great freedom to implement quickly decorrelating dynamics beyond Newtonian's dynamics of MD. Finally, we will demonstrate $\mathcal{O}(N \log N)$ scaling for ECMC's decorrelation of an N-body system of a commonly used long-range-interacting water model. This matches the performance of MD without ever discretizing time or space.

DY 6.4 Mon 10:45 ZEU 160

Virial coefficients of hard, anisotropic particles in two- to four-dimensional Euclidean spaces — •Markus Kulossa, Daniel Weidig, and Joachim Wagner — Institut für Chemie, Universität Rostock, 18051 Rostock, Germany

We compare virial coefficients up to order eight for anisotropic, hard particles in two- to four-dimensional Euclidean spaces in dependence on their aspect ratio. The virial coefficients of both, convex shapes such as stadia, spherocylinders and hyperspherocylinders and concave shapes such as dumbbells in two to four dimensions are analyzed. Since the second virial coefficient of hard objects equals their mutual excluded D-dimensional volume per particle, analytically obtained expressions for the second virial coefficients serve as a test for orientation-dependent overlap algorithms. In first approximation, a nearly universal dependence of reduced virial coefficients on the excess part of the mutual excluded volume is observed for third and higher order virial coefficients.

DY 6.5 Mon 11:00 ZEU 160

Geometric Bounds on the Power of Adiabatic Thermal Machines — •Joshua Eglinton[1,2] and Kay Brandner[1,2] — [1]School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, United Kingdom — [2]Centre for the Mathematical and Theoretical Physics of Quantum Non-equilibrium Systems, University of Nottingham, Nottingham NG7 2RD, United Kingdom

The laws of thermodynamics put fundamental bounds on the efficiencies of thermal machines. These Carnot bounds can typically be attained only if the machine is operated quasi-statically, which leads to vanishing power output. We present a new family of power-efficiency trade-off relations that imply a quadratic decay of power at Carnot efficiency, for devices operating between two fixed temperatures. Notably, these relations depend only on geometric quantities such as the thermodynamic length of the driving cycle and hold for essentially any thermodynamically consistent micro-dynamics such as classical Markov-jump processes, adiabatic Lindblad dynamics or coherent transport. This analysis is based on a new general scaling argument, with which we show that the efficiency of such devices reaches the Carnot bound only if heat-leaks between the baths can be fully suppressed. Furthermore, we find that their power is in fact determined by second-order terms in the temperature difference between the two baths, which are neglected in standard linear-response theory.

[1] - J. Eglinton and K. Brandner, Phys. Rev. E 105, L052102 (2022)

DY 6.6 Mon 11:15 ZEU 160

Hard rods on a 2D lattice system — •Michael Zimmermann — Universität Tübingen, Tübingen, Deutschland

An exact solution for the equilibrium density for a hard rod system on a 1D continuous system was found by Percus [1]. For lattice systems of hard rods, Lafuente and Cuesta established a method based on Rosenfeld's fundamental measure theory to find the exact solution in 1D and to extrapolate from this result to a density functional in higher dimensions [2,3]. But already in 2D theoretical properties differ from respective simulation results [4], such as the onset of demixing between rods of different orientation. In this talk we will discuss some possible extensions of the Lafuente-Cuesta functional for improving the excess free energy functional and for better approximations of density distributions in 2D hard rod lattice systems.

[1] Percus J. K. 1976 J. Stat. Phys. 15 505*11 [2] Rosenfeld Y. 1989 Phys. Rev. Lett. 63 980*3 [3] Lafuente L. and Cuesta J.A. 2002 J. Phys.: Condens. Matter 14 12079 [4] Oettel M., Klopotek M. et al 2016 J. Chem. Phys. 145 074902

15 min. break

DY 6.7 Mon 11:45 ZEU 160

Mean first-passage times of continuous-time random walkers determined through Wiener-Hopf integral equations — •Marcus Dahlenburg[1,2] and Gianni Pagnini[1,3] — [1]BCAM-Basque Center for Applied Mathematics, Alameda de Mazarredo 14, 48009 Bilbao, Basque Country, Spain — [2]Institute for Physics & Astronomy, University of Potsdam, 14476 Potsdam, Germany — [3]Ikerbasque-Basque Foundation for Science, Plaza Euskadi 5, 48009 Bilbao, Basque

Country, Spain

Asymmetric continuous-time random walks in continuous-space characterised by waiting-times with finite mean and by jump-amplitudes with both finite mean and finite variance are governed by an advection-diffusion equations in the asymptotic limit. The mean first-passage time (MFPT) of such an advective-diffusive system on a halfline results to be finite when the advecting drift is in the direction of the boundary. In our investigation we derive an inhomogeneous Wiener-Hopf integral equation that allows to avoids approximated results in the asymptotic limits and leads indeed to the exact determination of the MFPT. This quantity depends on the average of the waiting-times only but it conserves the information about the whole distribution of the jump-amplitudes. Through the case study of asymmetric double-exponential distributions of the jump-amplitudes one may identifies a length-scale, that defines the transition from starting points near the boundary to starting points far-away from the boundary where the MFPT loses the information about the exact shape of the jump-amplitudes' distribution and only conserves their mean.

DY 6.8 Mon 12:00 ZEU 160

A combinatorial approach to the many-body density of levels and the Bethe approximation — •Carolyn Echter, Georg Maier, Juan-Diego Urbina, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Regensburg, Germany

The Bethe formula, originally derived in [1] to estimate the density of levels of heavy nuclei, has become a widely used approximation for the many-body density of levels of a non-interacting fermionic system, appropriate for large numbers of particles and energies in a system-dependent range. Notably, in the case of equally spaced single-particle energy levels, it coincides with the asymptotic result for the number of unrestricted partitions of an integer known from analytic number theory [2]. An explanation is suggested by the combinatorics of distributing integer amounts of energy to particles obeying given statistics. We present a combinatorial derivation of the exact many-body density of levels for various particle statistics in the case of a constant single-particle density of states, thereby adding to existing discussions [3,4] and explaining the asymptotic agreement of Bethe's approximation with number theoretical partition functions. We compare numerically with semiclassical results and make suggestions towards a bosonic analogue of the Bethe formula based on our observations.

[1] H. A. Bethe, Phys. Rev. 50, 332-41 (1936). [2] G. H. Hardy, S. Ramanujan, Proc. London Math. Soc. (2) 17, 75-115 (1918). [3] F. C. Auluck, D. S. Kothari, Math. Proc. Camb. Philos. Soc. 42, 272-77 (1946). [4] A. Comtet, P. Leboeuf, S. N. Majumdar, Phy. Rev. Lett. 98, 070404 (2007).

DY 6.9 Mon 12:15 ZEU 160

Integral Equations in Statistical Mechanics: A Size-effect Study — •Jose Mauricio Sevilla Moreno and Robinson Cortes-Huerto — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Integral equations (IE) are in the core of statistical mechanics of liquids as they connect the local structure with thermodynamic properties as compressibility, activity coefficients and excess entropy. IE are normally defined in the grand canonical ensemble and calculated in the thermodynamic limit (TL). By contrast, computer simulations are performed with finite-size systems and mimic the TL using periodic boundary conditions (PBC). This proceeding introduces several finite-size contributions whose effects must be identified and corrected in order to approximate the simulation results to the TL. In this talk, we present a generic method to compute IE from molecular dynamics simulations. In our approach, we define finite-size IE, integrating them in Fourier space to trivially introduce PBC. This procedure allows us to identify and isolate ensemble, finite-volume domains and PBC effects and accurately obtain the corresponding thermodynamic quantities in the TL or artificially for any finite size system. To validate our method, we compute isothermal compressibilities, chemical potentials and excess entropies of simple liquids and liquid mixtures, including water and aqueous alcohol solutions, showing good agreement with results available in the literature.

DY 6.10 Mon 12:30 ZEU 160

A Multiscale Approach for Large-Scale Proton Dynamics Simulations — •Christian Dressler[1] and Daniel Sebastiani[2] — [1]TU Ilmenau, Institute of Physics, Theoretical Solid State Physics — [2]MLU Halle-Wittenberg, Institute of Chemistry, Theoretical Chemistry

We present a multiscale simulation approach for the calculation of proton diffusion/conduction in disordered organic and inorganic materials. We combine quantum chemical calculations for elementary reactions between the ions and surrounding molecules with molecular dynamics simulations for the incorporation of local dynamical heterogeneities at the nanometer/nanosecond scale. Data from both levels are integrated in a stochastic propagation scheme (Monte Carlo or Markov matrix approach) for the simulation of proton transfer at much larger time and length scales. The approach allows for an atom-level resolution of ion dynamics with quantum chemical accuracy but with final length- and time-scales of micrometers and milliseconds. As a proof-of-principle simulation, we have computed the explicit dynamics of a non-equilibrium process in an 8 μm CsH_2PO_4 system during 5 ms. Finally, we demonstrate the application potential of the scheme by computing the proton conductivity of a nanostructured CsH_2PO_4 fuel cell membrane with respect to the porosity.

DY 6.11 Mon 12:45 ZEU 160

Population Annealing and the Role of Resampling in Population Annealing — •Denis Gessert[1,2], Martin Weigel[3], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Leipzig University, Postfach 100920, D-04009 Leipzig, Germany — [2]Centre for Fluid and Complex Systems, Coventry University, Coventry CV1 5FB, United Kingdom — [3]Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

Studying equilibrium properties of thermodynamic systems with rough free-energy landscapes particularly challenges standard Markov chain Monte Carlo techniques such as the Metropolis algorithm. Sampling can be improved by using generalized ensemble methods, one of which is Population Annealing (PA). Although PA is not expected to outperform its contenders in terms of time complexity, it is particularly well suited for parallel execution with no theoretical limit on the level of parallelism, which makes it a viable option on modern HPC.

In PA a population of replicas is collectively cooled down. At each temperature a population control step is carried out before applying some replica-independent update moves. This population control is realized by means of resampling. Here, we compare various different resampling methods and their performance in PA applications. Using the $d = 2$ Ising model as a benchmark system, we identify two resampling methods that appear preferable over the widely used multinomial resampling. Further, we point out when different resampling choices affect the statistical quality of the simulation outcome and obtain some model-independent guiding principles for the choice of PA parameters.

DY 7: Granular Matter and Contact Dynamics

Time: Monday 10:00–12:45 Location: ZEU 147

DY 7.1 Mon 10:00 ZEU 147

Collective dipole reorganization in magnetostructures — •Wafflard Adrien, Vandewalle Nicolas, and Opsomer Eric — GRASP, Institut de Physique B5a, Université de Liège, Liège, BE

Playing with spherical neodymium magnets that you find in your favorite toy market is really addicting. By assuming they are uniformly magnetized, magnetic beads behave as point-like dipoles. For scientists, those inexpensive objects demonstrate how dipolar particles self-assemble into various structures ranging from 1D chains to 3D crystals. We show that magnetotubes and magnetocrystals can self-buckle, i.e. change their geometry, above a critical aspect ratio. The underlying dipolar ordering is found to exhibit a collective reorganization, altering the mechanical stability of the entire system. We identify the conditions in which these phenomena occur and conjecture that in chains, square or cubic magnetostructures, neighboring dipoles reorientate in order to form the longest possible chains. This suggests that a wide variety of magnetostructures, including well known stable structures, may collapse due to reorientation of dipoles.

DY 7.2 Mon 10:15 ZEU 147

How is the growth of ferromagnetic granular networks controlled by an orthogonal magnetic field? — Matthias Biersack[1], •Ali Lakkis[1], Oksana Bilous[2], Pedro A. Sanchez[2], Sofia S. Kantorovich[2], and Reinhard Richter[1] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]Computational and Soft Matter Physics, Faculty of Physics, University of Vienna, 1090 Vienna, Austria

We are exploring in experiments the aggregation process in a shaken granular mixture of glass and magnetized steel beads, occuring in a horizontal vessel after the shaking amplitude is suddenly decreased. Then the magnetized beads form a transient network that coarsens in time into compact clusters, following a viscoelastic phase separation [1]. A homogeneous magnetic field oriented in plane has been observed to "unknot" network structures orthogonal to the field [2]. Here we focus on the impact of a magnetic field B_z oriented orthogonally to the plain of the network. We measure the average number of neighbours $\bar{k}(t)$ and the efficiency $E(t)$ of the emerging networks. Both can be fitted by a logistic growth function for $B_z \in [0, 2]\,\mathrm{mT}$, unveiling that its characteristic time τ increases by about ten. Our results demonstrate that via dipole-dipole repulsion the field reduces the mobility of isolated steel beads, thus hindering the growth of the networks. The experimental results are compared with those of numerical simulations.

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

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

DY 7.3 Mon 10:30 ZEU 147

Dynamic light scattering from single macroscopic particles — Lisa Künstler[1], Raphael Kessler[1], Matthias Sperl[1,2], and •Philip Born[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170, Köln, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, 50937, Köln, Germany

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

[1] L. Dossow, R. Kessler, M. Sperl, & P. Born, Dynamic light scattering from single macroscopic particles. Applied Optics, 60(32), 10160-10167 (2021).

DY 7.4 Mon 10:45 ZEU 147

Shear jamming and free surface deformation enable reciprocal swimming in granular materials — •Hongyi Xiao, Achim Sack, and Thorsten Pöschel — Institute for Multiscale Simulations, Friedrich-Alexander-Universität Erlangen-Nürnberg, Cauerstraße 3, 91058 Erlangen, Germany

Swimming with reciprocal motion is desirable due to its simplicity, but it is prohibited in Newtonian fluids at low Reynolds number as stated by the scallop theorem. Such a constraint can be broken in fluids with complex rheology. In this study, we show that propulsion generation with reciprocal motion in granular materials is enabled by a prolonged hysteresis in the material response, which originates from a combination of jamming-induced material rigidity and plastic deformation of the free surface. Using both lab experiments and discrete element method simulations, a reciprocal swimmer mimicking a scallop was constructed and buried in a tank of polydisperse granular particles. The swimmer consists of two wings that open and close with geometrical and temporal symmetry. The resistive force, the swimmer's displacement, and the deformation of the free granular surface were measured. Results indicate that net propulsion force is generated when the swimmer is tethered, and net displacement is generated when the swimmer is released. Small amplitude oscillatory experiments confirm the existence of an elastic regime at small strains, and free surface deformation measurement reveals its influence at large strains. Furthermore, a secondary symmetry breaking mechanism due to a cooperative effect of the wings is also identified.

DY 7.5 Mon 11:00 ZEU 147

Phase space characterization of three-dimensional nucleation of glass spheres — •Frank Rietz[1,2] and Matthias Schröter[2] — [1]University of Magdeburg, Department of Nonlinear Phenomena — [2]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Göttingen

Packings of macroscopic spheres serve as a model system for studying atomic states. In many compactification protocols, the spheres do not form nuclei and remain in the state of random close packing. By cyclically shearing a packing of 50000 spheres, we can cross this boundary and observe a transition from a disordered to a crystallized state [1]. The three-dimensional temporal positions of the spheres are tracked by refractive index-matched scanning [2]. The description of disordered states and the nature of random close packing are open scientific problems. In our case, we describe the nucleation process by partitioning the packing into local groups of four touching spheres. These groups of spheres are tracked during the crystallization process and their contacts and relative orientation are recorded in a phase space diagram. By comparing the states before and after crystallization with the states that avoid crystallization, we show whether there are conditions under which the spheres statistically tend to crystallize.

[1] F. Rietz, C. Radin, H. L. Swinney, M. Schröter: Nucleation in sheared granular matter, Phys. Rev. Lett. 120, 055701 (2018)

[2] J. A. Dijksman, F. Rietz, K. A. Lőrincz, M. van Hecke, W. Losert: Refractive index matched scanning of dense granular materials, Rev. Sci. Instrum. 83, 011301 (2012)

15 min. break

DY 7.6 Mon 11:30 ZEU 147

Non-convex particles under shear in a split bottom cell — •Mahdieh Mohammadi[1], Ahmed Ashour[2], Dmitry Puzyrev[3], Torsten Trittel[3], and Ralf Stannarius[3] — [1]Technische Hochschule Brandenburg — [2]Future University of Egypt — [3]Otto-von-Guericke-Universität Magdeburg

We study dynamical features of surface flow in the top layer of a granular bed containing non-convex tetrapod and hexapod particles in a split-bottom shear cell. Different heights of granular beds were prepared and examined. Based on Particle Image Velocimetry and Particle Tracking Velocimetry, angular and radial displacements of particles on the surface of the ensemble were derived in dependence on the number of rotations of the bottom disk. Stereoscopic measurements of surface fluctuations of the bed during shearing turn out to be a key factor in this study to characterize heap and sink formation phenomena, which are related to the secondary flow of the grain ensembles in the bulk. We acknowledge support of DPG with project STA 425/40 and DLR with project EVA (50WM2048), and stimulating discussion

with K. Harth.

[1] Mahdieh Mohammadi, Dmitry Puzyrev, Torsten Trittel, and Ralf Stannarius, Phys. Rev. E 106, L052901 (2022).

DY 7.7 Mon 11:45 ZEU 147

Forces on obstacles suspended in flowing granular matter — •Jing Wang[1], Bo Fan[2], Tivadar Pongó[3], Tamás Börzsönyi[2], Raúl Cruz Hidalgo[3], and Ralf Stannarius[1] — [1]Institute of Physics, Otto von Guericke University Magdeburg, Magdeburg, Germany — [2]Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Budapest, Hungary — [3]Física y Matemática Aplicada, Facultad de Ciencias, Universidad de Navarra, Pamplona, Spain

We investigate the force on a spherical obstacle exerted by a flowing granular material. A sphere suspended in a discharging silo experiences mechanical forces both from the weight of the overlaying layers and from friction of the surrounding moving granular material. When the flow stops due to clogging of the silo, in experiments with hard frictional glass beads, the force on the obstacle remains exactly the same as during flow. In contrast, for nearly frictionless soft hydrogel particles the force decreased considerably after the flow stopped. The dependence of the total force on the obstacle diameter is qualitatively different for the two types of material: It grows quadratically with the sphere diameter of the obstacle for hydrogel spheres, while it grows much weaker, nearly linearly with the obstacle diameter, in a bed of hard frictional glass spheres.

DY 7.8 Mon 12:00 ZEU 147

Free cooling dynamics and energy partition in 3D granular gas mixtures — •Dmitry Puzyrev[1], Adrian Niemann[1], Kirsten Harth[2,3], Torsten Trittel[1], and Ralf Stannarius[1] — [1]Institute of Physics and MARS, Otto von Guericke University, 39106 Magdeburg — [2]Department of Engineering, TH Brandenburg, 14770 Brandenburg an der Havel — [3]MARS and MRTM, OVGU, 39106 Magdeburg

Granular gases are nonlinear systems that exhibit fascinating dynamical behavior far from equilibrium, including unusual cooling properties, clustering and violation of energy equipartition. Our study focuses on 3D microgravity experiments with dilute ensembles of rod-like particles and their mixtures. In drop tower experiments at ZARM, we studied granular cooling of mixtures of rods with two different diameters. The confirmation of Haff's equation [2] describing the energy decay is of particular interest. Experimental data analysis suggests different cooling rates, and the violation of energy equipartition between the rotational and translational degrees of freedom for the mixture components. Particle detection and tracking was performed with Machine Learning-aided approach [3]. The software will be available as a Python library that can be extended to other 3D and 2D particle tracking problems.

The authors acknowledge support from DLR in projects EVA (50WM2048) and VICKI (50WM2252).

References: [1] K. Harth et al., Phys. Rev. Lett., 120 (2018), 214301 [2] P. K. Haff, J. Fluid Mech., 134 (1983), 401-430 [3] Puzyrev et al., Microgravity Sci. Technol., 32 (2020), 897

DY 7.9 Mon 12:15 ZEU 147

Effect of particle size on the suction mechanism in granular grippers — •Angel Santarossa, Olfa D'Angelo, Achim Sack, and Thorsten Pöschel — Institute for Multiscale Simulation, Friedrich-Alexander Universität Erlangen-Nürnberg, Cauerstraße 3, 91058 Erlangen, Germany

Granular grippers are highly adaptable soft actuators able to grasp objects of different shapes and sizes. They consist of an elastic membrane partially filled with a granulate. Their operating principle relies on the reversible jamming transition of granular materials. The filled membrane can be deformed and reshaped when pressed onto an object. When the air within the membrane is evacuated, the granulate hardens, creating forces to hold and manipulate the object. Three mechanisms contribute to the holding force of granular grippers: frictional forces, geometrical constraints, and suction effects. Using X-ray computed tomography, we link the activation of suction to the size of the particles. We show that a gripper filled with small particles (average diameter $d \approx 0.12$ mm) conforms to a high degree around the object than with larger particles (average diameter $d \approx 4$ mm), thus enabling the formation of air-tight seals. When the gripper is pulled off, simulating the lifting of an object, vacuum pressure is generated in the sealed cavity at the interface gripper-object. If the particles are too large, the gripper does not conform tightly enough around the object, leaving gaps at the interface gripper-object. These gaps prevent the creation of sealed vacuum cavities between the object and the gripper, impeding the suction mechanism from operating.

DY 7.10 Mon 12:30 ZEU 147

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

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

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

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

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

DY 8: Invited Talk: Dynamics of Networks (joint session DY/SOE)

Time: Monday 12:30–13:00 Location: ZEU 250

Invited Talk DY 8.1 Mon 12:30 ZEU 250

Novel phenomena and analysis methods in oscillator networks: higher-order interactions, higher-order averaging, and inference — •Hiroshi Kori — The University of Tokyo, Japan

Synchronization of oscillator networks is essential for functionalization of systems. Examples include heart pacemaker, circadian clock, and locomotion, to name a few. In this talk, after reviewing a general background, I will present recent studies with an emphasis on novel phenomena and analysis techniques. (i) A network of three oscillators shows complex synchronization transitions when the network structure or overall coupling intensity is varied [1]. The transition is analyzed using a higher-order averaging method. (ii) In the assembly of noisy oscillators with a three-body interaction, synchronized state appears only transiently and its persistent time increases exponentially with the interaction strength of three-body coupling. (iii) I will present our proposed inference methods of coupling intensity from spike data [2] and the phase from oscillatory time series [3].

[1] M. Kato, H. Kori, PRE (2023)
[2] F. Mori and H. Kori, PNAS (2022)
[3] A. Matsuki, H. Kori, R. Kobayashi. arXiv (2022)

DY 9: Quantum Dynamics, Decoherence and Quantum Information

Time: Monday 14:00–17:15 Location: MOL 213

DY 9.1 Mon 14:00 MOL 213

From Dual Unitarity to Generic Quantum Operator Spreading — •Michael A. Rampp, Roderich Moessner, and Pieter W. Claeys — Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Dual-unitary circuits are paradigmatic examples of exactly solvable yet chaotic quantum many- body systems, but solvability naturally goes along with a degree of non-generic behaviour. By investigating the effect of weakly broken dual-unitarity on the spreading of local operators we study whether, and how, small deviations from dual-unitarity recover fully generic many-body dynamics. We present a discrete path-integral formula for the out-of-time-order correlator and use it to recover a butterfly velocity smaller than the light-cone velocity, $v_B < v_{LC}$, and a diffusively broadening operator front, two generic features of ergodic quantum spin chains absent in dual-unitary circuit dynamics. We find that the butterfly velocity and diffusion constant are determined by a small set of microscopic quantities and that the operator entanglement of the gates plays a crucial role.

DY 9.2 Mon 14:15 MOL 213

Harnessing the exponential Hilbert space dimension of quantum systems for reservoir computing — •Niclas Götting[1,2], Frederik Lohof[1,2], and Christopher Gies[1,2] — [1]Institute for Theoretical Physics, University of Bremen, Bremen — [2]Bremen Center for Computational Material Science, University of Bremen, Bremen

With the ever growing prevalence of machine learning in science and industry, the machine learning paradigm of reservoir computing has gained new attention. While classical reservoir computers have proven to be able to solve various prediction tasks by exploiting the complex dynamics of classical systems, their quantum counterparts are yet to be fully explored.

Coherent quantum systems exhibit properties like superposition and quantum entanglement, which in principle lead to an exponential scaling of the reservoir phase space dimension with respect to the number of quantum particles. The question arises if these quantum reservoir computers (QRCs) can energy and space efficiently outperform their classical analogues in complex prediction tasks.

As a first step we investigate the transverse-field Ising model as a QRC to find the link between the properties of the quantum network, the phase space dimension, and the performance of the QRC.

DY 9.3 Mon 14:30 MOL 213

Giant Residual Current from Ultrafast AC Driving of Bloch Electrons — •Adrian Seith, Jan Wilhelm, and Ferdinand Evers — Institut für Theoretische Physik, Universität Regensburg

In recent experiments, residual currents were seen to survive long after the laser illumination has died out[1]. Motivated by a vision of a "light-wave electronics", the effect has been utilized to design a petahertz logical gate[2].

In this work, we theoretically study residual currents of Bloch electrons and demonstrate that residual currents can be as large as the maximum current during illumination.

Based on a perturbative expansion of the semiconductor-Bloch equations, we derive an analytical formula; it explains the strong dependence of residual currents on the model parameters and the laser pulse shape. In particular, our formula allows to optimize pulse shapes for maximizing the residual currents' magnitude reaching values order of magnitudes larger than observed in recent experiments.

[1] Higuchi et. al., Nature 550, 224 (2017)
[2] Boolakee et. al., Nature 605, 251 (2022)

DY 9.4 Mon 14:45 MOL 213

Time-local generator of non-Markovian quantum dynamics by iterating its memory kernel — Maarten Wegewijs[1], Jan Vanberg[2], and •Konstantin Nestmann[2] — [1]Peter Grünberg Institute, Forschungszentrum Jülich, Germany — [2]Institute for Theory of Statistical Physics, RWTH Aachen University

The time-convolutionless generator (TCL) $\mathcal{G}$ of a quantum master equation (QME) has been found to be the fixed point $\mathcal{G} = \hat{\mathcal{K}}[\mathcal{G}]$ of the Nakajima-Zwanzig memory kernel $\mathcal{K}$ of the equivalent QME with time-convolution[a]. Here we investigate the calculation of $\mathcal{G}$ by iterating $\mathcal{K}$ directly in the stationary limit starting from any initial guess to construct approximations to the dynamics. We show that the local stability of the iteration is connected to the long-time dynamics using an extended but still tractable version of the dissipative Jaynes-Cummings model. The iteration automatically selects the asymptotically most relevant decay and oscillation frequency, providing a non-perturbative Markovian semigroup approximation. Linearization about the fixed point allows to extract the amplitude of this approximation in the full dynamics, providing a non-perturbative initial-slip correction. Around the strongly non-Markovian regime (non-CP divisibility) the iteration stability can be either lost, or, remarkably, enhanced, yielding an additional fixed point. The global iteration stability is counter-intuitive: convergence to the main locally stable fixed point is guaranteed by starting from an initial guess "far away" with frequencies in the "wrong", *non*-physical half-plane. [a]Phys. Rev. X 11, 021041 (2021), Phys. Rev. B 104, 155407 (2021) [b]SciPost Phys. 11, 053 (2021)

DY 9.5 Mon 15:00 MOL 213

Performance of quantum registers in diamond in the presence of spin impurities — •Dominik Maile and Joachim Ankerhold — Institut for Complex Quantum Systems, Ulm University

The Nitrogen Vacancy Center in diamond coupled to addressable surrounding nuclear spins forms a versatile building block for future quantum technologies. While previous activities focused on sensing with only a single or very few spins in operation, recently multi-qubit registers have been successfully implemented for quantum information processing. Further progress requires a detailed understanding of the performance of quantum protocols for consecutive gate operations and thus, beyond established treatments for relaxation and dephasing. In this talk (see also [1]), we provide such an analysis for a small spin registers with up to four spins built out of NV and environmental constituents in presence of ensembles of interacting impurity spins. Adapting a cluster correlation expansion, we predict coherence properties as well as fidelities for GHZ- and Bell-gate operations. The influence of the volume density and the geometry of the spin-bath consisting of substitutional nitrogen atoms are also taken into account.

[1] D. Maile and J. Ankerhold, arXiv:2211.06234

DY 9.6 Mon 15:15 MOL 213

Quantum Zeno manipulation of quantum dots — Naser Ahmadiniaz[1], Martin Paul Geller[2], Jürgen König[2], Peter Kratzer[2], Axel Lorke[2], •Gernot Schaller[1], and Ralf Schützhold[1,3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany — [3]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

We investigate whether and how the quantum Zeno effect, i.e., the inhibition of quantum evolution by frequent measurements, can be employed to isolate a quantum dot from its surrounding electron reservoir. In contrast to the often studied case of tunneling between discrete levels, we consider the tunneling of an electron from a continuum reservoir to a discrete level in the dot. Realizing the quantum Zeno effect in this scenario can be much harder because the measurements should be repeated before the wave packet of the hole left behind in the reservoir moves away from the vicinity of the dot. Thus the required repetition rate could be lowered by having a flat band (with a slow group velocity) in resonance with the dot or a sufficiently small Fermi velocity or a strong external magnetic field. We also consider the anti-Zeno effect, i.e., how measurements can accelerate or enable quantum evolution.

[1] N. Ahmadiniaz *et al.*, Phys. Rev. Res. **4**, L032045 (2022).

15 min. break

DY 9.7 Mon 15:45 MOL 213

Winding Number Statistics for Parametric Chiral Random Matrices — •Nico Hahn[1], Mario Kieburg[2], Omri Gat[3], and Thomas Guhr[1] — [1]University of Duisburg-Essen — [2]University of Melbourne — [3]The Hebrew University of Jerusalem

The winding number is a concept in complex analysis which has, in the presence of chiral symmetry, a physics interpretation as the topological invariant belonging to gapped phases of Fermions. We analytically study the statistical properties of this topological quantity. To this end, we set up a random matrix model for a chiral system with a parametric dependence. We address two chiral symmetry classes, the chiral unitary class without any further symmetries and the chiral symplectic class with additional time reversal symmetry. These classes are referred to as AIII and CII in the tenfold way of topological insulators and superconductors.

DY 9.8 Mon 16:00 MOL 213

Simulating Non-Markovian Qubit Dynamics on a Quantum Processor — •Mirko Rossini, Dominik Maile, Joachim Ankerhold, and Brecht Donvil — Institute for Complex Quantum Systems and IQST

We propose a novel scheme to simulate the open system dynamics of a qubit. We go beyond the completely positive framework and consider linear, trace and Hermicity-preserving but not necessarily positivity-preserving evolution maps. We call these maps general dynamical maps. These maps naturally arise as the solution of general time-local master equations and for finite-dimensional systems they can always be decomposed as the difference between two completely positivity maps. We bring this difference into a form suitable for quantum simulation.

We illustrate our scheme by implementing two examples on IBMQ quantum processors: in the first example, we simulate the evolution of a general time local master equation both from an initial time when the evolution map is guaranteed to be completely positive and from an intermediate time when it is not. With our second example, we show that the simulation of non-completely positive maps gives the ability to recover the initial state of Lindbladian evolution.

DY 9.9 Mon 16:15 MOL 213

Quantum Non-Markovianity made simple through extended states — Meng Xu[1], Yaming Yan[2], Qiang Shi[2], Joachim Ankerhold[1], and •Jürgen T. Stockburger[1] — [1]Institute for Complex Quantum Systems and IQST, Ulm University — [2]Beijing National Laboratory for Molecular Sciences, Chinese Academy of Sciences

We present a recent computational treatment of non-Markovianity [1] in open-system quantum dynamics. Focusing more on intrinsic timescales than on properties of a quantum channel and its generator, we extend the Hierarchical Equations of Motion (HEOM) approach through a highly efficient decomposition of environmental correlation functions into complex exponentials. Complex dynamics at ultralow temperatures and long reservoir timescales becomes tractable by this approach. We demonstrate that our version of the HEOM approach is closely related to an entire family of extended-state approaches, with our new approach being favored through a comparably low number of auxiliary dimensions. The accurate reproduction of long-time algebraic tails in an open-system correlation function provides a benchmark result.

[1] M. Xu *et al.*, Phys. Rev. Lett. **129**, 230601 (2022).

DY 9.10 Mon 16:30 MOL 213

The Influence of Dynamical Phases on a Quantum Processor based Reservoir Computer — •Brecht Donvil, Mirko Rossini, Dominik Maile, and Joachim Ankerhold — ICQ and IQST, University of Ulm, Ulm, Germany

Reservoir computing is subbranch of machine learning where a physical system, the reservoir, is used to perform computational tasks instead of a large neural network which has to be trained. In the last years, quantum systems systems are being explored as potential reservoirs[1,2,3]. While most of the research has focussed on Ising spin systems, recently it was shown that also quantum processors can serve as reservoirs. The authors of [3] illustrated this fact by successfully implementing reservoir computing on an IMBQ quantum processor.

The dynamical phase of the reservoir can influence its performance on certain information processing tasks. For example, the authors of [2] found that the transverse-field Ising model performs best on examples of memory related tasks on the edge of the ergodic phase. The work I present here concerns quantum processor based reservoir computing as proposed in [3]. I consider simple circuit layout which is know to exhibit a dynamical phase transition between a localised and ergodic phase. I show the influence of the dynamical phase of the circuit on its information processing capacity and its performance as a readout device.

[1] K. Fujii and K. Nakajimna, Phys. Rev. Applied **8**, 024030 (2017)
[2] R. Martínez-Peña et al., Phys. Rev. Lett. **127**, 100502 (2021)
[3] J. Chen et al., Phys. Rev. Applied **14**, 024065 (2020)

DY 9.11 Mon 16:45 MOL 213

String order in measurement-induced symmetry-protected topological phases — •Raúl Morral[1], Frank Pollmann[1,3], and Izabella Lovas[1,2] — [1]Department of Physics, TFK, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [2]Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106, USA — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany

We study measurement-induced symmetry protected topological (SPT) order in a wide class of quantum random circuit models, by combining calculations within the stabilizer formalism with tensor network simulations. We construct a family of quantum random circuits, generating the out-of-equilibrium version of all generalized cluster models, and derive a set of non-local string order parameters to distinguish symmetry protected topological phases. We apply this framework to study the random circuit realization of the XZX cluster model, and use the string order parameter to demonstrate that the phase diagram is strikingly stable against extending the class of unitary gates in the circuit, from Clifford gates to Haar unitaries. We then turn to the XZZX generalized cluster model, and demonstrate the coexistence of SPT order and spontaneous symmetry breaking, by relying on string order parameters and a connected correlation function. Our results pave the way to study the properties of a wide range SPT phases in quantum random circuit models with efficient tensor network methods.

DY 9.12 Mon 17:00 MOL 213

Quasiclassical and exact approaches to dissipative nonadiabatic quantum dynamics — •Graziano Amati[1], Johan Runeson[2], and Jerem Richardson[3] — [1]Albert Ludwigs Universitaet Freiburg, Hermann Herder Str. 3, 79104 Freiburg, Germany — [2]Physical and Theoretical Chemistry Laboratory, Oxford University, South Parks Road, Oxford, OX1 3QZ, UK — [3]Laboratory of Physical Chemistry, ETH Zuerich, 8093 Zuerich, Switzerland

The study of many relevant processes in nature from photosynthesis, to radiation damage, to vision, depends on an accurate description of the electronic nonadiabatic dynamics. The brute-force simulation of nonadiabatic systems happens to be a computationally intensive task,

given that the complexity of dynamic simulations scales exponentially with time and with the size of the system. Recently developed of 'spin mapping' approaches allow to recast a wide class of quantum nonadiabatic models onto quasiclassical systems of spins, whose dynamics exhibit a favorable linear or polynomial scaling in complexity. In my contribution I will firstly compare the accuracy in the long-time relaxation of several quasiclassical methods, borrowing ideas from classical ergodic theory. I will then discuss how to further improve the reliability of the long-time predictions of spin mapping techniques, by coupling these methods to the formalism of the non-Markovian generalized quantum master equation. I will then introduce the recent 'ellipsoid mapping' approach, a detailed-balance-preserving extension of spin mapping suited to study systems in thermal equilibrium.

DY 10: Active Matter II (joint session DY/BP/CPP)

Time: Monday 15:00–18:15 Location: ZEU 160

DY 10.1 Mon 15:00 ZEU 160

Chiral motion of actively driven objects in discrete steps towards a remote target — •Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

We address the motion of chiral actively driven objects that move in discrete steps on a flat substrate [1]. While closed polygon-shaped trajectories are found in the case of unperturbed motion, the dynamics becomes surprisingly rich and nonlinear, if the objects additionally head for a fixed remote target. In that situation, cycloidal-like, straight, zigzag-type, doubled zigzag, quadrupled zigzag, and further period-doubled types of trajectory emerge, besides chaotic behavior. Additionally, we investigate the motion of crowds of such objects under explicit mutual alignment interaction. In the absence of fluctuations, collective orientational ordering occurs also in the chaotic regime, in combination with spatial gathering of the particles. Conversely, fluctuations and polydispersity in target alignment counteract orientational ordering. Our results may apply to various types of actively driven objects, for instance, light-responsive bacteria, laser-controlled colloidal particles, or hoppers on vibrated substrates.

[1] A. M. Menzel, resubmitted.

DY 10.2 Mon 15:15 ZEU 160

Polar flocks with discretized directions: the active clock model approaching the Vicsek model — •Matthieu Mangeat, Swarnajit Chatterjee, and Heiko Rieger — Universität des Saarlandes, Saarbrücken, Germany

We study the off-lattice two-dimensional q-state active clock model (ACM) [EPL **138**, 41001 (2022)] as a natural discretization of the Vicsek model (VM) [PRL **75**, 1226 (1995)] describing flocking. The ACM consists of particles able to move in the plane in a discrete set of q equidistant angular directions, as in the active Potts model (APM) [EPL **130**, 66001 (2020); PRE **102**, 042601 (2020)], with a local alignment interaction inspired by the ferromagnetic equilibrium clock model. A collective motion emerges at high densities and low noise. We compute phase diagrams of the ACM and explore the flocking dynamics in the region, in which the high-density (polar liquid) phase coexists with the low-density (gas) phase. We find that for a small number of directions, the flocking transition of the ACM has the same phenomenology as the APM, including macrophase separation and reorientation transition from transversal to longitudinal band motion as a function of the particle self-propulsion velocity. For a larger number of directions, the flocking transition in the ACM becomes equivalent to the one of the VM and displays microphase separation and only transverse bands, i.e. no reorientation transition. Concomitantly also the transition of the $q \to \infty$ limit of the ACM, the active XY model, is in the same universality class as the VM. We also construct a coarse-grained hydrodynamic description akin to the VM.

DY 10.3 Mon 15:30 ZEU 160

Tracer-induced temperature difference in motility-induced phase separation — •Lukas Hecht, Iris Dong, and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstr. 8, D-64289 Darmstadt, Germany

Previous studies of overdamped active Brownian particles (ABPs) mixed with passive tracers have shown that self-propulsion can induce motility-induced phase separation (MIPS) for large enough particle density and self-propulsion speed [1]. Here, we present our study on overdamped ABPs mixed with inertial passive tracers. We show that MIPS features different kinetic temperatures in the dense and the dilute phase if the passive tracers are sufficiently heavy (inertial). Remarkably, unlike for underdamped ABPs [2,3], neither the overdamped ABPs nor the passive tracers alone would feature such a temperature difference in coexisting phases. The observed temperature difference is accompanied by a violation of the equipartition theorem and strongly depends on the self-propulsion speed and the particle density. This allows us to tune the temperature difference from a cold dense and hot dilute phase to the counterintuitive opposite case in which the dense phase is hotter than the dilute phase. These findings open a route to create active materials with a persistent temperature profile by inserting active particles and tuning their self-propulsion speed accordingly.

[1] J. Stenhammar et al., Phys. Rev. Lett. 114, 018301 (2015).
[2] S. Mandal et al., Phys. Rev. Lett. 123, 228001 (2019).
[3] L. Hecht et al., Phys. Rev. Lett. 129, 178001 (2022).

DY 10.4 Mon 15:45 ZEU 160

Collective motion in two-dimensional colloidal systems with effective (active) self-propulsion due to time-delayed feedback — •Robin A. Kopp and Sabine H. L. Klapp — ITP, TU Berlin, Berlin, Germany

In recent years, delayed feedback in colloidal systems has become an active and promising field of study [1,2], key topics being history dependence and the manipulation of transport properties. Here we study the dynamics of a two-dimensional colloidal suspension, subject to time-delayed feedback, where time-delayed feedback can be interpreted as a mechanism of effective self-propulsion, i.e., activity [3]. To this end we perform overdamped Brownian dynamics simulations, where the particles interact through a Weeks-Chandler-Andersen potential. Furthermore, each particle is subject to a Gaussian, repulsive feedback potential, that depends on the difference of the particle position at the current time, and at an earlier time. We observe and quantitatively study the emergence of dynamical clustering and collective motion characterized by a nonzero mean velocity and provide a possible explanation for the underlying mechanism combining single-particle and mean-field-like effects.

[1] S. A. M. Loos, and S. H. L. Klapp, Scientific Reports **9**, 2491 (2019)
[2] M. A. Fernandez-Rodriguez et al., Nature Communications **11**, 4223 (2020)
[3] R. A. Kopp and S. H. L. Klapp, arXiv:2210.03182 (2022)

DY 10.5 Mon 16:00 ZEU 160

Inverted Sedimentation of Active Particles in Unbiased ac Fields — •José Carlos Ureña Marcos and Benno Liebchen — Institut für Physik Kondensierter Materie, TU Darmstadt, Darmstadt, Germany

Biological microswimmers can steer autonomously and use this ability to perform sophisticated tasks. Synthetic microswimmers do not yet reach the same degree of autonomy, and need to be controlled externally if they are to carry out tasks such as targeted cargo delivery or microsurgery. While much progress has been made recently to control their motion based on external forces or gradients, e.g. in light intensity, which have a well-defined direction or bias, little is known about how to steer APs in situations where no permanent bias can be realized.

Here, we show that ac fields with a vanishing time average provide an alternative route to steering APs. We exemplify this route for inertial APs in a gravitational field, observing that a substantial fraction of them persistently travels in the upward direction upon switching on the ac field, resulting in an inverted sedimentation profile at the top wall of a confining container. Our results offer a generic control principle which could be used in the future to steer active motion, to direct collective behaviors and to purify mixtures.

15 min. break

Invited Talk DY 10.6 Mon 16:30 ZEU 160

Long-range communications enable the hierarchical self-organization of active matter — •Igor Aronson[1], Alexander Ziepke[2], Ivan Maryshev[2], and Erwin Frey[2] — [1]Pennsylvania State University, USA — [2]Ludwig-Maximilians-University, Munich, Germany

The most distinct markers of life are the ability to move (locomotion), consume energy (metabolism), process information, and form multi-cellular aggregates. Many biological systems exhibit long-range signaling strategies for evolutionary advantage. We explore the multiscale self-organization of interacting self-propelled agents that locally process information transmitted by chemical signals. The communication capacity dramatically expands their ability to form complex structures, allowing them to self-organize through a series of collective dynamical states at multiple hierarchical levels.

The consequent study shows that information exchange by acoustic waves between the self-propelled units creates a slew of multifunctional structures. Each unit is equipped with an acoustic emitter and a detector in this realization. The swarmers respond to the resulting acoustic field by adjusting their emission frequency and migrating toward the strongest signal. We find self-organized structures with different morphology, including snake-like self-propelled entities, localized aggregates, and spinning vortices. Our results provide insights into the design principles of communicating active particles capable of performing complex tasks.

DY 10.7 Mon 17:00 ZEU 160

Arrested by heating — •Corinna C. Maass[1,2], Prashanth Ramesh[2,1], and Maziyar Jalaal[3] — [1]University of Twente, Enschede, Netherlands — [2]MPI for Dynamics and Self-organization, Göttingen, Germany — [3]Universiteit van Amsterdam, Amsterdam, Netherlands

Active droplets are a class of microswimmers driven by chemical reactions at the droplet interface. Typically, the activity is powered by an advection-diffusion instability in the chemohydrodynamic fields around the droplet that is characterised by the Péclet number Pe of chemical transport. With increasing Pe, higher hydrodynamic modes at the interface cause the droplet to transition from inactivity, to steady, to reorienting, to fully unsteady motion. Here, we demonstrate that it is possible to change Pe reversibly and in situ by thermally activated changes in the chemical enviroment, and thereby to control the motility of the droplet.

DY 10.8 Mon 17:15 ZEU 160

Chiral active particles with non-reciprocal couplings: results from particle-based simulations — •Kim L. Kreienkamp and Sabine H. L. Klapp — Technische Universität Berlin, Germany

Non-reciprocal interactions manifest their drastic impact on the collective dynamics of active matter systems by changing, for example, the general type of observed instabilities [1] and leading to time-dependent states [2,3]. In particular, the combination of non-reciprocity and chirality in terms of intrinsically rotating chiral active particles ("circle swimmers") reveals intriguing non-trivial time-dependent collective dynamics [1].

After having developed an understanding of the collective dynamics on the continuum level in previous work [1], we here present first results of particle-based simulations of chiral active particle systems with non-reciprocal alignment couplings. Indeed, quantitative predictions from continuum approaches are somewhat limited by the approximations made during the coarse-graining process. Thus, the first goal of our particle-based simulations is to explore the validity of the previously obtained continuum results regarding the overall state diagram. Second, we aim at investigating microscopic aspects of the various time-dependent states. Finally, we discuss possibilities to characterize the thermodynamic behavior of the non-reciprocal chiral system based on the stochastic trajectories obtained in particle-resolved simulations.

[1] K. L. Kreienkamp and S. H. L. Klapp, New J. Phys. (2022).
[2] M. Fruchart et al., Nature 592, 363 (2021).
[3] Z. You et al., PNAS 117, 19767 (2020).

DY 10.9 Mon 17:30 ZEU 160

Lattice-induced freezing in active systems unveils dynamic crystallites with square ordering — •Aritra K. Mukhopadhyay[1], Peter Schmelcher[2,3], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, 64289 Darmstadt, Germany. — [2]Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany. — [3]The Hamburg Centre for Ultrafast Imaging, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany.

Active matter, comprising self-propelled particles like bacteria, colloidal microswimmers, or granular microflyers is currently attracting enormous attention for its ability to self-organize into complex nonequilibrium structures. In this work, we report on a new state of dynamic active crystallites, which occurs when exposing active particles to a spatially periodic potential. These crystallites require activity to emerge, adopt the structure of the underlying lattice (e.g. square rather than hexagonal close packing), and are continuously in motion. This new phase unifies the structural properties of crystals with the dynamical properties of disordered fluids. Our work thus unveils a route to creating a new state of active materials with an intrinsic structure that can be externally controlled.

DY 10.10 Mon 17:45 ZEU 160

Shape-dependent collective motion: cohesive groups and cargo transport of colloidal rods — Philipp Stengele, •Anton Lüders, and Peter Nielaba — Universität Konstanz, Konstanz, Deutschland

In active toy model systems where colloids interact via predefined social interaction rules as well as steric collisions, the shape of the individual particles strongly influences emerging collective behavior. We study this based on two example systems using Brownian dynamics simulations (without hydrodynamic interactions). Firstly, we investigate a simple perception model in which colloidal rods move actively if predefined visual stimuli exceed a certain threshold. Here, we find an aspect ratio range where the rods form a dilute cohesive group with a time-independent particle distribution. If the aspect ratio surpasses this range, the rods slowly drift apart. Secondly, we look into the cargo capture and transport of a passive rod using a dense swarm of active spheres which form a hexagonal cage with a cavity for the cargo. Again, the aspect ratio of the rod proves to be crucial, as we find geometric restrictions that must be met to stabilize the cavity. Our work underlines that the shape (here, the aspect ratio) of the particles in active matter systems must be carefully considered while defining interaction rules to perform specific tasks.

DY 10.11 Mon 18:00 ZEU 160

Active Chiral Nematics — •Rüdiger Kürsten[1,2,3] and Demian Levis[1,2] — [1]Departament de Física de la Matèria Condensada, Universitat de Barcelona, Barcelona, Spain — [2]Universitat de Barcelona Institute of Complex Systems (UBICS), Barcelona, Spain — [3]Institut für Physik, Universität Greifswald, Greifswald, Germany

We study inherently chiral self-propelled particles in two dimensions that are subjected to nematic alignment interactions and rotational noise. By means of both, homogeneous and spatially resolved mean field theory we identify various different flocking states. We confirm the presence of the predicted phases using agent-based simulations. We emphasize that special care has to be taken within the simulations in order to avoid artifacts. We present a non-standard simulation technique in order to avoid those artifacts.

DY 11: Focus Session: Physics Meets ML II – Understanding Machine Learning as Complex Interacting Systems (joint session DY/TT)

Machine-learning has recently entered and is now transforming many fields of science, enabling discoveries in a data-driven manner. As a scientific method, however, ML often lacks one defining feature: Explainability. We here seek discussions with pioneers in understanding, explaining, and improving machine learning methods from the point of view as a physical system of interacting elements. In fact, the history of approaching neuronal networks and problems of inference and learning as a problem of statistical physics has a long history, with a number of important discoveries early on. The close relation between spin glasses and neuronal networks are being currently exploited to address pressing questions, such as the remarkable generalization properties of neuronal networks despite their massive overparameterization and their behavior reminiscent of renormalization group transformations.

Organized by Sabine Andergassen (Tübingen) and Moritz Helias (Jülich)

Time: Monday 15:00–18:30 Location: ZEU 250

Invited Talk DY 11.1 Mon 15:00 ZEU 250
The challenge of structured disorder in statistical physics — •Marc Mezard — Bocconi University, Milano

Statistical physics offers many interesting tools to study machine learning. In most cases it needs to use a statistical ensemble of data. Most of the theoretical work has relied on unstructured data. Yet, the highly structured character of data used in training deep networks is a crucial ingredient of their performance. Modelling structured data, analyzing the learning and the generalization of deep networks trained on this data, are major challenges. This talk will describe several recent developments in this direction.

Invited Talk DY 11.2 Mon 15:30 ZEU 250
The emergence of concepts in shallow neural-networks — •Elena Agliari — Piazzale A. Moro 5, 00185 Roma

In the first part of the seminar I will introduce shallow neural-networks from a statistical-mechanics perspective, focusing on simple cases and on a naive scenario where information to be learnt is structureless. Then, inspired by biological information-processing, I will enrich the framework and make the network able to successfully and cheaply handle structured datasets. Results presented are both analytical and numerical.

Invited Talk DY 11.3 Mon 16:00 ZEU 250
Adaptive Kernel Approaches to Feature Learning in Deep Neural Networks — •Zohar Ringel — Racah Institute of Physics, Hebrew University in Jerusalem

Following the ever-increasing role of deep neural networks (DNNs) in our world, a better theoretical understanding of these complex artificial objects is desirable. Some progress in this direction has been seen lately in the realm of infinitely overparameterized DNNs. The outputs of such trained DNNs behave essentially as multivariate Gaussians governed by a certain covariance matrix called the kernel. While such infinite DNNs share many similarities with the finite ones used in practice, various important discrepancies exist. Most notably the fixed kernels of such DNNs stand in contrast to feature learning effects observed in finite DNNs. Such effects are crucial as they are the key to understanding how DNNs process data. To accommodate such effects within the Gaussian/kernel viewpoint, various ideas have been put forward. Here I will provide a short overview of those efforts and then discuss in some detail a general set of equations we developed for feature learning in fully trained/equilibrated DNNs. Interestingly, our approach shows that DNNs accommodate strong feature learning via mean-field effects while having decoupled layers and decoupled neurons within a layer. Furthermore, learning is achieved not by compression of information but rather by increasing neuron variance along label-relevant directions in function space.

DY 11.4 Mon 16:30 ZEU 250
Interpreting black-box ML with the help of physics — •Miriam Klopotek — University of Stuttgart, SimTech Cluster of Excellence EXC 2075, Stuttgart, Germany

Complexity is an unavoidable part of systems with emergent or even so-called intelligent capabilities. Ultimately, it stems from the many microscopic constituents with multiple possible states, which introduces a vast space of degrees of freedom. This is true both for many-body systems as well as modern machine learning (ML) systems. Today, the latter suffer notoriously from the 'black-box problem', i.e. they are inherently opaque. We argue that an engagement with physics can offer deep insights ultimately for a theory of operation and thus an interpretation, as well as powerful ways to assess their reliability and shortcomings. We show some results for a case study with beta-variational autoencoders (β-VAEs) [1], which we trained on data from a well-characterized model system of hard rods confined to 2D lattices [2].

[1] D. P. Kingma and M. Welling, ICLR 2014. D. J. Rezende, S. Mohamed, and D. Wierstra, ICML 2014, p. 1278-1286.
[2] P. Quiring, M. Klopotek and M. Oettel, Phys. Rev. E 100, 012707 (2019).

15 min. break

Invited Talk DY 11.5 Mon 17:00 ZEU 250
Analysing the dynamics of message passing algorithms — •Manfred Opper[1,2] and Burak Cakmak[1] — [1]Institut für Softwaretechnik und Theoretische Informatik, Technische Universität Berlin, 10587, Germany — [2]Centre for Systems Modelling and Quantitative Biomedicine, University of Birmingham, B15 2TT, United Kingdom

Message passing algorithms are deterministic methods which are designed for efficiently computing marginal statistics for probabilistic, Bayesian data models used in machine learning and statistics. Such algorithms have been developed in parallel within the machine learning and the statistical physics communities. They often provide highly accurate approximations at a much higher speed compared to exact Monte Carlo sampling. The fixed points of such algorithms can be analysed for high dimensional models (under the assumption of specific data distributions) using the replica method of statistical physics. In this talk we will focus on the dynamical properties of the algorithms. Applying dynamical functional techniques to the nonlinear dynamics, the degrees of freedom which interact via a random matrix can be decoupled in the limit of large systems resulting in exact stochastic single node dynamics. For general dynamical models, it is hard to further analyse this effective dynamics due to the occurence of memory terms. Surprisingly, for message passing algorithms memory terms are absent and exact results for convergence rates and stability can be derived for specific data distributions.

Invited Talk DY 11.6 Mon 17:30 ZEU 250
Deep Learning Theory Beyond the Kernel Limit — •Cengiz Pehlevan — Harvard University, USA

Deep learning has emerged as a successful paradigm for solving challenging machine learning and computational problems across a variety of domains. However, theoretical understanding of the training and generalization of modern deep learning methods lags behind current practice. I will give an overview of our recent results in this domain, including a new theory that we derived by applying dynamical field theory to deep learning dynamics. This theory gives insight into internal representations learned by the network under different learning rules.

DY 11.7 Mon 18:00 ZEU 250
Solving the Bethe–Salpeter equation with exponential con-

vergence — •Markus Wallerberger[1], Hiroshi Shinaoka[2], and Anna Kauch[1] — [1]TU Wien, Vienna, Austria — [2]Saitama University, Japan

The Bethe–Salpeter equation plays a crucial role in understanding the physics of correlated fermions, relating to optical excitations in solids as well as resonances in high-energy physics. Yet, it is notoriously difficult to control numerically, typically requiring an effort that scales polynomially with energy scales and accuracy. This puts many interesting systems out of computational reach.

Using the intermediate representation and sparse modeling for two-particle objects on the Matsubara axis, we develop an algorithm that solves the Bethe–Salpeter equation in $O(L^8)$ time with $O(L^4)$ memory, where L grows only logarithmically with inverse temperature, bandwidth, and desired accuracy. This opens the door for computations in hitherto inaccessible regimes. We benchmark the method on the Hubbard atom and on the multiorbital weak-coupling limit, where we observe the expected exponential convergence to the analytical results. We then showcase the method for a realistic impurity problem.

[1] M. Wallerberger et al., Phys. Rev. Research 3, 033168 (2021)

DY 11.8 Mon 18:15 ZEU 250

Making machines untangle the parquet equations — •Samuel Badr[1], Anna Kauch[1], Hiroshi Shinaoka[2], Karsten Held[1], and Markus Wallerberger[1] — [1]TU Wien, Vienna, Austria — [2]Saitama University, Saitama, Japan

Diagrammatic theories at the two-particle level are increasingly important in understanding the subtle interplay of phenomena occurring in strongly correlated electron systems. The parquet equations are a centerpiece of many such theories, since they are the simplest unbiased topological classification of two-particle diagrams. However, due to their eponymous interlocking structure, the parquet equations are vexingly difficult to solve, requiring prohibitive amounts of memory.

We tackle this problem using the recently developed, machine learning inspired, techniques: firstly, the overcomplete intermediate representation, a highly compressed model for two-particle objects which is guaranteed to converge exponentially; secondly, a sparse set of Matsubara frequencies tailored to the structure of the parquet equations. This allows us to perform convolutions and frequency shifts at no loss of accuracy.

We benchmark our solver for the Hubbard atom, where we reproduce analytic results, and then showcase the solver for more extended systems.

DY 12: Nonequilibrium Quantum Many-Body Systems I (joint session TT/DY)

Time: Tuesday 9:30–13:15 Location: HSZ 204

DY 12.1 Tue 9:30 HSZ 204

Ultrafast dynamics of quantum many-body systems including dynamical screening and strong coupling — •Michael Bonitz[1], Jan-Philip Joost[1], Hannes Ohldag[1], Erik Schroedter[1], and Iva Brezinova[2] — [1]CAU Kiel, Institute for Theoretical Physics and Astrophysics — [2]TU Wien, Institute of Applied Physics, Vienna, Austria

Dynamical screening is a key property of charged many-particle systems. Its theoretical description is based on the GW approximation that is extensively applied for ground-state and equilibrium situations. The main limitation of the GW approximation is the neglect of strong electronic correlation effects. Here we derive the nonequilibrium dynamically screened ladder (DSL) approximation that self-consistently includes, in addition to the GW diagrams, also particle-particle and particle-hole T-matrix diagrams. Our DSL approach is formulated within the G1-G2 scheme [1,2] that is linear in time, in contrast to the cubic scaling of standard Nonequilibrium Green functions simulations. The price to pay for this speedup is the need to store the two-particle Green function. This can be avoided with a recently developed quantum fluctuations approach [3].

[1] N. Schluenzen et al., Phys. Rev. Lett. 124, 076601 (2020)
[2] J.-P. Joost al., Phys. Rev. B 105, 165155 (2022)
[3] E. Schroedter et al., Cond. Mat. Phys. 25 , 23401 (2022)

DY 12.2 Tue 9:45 HSZ 204

Spectral response of a charge density wave insulator to periodic driving — •Alexander Osterkorn, Constantin Meyer, and Salvatore Manmana — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

Periodically driven quantum many-body systems host unconventional behavior not realized at equilibrium. Here we address in detail the emergence of a cosine-like band in the gap region of the nonequilibrium single-particle spectral function of strongly interacting spinless fermions on a chain in the charge density wave phase [1]. We compare the dynamics of the periodically driven system to the quench dynamics with an effective Floquet Hamiltonian and discuss the role of doublon excitations in both cases. This is investigated using both matrix product state based time evolution techniques as well as time-dependent Hartree-Fock. [1] arXiv:2205.09557

DY 12.3 Tue 10:00 HSZ 204

Floquet engineering in tilted lattices — •Melissa Will[1], Pablo Sala[2,3], and Frank Pollmann[1] — [1]Department of Physics, T42, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [2]Department of Physics and Institute for Quantum Information and Matter, California Institute of Technology, Pasadena, California 91125, USA — [3]Walter Burke Institute for Theoretical Physics, California Institute of Technology, Pasadena, California 91125, USA

Quantum many-body systems out of equilibrium can exhibit very rich and exciting phenomena. A particularly important question is whether and how a quantum system thermalizes under unitary evolution. In this context three classes of systems have been identified: ergodic, localized and an intermediate regime exhibiting so called quantum many-body scars. In this talk we discuss whether a time-periodic, local drive can induce thermalization of a localized system. We consider interacting hard-core bosons in an one dimensional, tilted system with periodic driving. We find that the system becomes ergodic for resonant driving frequencies. In contrast, if the tilt is not close to a multiple of driving frequency, the system stays localized. This observation can theoretically be understood by deriving an effective Hamiltonian using a Magnus expansion. Using large scale numerical methods, we explore entanglement entropy and imbalance over time. Our theoretical predictions are in good agreement with numerics.

DY 12.4 Tue 10:15 HSZ 204

Photoinduced spinful excitons in Hubbard systems with magnetic superstructures — Constantin Meyer and •Salvatore R. Manmana — Institute for Theoretical Physics, Göttingen University, Friedrich-Hund-Platz 1, 37077 Göttingen

The possibility to form excitons in photo-illuminated correlated materials is central from fundamental and application oriented perspectives. We show how the interplay of electron-electron interactions and a magnetic superstructure leads to the formation of a peculiar spinful exciton, which can be detected in the nonequilibrium spectral function and the time-dependent optical conductivity. We study these quantities by using matrix product states (MPS) following an electron-hole excitation in a class of one-dimensional Hubbard models with on-site interactions and alternating local magnetic fields, which realize correlated band insulators. An excitation in only one specific spin direction leads to an additional band in the gap region of the spectral function only in the opposite spin direction, and to an additional peak in the optical conductivity. We discuss implications for experimental studies in correlated insulator systems.

DY 12.5 Tue 10:30 HSZ 204

Photoinduced pairing states of excitonic insulators — •Satoshi Ejima — DLR Quantencomputing-Initiative, Hamburg, Germany

Applying the time-dependent density-matrix renormalization group technique, we explore photoinduced pairing states in the half-filled extended Falicov-Kimball model (EFKM) in one dimension, both with and without internal SU(2) symmetry. In the time-dependent photoemission spectra simulated with the optimal pump pulse parameters, an extra band appears above the Fermi energy after pulse irradiation, implying a photoinduced metallization. Even in the absence of the SU(2) structure, the electron-electron pair correlations can also be enhanced

during the pump, while they decrease over time after pulse irradiation. This suggests a possible photoexcited metallization of Ta_2NiSe_5, a strong candidate for an excitonic insulator material, for which the EFKM is considered to be the minimal theoretical model. Computing the time-dependent photoemission spectra with the parameter set for this material, i.e., in the EFKM without SU(2) symmetry, we demonstrate the photoinduced insulator-to-metal transition, in accord with recent findings in time- and angle-resolved photoemission spectroscopy experiments on Ta_2NiSe_5.
[1] S. Ejima, F. Lange, H. Fehske, Phys. Rev. B **105**, 245126 (2022)

15 min. break

Invited Talk DY 12.6 Tue 11:00 HSZ 204
Higgs spectroscopy of superconductors in nonequilibrium — •Dirk Manske — Max-Planck-Institut für Festkörperforschung

Higgs spectroscopy is a new and emergent field [1-3] that allows to classify and determine the superconducting order parameter by means of ultra-fast optical spectroscopy. There are two important ways to activate the Higgs mode in superconductors, namely a single-cycle *quench* or an adiabatic, multicycle *drive* pulse, which I will discuss in detail. Furthermore, I will review and report on the latest progress on Higgs spectroscopy, in particular on the role of the third-harmonic-generation (THG) [4-6] and the possible IR-activation of the Higgs mode by impurities or external dc current [7,8]. I also provide new predictions for time-resolved ARPES experiments in which, after a quench, a continuum of Higgs mode is observable and a phase information of the superconducting gap function would be possible to extract [9]. Finally, I show that the Higgs mode may shed some light on the 25-years-old A1g-puzzle in equilibrium Raman scattering on high-T_c cuprates [10].
[1] Nat. Commun. 11, 287 (2020)
[2] Phys. Rev. B 101, 184519 (2020)
[3] Nat. Commun. 11, 1793 (2020)
[4] Phys. Rev. B 104, 174508 (2021)
[5] Nature Commun., accepted (2022)
[6] Nature Commun., submitted (2022)
[7] Phys. Rev. B 101, 220507 (2020)
[8] Phys. Rev. B 104, 134504 (2021)
[9] Phys. Rev. B 101, 224510 (2020)
[10] Phys. Rev. Lett. 127, 197001 (2021)

DY 12.7 Tue 11:30 HSZ 204
Periodically driven spin-1/2 XXZ antiferromagnetic chains — •Aslam Parvej, Imke Schneider, and Sebastian Eggert — Technische Universität Kaiserslautern, Kaiserslautern, Germany

Time-periodically driven quantum systems are of great interest due to the possibility of unconventional states of matter and Floquet engineering. The interplay of many-body interactions and time-periodic manipulations facilitate new phenomena in the steady state. We analyze the Floquet steady states of finite spin-1/2 XXZ antiferromagnetic chains with periodically driven anisotropy parameter at frequencies below the band width, so that resonances are in principle possible. We use a numerical real-time approach with an adiabatic time evolution protocol by ramping up the driving amplitude of the external periodic drive to prepare a non-equilibrium Floquet steady state. Parametric resonances are expected when the driving frequencies are equal to twice the energy gaps in a finite system. However, the observed resonance absorption of energy and heating is surprisingly weak in our system even for large driving amplitude. This changes if a square wave is used for driving.

DY 12.8 Tue 11:45 HSZ 204
Controllable effects of the mass term in time-periodic driven sine-Gordon models. — •Dimo Claude[1], Simon Jäger[1], Christoph Dauer[1], Piotr Chudzinski[2], Imke Schneider[1], and Sebastian Eggert[1] — [1]Physics Department and Research Center OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany. — [2]Institute of Fundamental Technological Research, Polish Academy of Science, 02-106 Warszawa, Poland.

Recently, the full Floquet solution of a Luttinger Liquid with periodically modulated interactions has been derived and resonant wavevectors have been identified. There, the quantum state can only be stabilized when damping mechanisms of the one-dimensional systems are included. In our work, we investigate the time-periodic Luttinger Liquid under a non-linear perturbation which originates from the Sine-Gordon potential. This term provides interactions among the different modes of the Luttinger Liquid and can potentially confine the parametrically amplified modes. We investigate this model up to fourth order of the phase field using a mean-field approach. The resulting effective model is quadratic in the field operators while the non-linearity remains, due to the explicit dependence of the frequencies on the time-dependent quantum state. Using a self-consistency relation between the number of density wave excitations and the systems' energy, we discuss the formation of a non-equilibrium steady state and study its stability.

DY 12.9 Tue 12:00 HSZ 204
Influence of phononic dissipation on impact ionization processes in a photodriven Mott insulator — •Paolo Gazzaneo, Tommaso Maria Mazzocchi, Jan Lotze, and Enrico Arrigoni — Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz, Austria

It has been suggested that in strongly correlated materials, highly photoexcited charge carriers could use their extra energy to excite additional carriers across the Mott gap via impact ionization [1,2]. However, the influence of electron-phonon scattering on photocurrent and impact ionization in Mott photovoltaic setups is still an open question.

We address this issue in a nonequilibrium steady state study on the occurrence of impact ionization in a simplified model of a Mott photovoltaic device in presence of acoustic phonons [3], consisting of a Mott-insulating layer coupled to two wide-band fermion leads.

For a small hybridization to the leads, we obtain a peak in the photocurrent as a function of the driving frequency which can be associated with impact ionization processes, while for larger hybridizations we find a suppression of impact ionization with respect to direct photovoltaic excitations. The effect of acoustic phonons produces a slight enhancement of the photocurrent for small driving frequencies and a suppression at frequencies around the main peak at all considered hybridization strengths.
[1] E. Manousakis, Phys. Rev. B 82, 125109 (2010)
[2] J. E. Coulter et al., Phys. Rev. B 90, 165142 (2014)
[3] Gazzaneo et al., Phys. Rev. B 106, 195140 (2022)

DY 12.10 Tue 12:15 HSZ 204
Correlated Mott insulators in strong electric fields: Role of phonons in heat dissipation — •Tommaso Maria Mazzocchi, Paolo Gazzaneo, Jan Lotze, and Enrico Arrigoni — Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz, Austria

Mott-insulating models can undergo an insulator-to-metal transition when subject to a constant bias voltage [1], which makes them suitable to describe the resistive switch observed in correlated insulators [2]. Nonequilibrium state-of-the-art techniques rely on the coupling to fermion baths to dissipate the field-induced excess energy [1,3]. However, a realistic description of heat-exchange requires the inclusion of phonons. In [4] we study a single-band Hubbard model in a static electric field coupled to electron and acoustic phonon baths. The nonequilibrium steady-state is addressed via the dynamical mean-field theory using the auxiliary master equation approach as impurity solver. Phonons are included via the Migdal approximation. Using both the electron and phonon baths the steady-state current is slightly enhanced by phonons for field strengths close to half of the gap and suppressed at the gap resonance. With phonons alone, dissipation can occur only at the resonances and the current at the metallic phase is suppressed by almost one order of magnitude.
[1] C. Aron, Phys. Rev. B 86, 085127 (2012)
[2] E. Janod et al., Adv. Funct. Mater. 25, 6277 (2015)
[3] Y. Murakami et al., Phys. Rev. B 98, 075102 (2018)
[4] T.M. Mazzocchi et al., Phys. Rev. B 106, 125123 (2022)

DY 12.11 Tue 12:30 HSZ 204
Correlated Mott insulators and photovoltaics out of equilibrium: phonons and heat dissipation — •Enrico Arrigoni, Tommaso Mazzocchi, Paolo Gazzaneo, Daniel Werner, and Jan Lotze — Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz Austria

I will present recent results for correlated Mott systems in a nonequilibrium driven steady state. Results are obtained via nonequilibrium Dynamical Mean Field Theory with an impurity solver based upon a combination of Keldysh Green's functions and Lindblad formalism for open quantum systems [1]. Recent improvements based upon a Configuration Interaction treatment of the many body Lindblad equa-

tion allow for an efficient solution of the impurity problem deep in the Kondo regime [2].

In particular, I will discuss the interplay of strong correlation and Joule dissipation by phonons near the Mott dielectric breakdown [3] and in photoexcitation induced transport across a Mott insulating gap [4].

[1] E. Arrigoni et al., Phys. Rev. Lett. 110, 086403 (2013)
A. Dorda et al., Phys. Rev. B 89 165105 (2014)
A. Dorda et al., Phys. Rev. B 92, 125145 (2015)
[2] D. Werner et al., arXiv:2210.09623 (2022)
[3] T. Mazzocchi at al., Phys. Rev. B 106, 125123 (2022)
[4] M. Sorantin et al., Phys. Rev. B 97, 115113 (2018)
P. Gazzaneo et al. Phys. Rev. B 106, 195140 (2022)

DY 12.12 Tue 12:45 HSZ 204

Photoinduced prethermal order parameter dynamics in the two-dimensional large-N Hubbard-Heisenberg model — •Alexander Osterkorn and Stefan Kehrein — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

We study the microscopic dynamics of competing ordered phases in a two-dimensional correlated electron model [1], which is driven with a pulsed electric field of finite duration. In order to go beyond a mean-field treatment of the electronic interactions we adopt a large-N generalization of the Hubbard model and combine it with the semi-classical fermionic truncated Wigner approximation as a time evolution method. This allows us to calculate dephasing corrections to the mean-field dynamics and to obtain stationary states, which we interpret as prethermal order. We use this framework to simulate the light-induced transition between two competing phases (bond density wave and staggered flux) and find that the post-pulse stationary state order parameter values are not determined alone by the amount of absorbed energy but depend explicitly on the driving frequency and field direction. While the transition between the two prethermal phases takes place at similar total energies in the low- and high-frequency regimes, we identify an intermediate frequency regime for which it occurs with minimal heating [2].

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

DY 12.13 Tue 13:00 HSZ 204

Observation of magnon bound states in the long-range, anisotropic Heisenberg model — Florian Kranzl[1], •Stefan Birnkammer[2], Manoj Joshi[1], Alvise Bastianello[2], Rainer Blatt[1], Michael Knap[2], and Christian Roos[1] — [1]Universität Innsbruck, Innsbruck, Austria — [2]Technische Universität München, Garching, Germany

Over the recent years coherent, time-periodic modulation has been established as a versatile tool for realizing novel Hamiltonians. Using this approach, known as Floquet engineering, we experimentally realize a long-ranged, anisotropic Heisenberg model with tunable interactions in a trapped ion quantum simulator. We demonstrate that the spectrum of the model contains not only single magnon excitations but also composite magnon bound states. For the experimentally realized long-range interactions, the group velocity of magnons is unbounded. Nonetheless, for sufficiently strong interactions we observe bound states of these unconventional magnons which possess a non-diverging group velocity. By measuring the configurational mutual information between two disjoint intervals, we demonstrate the implications of the bound state formation on the entanglement dynamics of the system. Our observations provide key insights into the peculiar role of composite excitations in the non-equilibrium dynamics of quantum many-body systems.

DY 13: Active Matter III (joint session BP/CPP/DY)

Time: Tuesday 9:30–12:30 Location: TOE 317

DY 13.1 Tue 9:30 TOE 317

Gliding motility and reorientation of flagellated microbes on curved surfaces — •Alexandros Fragkopoulos[1], Nicolas Fares[1,2], and Oliver Bäumchen[1] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]University of Bordeaux, CNRS, LOMA, UMR 5798, 33400 Talence, France

The model organism *Chlamydomonas reinhardtii*, a unicellular biflagellated microalga, can adhere and colonize almost any surface under particular light conditions. Once the cells attach to a surface, an intraflagellar transport machinery translocates the cell body along the flagella, which are oriented in a 180° configuration. This motion is known as gliding motility. Even though the cells firmly adhere to surfaces, they are able to reorient through different physical mechanisms [1]. With the use of the orientation autocorrelation function, we find that cells exhibit large reorientation events shortly after their initial attachment to a surface, while at longer time scales they are primarily constrained to 1D motion. On cylindrical surfaces, the large reoriations cause the cells to predominantely align in the direction of the minimum principle curvature. We quantify the curvature-induced alignment using the nematic order parameter and reveal that the minimum surface curvature required for cell alignment is comparable to the static flagella curvature.

[1] S. Till, et al., *Phys. Rev. Res.*, (Accepted)

DY 13.2 Tue 9:45 TOE 317

Efficiency of navigation strategies for active particles — •Lorenzo Piro[1], Ramin Golestanian[1,2], and Benoit Mahault[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, United Kingdom

Optimal navigation in complex environments is a problem with multiple applications ranging from designing efficient search strategies to engineering microscopic cargo delivery. When motion happens in presence of strong external forces, route optimization is particularly important as active particles may encounter trapping regions that would substantially slow down their progress.

Here, considering a self-propelled agent moving at a constant speed, we study the efficiency of Zermelo's classical solution. Investigating both cases of motion on the plane and on curved surfaces, we focus on the regime where the external force exceeds self-propulsion in finite regions. There, we show that, despite the fact that most trajectories following the trivial policy of going straight get arrested, the Zermelo policy allows for a comprehensive exploration of the environment.

However, our results also indicate an increased sensitivity of the Zermelo strategy to initial conditions, which limits its robustness and long-time efficiency, particularly in presence of fluctuations. These results suggest an interesting trade-off between exploration efficiency and stability for the design of control strategies to be implemented in real systems.

DY 13.3 Tue 10:00 TOE 317

Run with the Brownian Hare, Hunt with the Deterministic Hounds — •Davide Bernardi[1] and Benjamin Lindner[2,3] — [1]Italian Institute of Technology, Ferrara, Italy — [2]Bernstein Center for Computational Neuroscience, Berlin, Germany — [3]Institut für Physik, Humboldt-Universität zu Berlin

Pursuit and evasion are vital to most animal species and play an important role in many human activities. Traditionally, chase-and-escape models have been studied in the framework of game theory, or in detailed models that can be studied only through numerical simulations and that lack generalization power.

Here, we present analytic results for the mean time and energy used by a pack of deterministic hounds to capture a prey that undergoes Brownian diffusion. Depending on the number of chasers, we find that the mean capture time as a function of the prey's diffusion coefficient can be monotonically increasing, decreasing, or attain a minimum at a finite value. Furthermore, an optimal speed and number of chasing hounds exist, that depend on the baseline power consumption and drag coefficient of each chaser.

The present model can be seen as an analytically tractable basis for the theoretician's perspective on the growing field of smart microswimmers and autonomous robots.

DY 13.4 Tue 10:15 TOE 317

Function of Morphodynamics in Foraging *Physarum polycephalum* — •Lisa Schick[1], Mirna Kramar[2], and Karen Alim[1] — [1]School of Natural Sciences, Technical University of Munich, Ger-

many — [2]Institute Curie, Paris, France

How network-forming fungi structure and reorganize their network morphology and thereby the carbon flows in the soil is key to understanding climate - yet hidden from us due to the long time scales of network dynamics and the soil itself. Here, the network-forming slime mold *Physarum polycephalum* serves as a model of network dynamics of a foraging network-forming life. We follow and quantify the network migration velocity and morphology of foraging *P. polycephalum*. We identify three distinct morphological states characterized by network compactness and density of moving fronts. Estimating the energetic cost of distinct states, we find that morphological variability allows the organism to balance the energetic costs of foraging and search strategy. Our observations allow us to project how resource availability might shift the balance and thereby affect network extension in foraging network-forming organisms.

DY 13.5 Tue 10:30 TOE 317

Unraveling the migratory behavior of a large single-celled organism — •Lucas Tröger, Florian Goirand, and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

Many cells face search problems, such as finding food, conspecifics, or shelter, and different search strategies can provide different chances for success. In contrast to most single-celled organisms the slime mold *Physarum polycephalum* forms a giant network-shaped cell while foraging for food. Which advantage does the giant cell at the verge to multicellularity provide? We experimentally investigate and quantify the long-time migratory behavior of small networks of *P. polycephalum* in the absence and in the presence of food, and develop a simple mechanistic model that successfully describes its migration. We find that *P. polycephalum* performs a run-and-tumble-like motion modified by self-avoidance to achieve superdiffusive migration. Furthermore, it tunes its short-time dynamics in order to adapt to environments with different amounts of available nutrients, while its long-time dynamics remain unchanged. This work shows how *P. polycephalum* controls the inherent stochasticity of its movement by simple rules, which may represent an evolutionary advantage.

15 min. break

DY 13.6 Tue 11:00 TOE 317

Controlling active turbulence by activity patterns — •arghavan partovifard, josua grawitter, and holger stark — Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Active fluids exhibit spontaneous and chaotic flow patterns which are known as active turbulence [1]. One of the current challenges in active matter is controlling and harnessing these flow patterns for powering processes at small scales [2]. As a simple realization of an active fluid, we consider a semi-dilute solution of active rods and study it within a numerical simulation of the governing equations that are formulated in terms of velocity and the orientational order tensor parameter fields.

We find that for a solution of pusher active rods there is a critical magnitude of activity above which the initially isotropic solution develops locally varying nematic order and turbulent-like fluid flow. Aiming to control the turbulent flow state, we pattern the activity with a square lattice of circular inactivity spots. We find that for a specific range of lattice parameters the flow field develops lanes of unidirectional flow with alternating directions while between them a row of corotating vortexes emerges; We call this state the laning state and it is multistable since different realizations of the random initial state of rods lead to different configurations of the laning state with various widths of the lanes. In this state, the director field develops nematic domains oriented toward the Leslie angle with respect to the flow.

[1] Wensink *et al.*, Proc. Natl. Acad. Sci. **109**, 14308-14313 (2012)
[2] Bowick *et al.*, Phys. Rev. X **12**, 010501 (2022)

DY 13.7 Tue 11:15 TOE 317

Active matter: From spontaneous to controlled phenomena. — •Daniel Pearce — University of Geneva

Active matter is the study of materials able to move themselves. During this talk I will discuss how we can take advantage of the interplay between topological defects, geometry and topology to exercise control over active materials. By studying active nematic fluids on a curved surface, we can influence the position and orientation of topological defects according to their charge. This means specific nematic textures can be generated. By studying active contractile actomyosin gels, it is possible to show that only active topological defects with charge +1 can generate curvature, and the sign is related to the phase of the defect. This frees the process from the constraints of the Poincare-Hopf theorem and allows complex surfaces to be generated. This is demonstrated by recreating the shape of a freshwater hydra from the positions of the topological defects

DY 13.8 Tue 11:30 TOE 317

Nucleation of chemically active droplets — •Noah Ziethen and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Liquid-liquid phase separation emerged as a crucial organizing principle inside biological cells giving rise to a plethora of intracellular compartments. Unique to the cellular context, these condensates can consist of only a few hundred molecules and are affected by non-equilibrium processes. In particular, active chemical conversion between condensate material and proteins in the surrounding cytoplasm can control multiple aspects of the condensates. Yet, it is unclear how these reactions affect the spontaneous nucleation and dissolution associated with low particle numbers. Here, we investigate the influence of chemical reactions on the bistable region of active droplets using a stochastic field theory. We find an effective increase in the energy barrier and thus decelerated transitions between the homogeneous and the droplet state. Using classical nucleation theory, we approximate the full dynamics by diffusion in a free energy potential described by an analytical expression only depending on droplet radius and reaction rate. This analogy also allows us to determine the equivalence of the binodal line, so we can propose an extension of the equilibrium phase diagram to capture driven chemical reactions. Cells might use these effects to control the nucleation of intracellular droplets.

DY 13.9 Tue 11:45 TOE 317

Hydrodynamic description and transport coefficients in a model of active cellular aggregates — •Subhadip Chakraborti[1,2] and Vasily Zaburdaev[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany

Complex multicellular aggregates consisting of a large number of interacting cells are ubiquitous in biology, ranging from bacterial biofilms to organoids, cell spheroids, and tumors. We consider colonies of *N. gonorrhoeae* bacteria as a prototypical example of cells that use retractile cell appendages to actively interact with a substrate and with each other. We construct a microscopic model on a 1D lattice taking into account the non-equilibrium bacterial motility driven by two crucial forces – cell-substrate and cell-cell interactions. We observe a phase transition from a homogeneous state to a clusterized state upon tuning the density and activity parameters. Using macroscopic fluctuation theory (MFT), we analytically derive hydrodynamics for the model system and calculate two density-dependent transport coefficients – the bulk-diffusion coefficient and the conductivity. The behavior of these transport coefficients successfully explains the non-equilibrium phase transition. We support our analytical findings with the results obtained numerically. Our theory provides a general framework for studying the non-equilibrium collective behavior of other dense cellular aggregates also, in the context of dynamics and their transport properties.

DY 13.10 Tue 12:00 TOE 317

Flocking of unfriendly species: The two-species Vicsek model — •Swarnajit Chatterjee[1], Matthieu Mangeat[1], Chul-Ung Woo[2], Heiko Rieger[1], and Jae Dong Noh[2] — [1]Saarland University, Saarbrücken, Germany — [2]University of Seoul, Seoul, Korea

We consider the two-species Vicsek model (TSVM) consisting of two kinds of self-propelled particles, A and B, that tend to align with particles from the same species and to anti-align with the other. The model shows a flocking transition that is reminiscent of the original Vicsek model [1]: it has a liquid-gas phase transition and displays micro-phase separation in the coexistence region where multiple dense liquid bands propagate in a gaseous background. The novel feature of the TSVM is the existence of two kinds of bands, one composed of mainly A-particles and one mainly of B- particles and the appearance of two dynamical states in the coexistence region: the PF (parallel flocking) state in which all bands of the two species propagate in the same direction, and the APF (anti-parallel flocking) state in which the bands of species A and species B move in opposite directions. When PF and APF states exist in the low-density part of the coexistence region they perform stochastic transitions from one to the other. The system size

dependence of the transition frequency and dwell times shows a pronounced crossover that is determined by the ratio of the band width and the longitudinal system size. Our work paves the way for studying multispecies models with heterogeneous alignment interactions.

[1] T. Vicsek, A. Czirók, E. Ben-Jacob, I. Cohen, and O. Shochet, Phys. Rev. Lett. 75, 1226 (1995).

DY 13.11 Tue 12:15 TOE 317

Two-potential model for molecular motors — •Sophie Klempahn and Helmut Schiessel — Cluster of Excellence Physics of Life, Technical University of Dresden, Germany

Molecular motors are highly efficient biological machines, which drive systems away from equilibrium and realise key biological processes. For the description of the molecular motor action, discrete jump processes as well as energy barriers with height differences can be used. However, these models are based on symmetric conditions or unidirectional motion and therefore do not capture real biological systems with fuel gradients or where the motion is not unidirectional. To predict the effect of molecular motors on the density distribution of cargo particles in one dimension, we introduce a two potential model. This model represents the cargo particles as active particles, in which the binding of molecular motors to the cargo particle causes the active part of motion. Furthermore, we use two different energy landscapes for jumps to the left or right side, to include motors moving back- and forward, asymmetric environment or two different molecular motors acting on the same cargo particle in different directions. The solution of a master equation with different energy landscapes for jumps to the left and right side results in specific extremal points in the probability density of the cargo particles and shows a ratchet effect in case of periodic potentials.

DY 14: Invited Talk: Machine Learning and Complex Fluids

Time: Tuesday 9:30–10:00 Location: MOL 213

Invited Talk DY 14.1 Tue 9:30 MOL 213

Unraveling structural and dynamical features in glassy fluids using machine learning — •Laura Filion[1], Frank Smallenburg[2], and Rinske Alkemade[1] — [1]Debye Institute for Nanomaterials Science, Utrecht University, Netherlands — [2]Laboratoire de physique des Solides, Université Paris-Saclay, France

Developments in machine learning (ML) have opened the door to fully new methods for studying phase transitions due to their ability to extremely efficiently identify complex patterns in systems of many particles. Applications of machine learning techniques vary from the use of developing new ML-based order parameters for complex crystal structures, to locating phase transitions, to speeding up simulations. The rapid emergence of multiple applications of machine learning to statistical mechanics and materials science demonstrates that these techniques are destined to become an important tool for soft matter physics. In this talk, I will briefly present an overview of the work my group is doing on using ML to study soft matter systems, with a focus on how ML can be used to explore new connections between structure and dynamics in supercooled liquids. In particular, I will present a strategy to fit the dynamics in glassy systems using advanced hierarchical order parameters combined with simple linear regression. Additionally, I will present a method for extracting the cage structure of a glassy configuration, and demonstrate that this information significantly improves our ability to predict glassy dynamics over a broad range of time scales.

DY 15: Physics of Contagion Processes I (joint session SOE/DY)

Time: Tuesday 9:30–10:00 Location: ZEU 260

Invited Talk DY 15.1 Tue 9:30 ZEU 260

Digital Pandemiology – Is that physics? — •Dirk Brockmann — Humboldt University of Berlin, Berlin, Germany

Three years of COVID-19 lie behind us. Experts from various fields worked constantly on understanding, mitigating and making sense of the pandemic. Novel digital tools became an essential part and complemented traditional, epidemiological methods. I will report on research activities and digital projects we launched during the past years that delivered important insights and were helpful as real-time assessment tools during the pandemic. These include the Covid-19-mobility monitor and the Corona Data Donation Project in which more than 500,000 participants donated daily data collected by their smartwatch or wearable device. I will summarize the results we obtained from these technologies and discuss why physics, as a mindset, is helpful for understanding phenomena that unfold across the borders of traditional scientific disciplines.

DY 16: Complex Fluids and Soft Matter (joint session DY/CPP)

Time: Tuesday 10:00–13:00 Location: MOL 213

DY 16.1 Tue 10:00 MOL 213

How are mobility and friction related in viscoelastic fluids? — •Juliana Caspers[1], Nikolas Ditz[2], Karthika Krishna Kumar[2], Felix Ginot[2], Clemens Bechinger[2], Matthias Fuchs[2], and Matthias Krüger[1] — [1]Institute for Theoretical Physics, Georg-August Universität Göttingen, 37073 Göttingen, Germany — [2]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

The motion of a colloidal probe in a viscoelastic fluid is described by friction or mobility, depending on whether the probe is moving with a velocity or feeling a force. While the Einstein relation describes an inverse relationship valid for Newtonian solvents, both concepts are generalized to time-dependent memory kernels in viscoelastic fluids. We theoretically and experimentally investigate their relation by considering two observables: the recoil after releasing a probe that was moved through the fluid and the equilibrium mean squared displacement (MSD). Applying concepts of linear response theory, we generalize Einstein's relation and thereby relate recoil and MSD, which both provide access to the mobility kernel. With increasing concentration, however, MSD and recoil show distinct behaviors, rooted in different behaviors of the two kernels. Using two theoretical models, a linear two-bath particle model and hard spheres treated by mode-coupling theory, we find a Volterra relation between the two kernels, explaining differing timescales in friction and mobility kernels under variation of concentration.

DY 16.2 Tue 10:15 MOL 213

Can liquid-state theory predict jamming of hard particles? — •Carmine Anzivino[1], Mathias Casiulis[2], Amgad Moussa[3], Stefano Martiniani[2], and Alessio Zaccone[1] — [1]Department of Physics "A. Pontremoli", University of Milan, via Celoria 16, 20133 Milan, Italy — [2]Center for Soft Matter Research, Department of Physics, New York University, New York 10003, USA — [3]Syngenta AG, 4058 Basel, Switzerland

By generalizing the notion of maximally random jammed (MRJ) state [1,2] to that of MRJ-line, we show [3] that it is reasonable to assume the most random branch of jammed states to undergo crowding in a way qualitatively similar to an equilibrium liquid. We then prove that,

for hard-sphere systems, liquid-state theories can be succesfully used to estimate the RCP density, when the latter is identified with the densest isostatic point, i. e. the densest among the MRJ states with z=6.

Our finding is further enforced by the analysis of polydisperse systems. Either in the case of bidisperse and polydisperse hard spheres our prediction of the RCP density is in very good agreement with simulations, for a large values of size ratios and polydispersity.

[1] S. Toquato, T. M. Truskett, and P. G. Debenedetti, Phys. Rev. Lett. 84, 2064 (2000). [2] S. Torquato and F. H. Stillinger, Reviews of Modern Physics 82, 2633 (2010). [3] C. Anzivino, M. Casiulis, T. Zhang, A. S. Moussa, S. Martiniani and A. Zaccone, "Estimating RCP as the densest isostatic packing in bidisperse and polydisperse hard spheres", manuscript submitted (2022).

DY 16.3 Tue 10:30 MOL 213

2D crystals of squares and the tetraic phase — •Peter Keim — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen

Squares (5 micron edge-length) were manufactured from a photo-resist using a 3D nanoprinter (nanoscribe GT). In aqueous solution, particles sediment by gravity to a thin cover slide where they form a mono-layer of Brownian particles. The curvature of the cover slide can be adjusted from convex to concave, which allows to vary the area-density of the mono-layer from 700 to 1500 particles in the field of view. For low densities, the squares are free to diffuse and form a 2D fluid while for high densities they form a quadratic crystal. In analogy to 2D-melting by topological defects with an intermediate hexatic phase for isotropic particles (KTHNY-theory and Nobel-price 2016), a four-folded bond-order correlation function is used to resolve a tetratic phase with quasi-long-range orientational order but short rang translational order.

DY 16.4 Tue 10:45 MOL 213

Transient microrheology unveils the presence of two relaxation processes in viscoelastic fluids — •Félix Ginot[1], Juliana Caspers[2], Luis Frieder Reinalter[1], Karthika Krishna Kumar[1], Matthias Krüger[2], and Clemens Bechinger[1] — [1]Fachbereich Physiks Universität Konstanz, 78457 Konstanz, Germany — [2]Institute for Theoretical Physics, Georg-August Universität Göttingen, 37073 Göttingen, Germany

We experimentally investigate the transient dynamics of a colloidal probe particle in a viscoelastic fluid after the driving force acting on the probe is suddenly removed. In this situation, the probe exhibits a strong backward recoil, with two distinct timescales. While the first timescale naturally originates from the viscoelastic properties of the fluid, the second timescale arises from the coupling between the probe and the bath. These experimental observations are in excellent agreement with a microscopic model which considers the probe particle to be coupled to two bath particles via harmonic springs. Interestingly, this model exhibits two sets of eigenmodes corresponding to reciprocal and non-reciprocal force conditions, and which can be experimentally confirmed in our experiments. We expect our findings to be relevant under conditions where particles are exposed to non-steady shear forces as this is encountered e.g. in microfluidic sorting devices or the intermittent motion of motile bacteria within their natural viscoelastic surroundings.

15 min. break

DY 16.5 Tue 11:15 MOL 213

Phason strain-free growth of quasicrystals based on purely local rules and without repair mechanism — Stefan Wolf[1], Michael Engel[2], and •Michael Schmiedeberg[1] — [1]Institute of Theoretical Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

We introduce a simple model for the growth of colloidal quasicrystals where new particles are sequentially added according to specific local rules to the system in three dimensions. Subsequent changes to the particles are not allowed, i.e., no phasonic rearrangements can occur once a particle has been placed into the system. Our findings demonstrate that the purely local energetic rules are sufficient to obtain complex long-ranged order. Thus, phasonic rearrangements or fluctuations might be important to facilitate the formation of almost perfect quasicrystals [1-3] but they are not indispensable.

[1] C.V. Achim, M. Schmiedeberg, and H. Löwen, Phys. Rev. Lett. 112, 255501 (2014).

[2] A. Gemeinhardt, M. Martinsons, and M. Schmiedeberg, Eur. Phys. J. E 41, 126 (2018).

[3] K. Nagao, T. Inuzuka, K. Nishimoto, and K. Edagawa, Phys. Rev. Lett. 115, 075501 (2015).

DY 16.6 Tue 11:30 MOL 213

Magnus force on microscopic spinning objects moving through non-Markovian baths — Xin Cao[1], •Debankur Das[2], Niklas Windbacher[1], Felix Ginot[1], Matthias Kruger[2], and Clemens Bechinger[1] — [1]Fachbereich Physik, University Konstanz, 78464 Konstanz, Germany — [2]Institut für Theoretische Physik, Universität Göttingen, 37077 Göttingen Germany

When a spinning object moves through a fluid or air, its direction of motion becomes deflected due to the Magnus force that is perpendicular both to the moving direction and the spinning axis. Since the Magnus effect is caused by inertial effects within the surrounding medium, it should vanish at micro scales where viscous forces dominate over inertia. Recent experiments have observed the phenomenon similar to Magnus effect when a spinning colloids and there aggregates are externally driven through a viscoelastic fluid. Even though the deflection force shows a similar dependence on the spinning and translating velocity of the particles as in case of Magnus forces, its sign is reversed. Here, we have developed a theory of such motions which doesnot rely on the inertial effects but caused explicitly by the memory effect of the viscoelastic fluid. To better elucidate our theory we corroborate our results with experiments. Our theory successfully captures the density relaxation timescales of the viscoelastic fluid. Further we proposed viable theoretical predictions which can be verified with further experiments.

DY 16.7 Tue 11:45 MOL 213

Preferential alignment of colloidal dumbbells with recoil direction — •Karthika Krishna Kumar[1], Félix Ginot[1], Juliana Caspers[2], Matthias Krüger[2], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, Germany — [2]Institute for Theoretical Physics, Georg-August Universität Göttingen, Germany

Unlike Newtonian fluids, viscoelastic fluids can store and dissipate energy on much longer timescales leading to non-Markovian dynamics. Hence, probing viscoelastic fluids using colloidal particles reveal complex dynamics in microscopic lengthscales. A consequence of this is the recoil behavior of a colloidal particle after dragging it through a viscoelastic fluid. In this work, we use a pair of colloidal particles stuck together due to depletion interactions forming a dumbbell-shaped structure. This gives the advantage of resolving the orientational component in addition to the translational components of the particle motion. Surprisingly, we report that the axis of the dumbbell tends to align with the direction of the motion during a recoil. The amplitude of this orientational component follows a non-linear trend even in the regime where translational recoil amplitudes show a linear increase with shear velocity. This behavior can no longer be explained by the linear two-bath particle model which is able to explain the bi-exponential translational recoils. Furthermore, the amplitude of this re-orientation increases with the initial angle at which the dumbbell is dragged. This points to an asymmetric distribution of elastic energy between the two particles of the dumbbell which might cause this effect.

DY 16.8 Tue 12:00 MOL 213

Entropic phase diagram of twisted convex particles — •Poshika Gandhi and Anja Kuhnhold — Institute of Physics, University of Freiburg, Germany

The field of liquid crystal simulations has, over the years, benefitted immensely from the study of purely entropy driven systems. Since Onsager's[1] predictions of the existence of a nematic phase in long rods, the list of known phases of hard rod-like particles has grown to include phases like smectics and cholesterics.

An important parameter in the formation of these phases is the particle shape anisotropy. By considering unusual particle shapes new phases can be discovered. Recently, Dussi and Dijkstra[2] showed the formation of stable chiral nematic phase in twisted polyhedral particles using only entropic interactions.

We used Monte Carlo NVT simulations to produce phase diagrams of a different class of twisted particles - convex triangular and rectangular prisms. The results show a host of previously undiscovered phases arising from the shape anisotropy parameters like twist angle and aspect ratios.

[1] Onsager, L., Ann. N. Y. Acad. Sci., 51, 627 (1949).
[2] Dussi, S., Dijkstra, M., Nat Commun. 7, 11175 (2016).

DY 16.9 Tue 12:15 MOL 213

Optimizing the Structure of Acene Clusters — •Philipp Elsässer and Tanja Schilling — Institute of Physics, University of Freiburg, Germany

In the production of organic solar cells, neutral acene cluster beams are used to create thin films. The molecules in these clusters can be arranged in various ways. Most types of acene molecules are quasi two dimensional with one long axis - they prefer stacked or herring-bone structures. Additionally, the positions of the molecules in a cluster may vary. Thus, the exact way of how they arrange has a strong influence on the overall energy of the cluster.

We have investigated the structures of anthracene, tetracene, and pentacene clusters with up to 30 molecules. In order to find the configurations at the global minimum of the potential energy surface with respect to the positions of the atoms, we applied the Basin-Hopping Monte-Carlo (BH) algorithm to atoms described by the polymer-consistent force field - interface force field (PCFF-IFF). We studied for these cluster structures the relative stability between different sizes of clusters, as well as the accessibility of the global minimum at different temperatures.

DY 16.10 Tue 12:30 MOL 213

Ergodicity breaking in overpacked colloidal hard spheres — •Hans Joachim Schöpe — Universität Tübingen, Institut für angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

The ergodic hypothesis is an essential prerequisite for the applicability of statistical mechanics in thermodynamic equilibrium. Direct experimental evidence of the validity of the ergodic hypothesis is extremely rare. Furthermore, the question arises to what extent - if at all - ergodicity exists in non-equilibrium. We have realized a novel dynamic light scattering experiment, which makes it possible to determine the probability distribution of relaxation-times in colloidal suspensions. We present here a systematic study of the relaxation-time distribution in colloidal hard spheres at the transition from equilibrium to non-equilibrium. In thermodynamic equilibrium, we can impressively confirm the ergodic hypothesis and show that the fluctuations are of a Gaussian nature. Out of equilibrium, we can detect non-Gaussian behavior, which increases rapidly with increasing undercooling (overpacking). The ergodic hypothesis is no longer fulfilled in non-equilibrium. Furthermore, we observe that the metastable fluid ages in the induction stage, the non-Gaussian fluctuations increase in the time before crystallization sets in. To what extent these fluctuations cause crystallization must be clarified in the future.

DY 16.11 Tue 12:45 MOL 213

Coacervates from a polyelectrolye and a small polyion: preparation, phase behavior and theoretical modeling — Lucy Coria-Oriundo[1], Eugenia Apuzzo[2], Santiago Herrera[1], Marcelo Ceolín[2], Gabriel Debais[1], Fernando Battaglini[1], and •Mario Tagliazucchi[1] — [1]Universidad de Buenos Aires, Bs.As., Argentina — [2]Universidad Nacional de la Plata, Bs.As., Argentina.

A mixture of oppositely charged polyelectrolytes, under the proper experimental conditions, can undergo liquid-liquid phase separation. The resulting polymer-rich phase is usually known as polyelectrolyte coacervate. This work reports liquid coacervates composed of a small polyanion (ferricyanide) and branched poly(ethyleneimine) (BPEI), a polycation. The phase diagram of the system was measured as a function of the concentration of both components at fixed pH = 6 and a concentration of added NaCl of 0.5 M. The salt resistance of the coacervate was studied and it was found that the coacervate is stable up to [NaCl] = 1.35 M. The phase diagram and salt-resistance experiments were modeled with a statistical-thermodynamics formalism that models the association of the oppositely charged species as a pseudo-chemical-equilibrium. The model fits very well the experimental data and was used to analyze the differences between polymer-polymer and polymer-small ion coacervates. Finally, the diffusion coefficient of ferricyanide within the coacervated (measured with cyclic voltammetry) was shown to increase 10 times when the concentration of added NaCl was increased from 0 to 1.2 M.

DY 17: Machine Learning in Dynamics and Statistical Physics I

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

DY 17.1 Tue 10:00 ZEU 160

On-the-fly adaptive sparse grids for coupling high-fidelity and coarse-grained models — •Tobias Hülser, Sina Dortaj, and Sebastian Matera — Fritz-Haber-Institut der MPG, Berlin, Germany

Most simulations of continuum models require the repetitive evaluation of some non-linear functions. If the latter are only given by the outcome of some high-fidelity simulation, these evaluations can easily become the computational bottleneck of the coupled simulation. To overcome this limitation, computationally efficient machine-learning models have become popular as surrogates of the high-fidelity model in the continuum scale simulation. However, if the input dimension of these models is high, the training of the surrogate often requires infeasible numbers of simulations, the so-called curse of dimensionality. We present an on-the-fly adaptive sparse grids approach, which lifts these limitations. This exploits that, on the one hand, sparse grids are only mildly affected by the curse of dimensionality and allow for an adaptive, local error based training set design. On the other hand, we utilize that, during a continuum simulation, only a small low-dimensional subset of the high-dimensional input space of the high-fidelity model is visited. We therefore construct the surrogate on the fly during the continuum simulation, only generating the high-fidelity data which is needed to interpolate this subset.

We demonstrate the approach on exemplary physical-chemical models from the field of heterogeneous catalysis. We find that our approach can significantly reduce the number of high-fidelity evaluations compared to the direct coupling.

DY 17.2 Tue 10:15 ZEU 160

Reservoir Computing using Active Matter Model Systems: A Physics Viewpoint — •Mario U. Gaimann and Miriam Klopotek — Stuttgart Center for Simulation Science (SimTech), Cluster of Excellence EXC 2075, University of Stuttgart, Germany

Spatio-temporal prediction of chaotic systems is a challenging problem that is relevant for many fields (weather, finance, energy, and other dynamic systems). Recurrent neural networks and specifically neuron-based reservoir computing were previously used to approach this problem [1,2]. However, these learning systems are typically treated as black boxes, and do not incorporate reasoning or analysis in terms of physical laws and dynamics. Here we study the non-equilibrium dynamics of simple active matter models serving as reservoir computing substrates [3]. This allows us to determine and interpret the state of our reservoir and relate the learning problem to other generic phenomena in statistical physics. With this knowledge we aim to understand optimal conditions for learning in relation to critical states and physical constraints.

[1] Tanaka, G. *et al.* (2019), *Neural Networks* **115**, 100-123.
[2] Nakajima, K. and Fischer, I. (2021). *Reservoir Computing.* Springer Singapore.
[3] Lymburn, T. *et al.* (2021), *Chaos* **31(3)**, 033121.

DY 17.3 Tue 10:30 ZEU 160

Machine Learning Percolation: Does it understand the physics? — •Djénabou Bayo[1,2], Andreas Honecker[2], and Rudolf A. Römer[1] — [1]Departement of Physics, University of Warwick, Coventry, CV47AL, United Kingdom — [2]Laboratoire de Physique Théorique et Modélisation (LPTM) (CNRS UMR8089), CY Cergy Paris Université, 95302 Cergy-Pontoise, France

The percolation model is one of the simplest models in statistical physics displaying a phase transition at a critical site occupation probability p_c. The hallmark of the percolation transition is the emergence of a spanning cluster of connected neighboring sites across the lattice. Machine learning (ML) approaches to percolation have shown that the non-spanning ($p < p_c$) and the spanning ($p > p_c$) phases can be identified reasonably well with supervised deep learning (DL) strategies for classification based on convolutional neural networks (CNNs). Surprisingly, the role of the spanning cluster seems to be less prominent in such DL methods. Here, we show that CNNs, when trained with the

site occupation probabilities p as labels, can classify not only the two phases $p < p_c$ and $p > p_c$, but also according to the many individual p's. Nevertheless, the same CNNs struggle when trying to predict the emergence of the spanning cluster. Indeed, when we train with correlation lengths or the existence of the spanning cluster, the results suggest that the CNNs seem to rely mostly on the p's as a proxy measure. This suggests that the essential physics of the spanning cluster is not actually what determines the DL results.

DY 17.4 Tue 10:45 ZEU 160

Bayesian deep learning for error estimation in the analysis of anomalous diffusion — •Henrik Seckler[1] and Ralf Metzler[1,2] — [1]Institute for Physics & Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany. — [2]Asia Pacific Centre for Theoretical Physics, Pohang 37673, Republic of Korea

Modern single-particle-tracking techniques produce extensive time-series of diffusive motion in a wide variety of systems, from single-molecule motion in living-cells to movement ecology. The quest is to decipher the physical mechanisms encoded in the data and thus to better understand the probed systems. We here augment recently proposed machine-learning techniques for decoding anomalous-diffusion data to include an uncertainty estimate in addition to the predicted output. To avoid the Black-Box-Problem a Bayesian-Deep-Learning technique named Stochastic-Weight-Averaging-Gaussian is used to train models for both the classification of the diffusion model and the regression of the anomalous diffusion exponent of single-particle-trajectories. Evaluating their performance, we find that these models can achieve a well-calibrated error estimate while maintaining high prediction accuracies. In the analysis of the output uncertainty predictions we relate these to properties of the underlying diffusion models, thus providing insights into the learning process of the machine and the relevance of the output.

DY 17.5 Tue 11:00 ZEU 160

A machine learned classical density functional for orientational correlations in the Kern-Frenkel model for patchy particles — •Alessandro Simon[1,2] and Martin Oettel[1] — [1]Institute for Applied Physics, University of Tübingen, Germany — [2]Max Planck Institute for Intelligent Systems, Tübingen, Germany

Models of patchy particles in a generic form (hard spheres decorated with a fixed number of attraction sites), posses an interesting phase behaviour, despite their apparent simplicity. This includes gel-formation and a vanishing fluid density at the gas-liquid coexistance, as the number of attractive patches and temperature is decreased. Using simulations of a symmetric four-patch model, we examine the orientational order of the particles and the effects of their tetrahedral symmetry on the expansion of density profiles and pair correlations in rotational invariants. Building on an existing classical density functional model which is formulated on the basis of Wertheim's theory for associating liquids and does not resolve orientational correlations [Stopper et al. J. Chem. Phys. 149, 224503 (2018)], we construct an improved density functional using machine learning and show that it yields the correct orientation distribution in slit-like geometries.

15 min. break

DY 17.6 Tue 11:30 ZEU 160

Classification of Gel Networks using Graph Convolutional Neural Networks — •Matthias Gimperlein and Michael Schmiedeberg — FAU Erlangen-Nürnberg, Erlangen, Germany

The structural properties of gel networks are important for the mechanical properties of the corresponding gels. We analyze gel networks and their structure using a machine learning approach based on graph convolutional networks (GCN) employing only the local neighborhood of particles as input information.

Using these we define a GCN-Autoencoder to reconstruct adjacency matrices of networks and quantitatively analyze in which properties the prediction of the network differs from the original input. This includes analysis on the abstract graph level as well as on the real physical network level.

Furthermore we use GCNs to classify gel networks depending i.e. on the loopsizes which are present in the network. Our goals include getting robust classification of strongly or weakly connected gel networks, predictions of minimal connecting structures and an insight how - according to an artificial intelligence - gel networks look like.

DY 17.7 Tue 11:45 ZEU 160

A 3-layer injection-locked multimode semiconductor laser neural network — •Elizabeth Robertson[1,3], Romain Lance[2], Anas Skalli[2], Xavier Porte[2], Janik Wolters[1,3], and Daniel Brunner[2] — [1]Deutsches Zentrum für Luft-und Raumfahrt, 12489 Berlin, Germany — [2]Institut FEMTO-ST, Université Bourgogne Franche-Comté, CNRS UMR6174, Besançon, France — [3]Technische Universität Berlin, Institut für Optik und Atomare Physik, 10623 Berlin, Germany

Optical hardware implementations of artificial neural networks (ANNs) have become a hot topic of research due to the inherent parallelism, potentially high speed and energy efficiency of optics [1]. Semiconductor laser networks are of specific interest as they are highly non-linear systems, which can be modulated at high throughput [2]. Previous work using spatial modes as nodes of an ANN, illustrated the use of multimode large area VSCELs for neural network computing in a fully parallel substrate, without pre- or post-processing [3,4]. We further expand this concept to a three-layer network consisting of mutually coupled multimode VSCELs, injection locked to a DFB laser. Here, information is fed into the network by modulating the injection laser, and boolean output weights are implemented using a digital micromirror device. We present an outline of the system, investigate its locking behavior and non-linear response. [1] Huang C. et al., Advances in Physics: X 7, 1 (2022) [2] Skalli A. et al., Opt. Mater. Express 12, 2395-2414 (2022) [3] Porte X. et al., J. Phys. Photonics 3 024017 (2021) [4] Skalli A. et al., Opt. Mater. Express 12, 2793-2804 (2022)

DY 17.8 Tue 12:00 ZEU 160

Efficiently compressed time series approximations — •Paul Wilhelm[1] and Marc Timme[1,2] — [1]Chair for Network Dynamics, Institute of Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), TU Dresden, Germany — [2]Lakeside Labs, Klagenfurt, Austria

Time series emerge from a broad range of applications, for instance as stock market pricing, electrocardiographic recordings or trajectories in chaotic dynamical systems. Long time series require an approximation scheme for compressing and storing, analyzing or predicting them.

How can we construct efficient approximations? Continuous, piecewise linear functions with variable knots that mark the end points of each segment are easy to handle and often used. However, fitting the knots is highly nonlinear and only feasible with a lucky initial guess. Here we propose a novel method that exploits repeating motifs in the data and thereby avoids fitting each knot independently, significantly accelerating the construction of the approximation.

Starting from the beginning of a time series, the method iteratively integrates subsequent data points. For each extension, it tries to reuse parts of the already existing function to approximate the yet uncovered data points. If successful, each motif is approximated only once and reused multiple times. As a result, the knots of the function are interdependent and can thus be represented in compact form. In contrast to deep neural networks that also find a piecewise linear approximation, our approach offers a efficient and explainable method and thereby a novel perspective onto why and how deep neural networks may work.

DY 17.9 Tue 12:15 ZEU 160

Active Learning Strategies for Molecular Dynamics with Machine-learned Potentials — •Shubham Sharma[1] and Mariana Rossi[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Machine-learning potentials (MLPs) have allowed the efficient modelling of complex atomistic systems with ab-initio accuracy. Normally, the construction of sufficiently large and diverse reference datasets, using first-principles calculations, is a bottleneck for training. Therefore, several active-learning strategies have been proposed, which aim to make the training more efficient, especially when used together with molecular-dynamics techniques [1]. In this work, we explore building protocols for training sets of high-dimensional neural-network potentials (HDNNPs), targeting specifically weakly-bound condensed-phase systems. For that, we show how we can use and augment the committee-model framework within the i-PI code [2]. We show results for acene-based molecular crystals and discuss the advantages and limitations of different learning strategies to treat different crystal polymorphs, at various thermodynamic conditions. [1] C. Schran et. at., J. Chem. Phys. **153**, 104105 (2020). [2] V. Kapil et. al., Comput. Phys. Commun. **236**, 214 (2019).

DY 17.10 Tue 12:30 ZEU 160

Machine learning-based prediction of dynamical clustering in excited granular media — •Sai Preetham Sata, Dmitry Puzyrev, and Ralf Stannarius — Institute of Physics and MARS, Otto von Guericke University Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany

Granular gases excited by external force tend to undergo gas-like to cluster transitions when the filling fraction of particles reaches sufficient value. In order to understand the clustering dynamics, experiments were performed in microgravity [1,2]. A numerical simulation model based on DEM is available. By varying geometrical and material parameters, a phase diagram is obtained. Cumulative distribution functions of the density profiles and uniform distribution profiles are obtained and the maximum distance between these curves is compared to the Kolmogorov-Smirnov (KS) test threshold to detect gas-cluster transitions. We aim to predict the formation of dynamical clusters with the use of machine learning techniques as an alternative to DEM simulations, requiring much less computational effort. We confirm the reliability of the predictions for relatively well-studied spherical beads, with the perspective of analysis of clustering of more complicated particle shapes.

This study is supported by DLR projects VICKI and EVA (50WM2252 and 50WM2048)

References: [1] S. Aumaître, et al. Review of Scientific Instruments 89, 075103 (2018) [2] M. Noirhomme et al. EPL 123, 14003 (2018) [3] Puzyrev, D., Fischer, D., Harth, K. et al., Sci Rep 11, 10621 (2021).

DY 18: Nonlinear Dynamics, Synchronization and Chaos

Time: Tuesday 10:00–12:15 Location: ZEU 147

DY 18.1 Tue 10:00 ZEU 147

Synchrony at Weak Coupling in the Complexified Kuramoto Model — •Moritz Thümler[1], Shesha G.M. Sriniva[2], Malte Schröder[1], and Marc Timme[1,3] — [1]Chair for Network Dynamics, Institute of Theoretical Physics & Center for Advancing Electronics Dresden (cfaed), TU Dresden — [2]Institute of Physics and Material Sciences, Universite du Luxembourg — [3]Lakeside Labs, Klagenfurt, Austria

We present the finite-size Kuramoto model analytically continued from real to complex variables and analyze its collective dynamics. For strong coupling, synchrony appears through locked states that constitute attractors, as for the real-variable system. However, synchrony persists in the form of *complex locked states* for coupling strengths K below the transition $K^{(\mathrm{pl})}$ to classical *phase locking*. Where complex locked states are stable, their imaginary parts indicate which units belong to the locked population in the original, real-variable system. We uncover a second transition at $K' < K^{(\mathrm{pl})}$ below which complex locked states become linearly unstable yet still exist for arbitrarily small coupling strengths. The results open up a path towards a new field of network dynamics with variables complexified by analytic continuation.

DY 18.2 Tue 10:15 ZEU 147

Predicting tipping points in driven nonlinear systems — •Gwendolyn Quasebarth[1], Moritz Thümler[1], and Marc Timme[1,2] — [1]Chair for Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), Technical University of Dresden, Dresden, Germany — [2]Lakeside Labs, Lakeside B04b, Klagenfurt, Austria

Tipping points mark parameter values beyond which a system qualitatively changes its collective dynamics, often in undesired ways. Standard response theory for nonequilibrium nonlinear systems predicts local deviations around a stable fixed point via a polynomial in the amplitude ϵ of the driving signal. However, such standard response theories (of arbitrary order in ϵ) necessarily fail to predict nonequilibrium tipping points. Here, we propose a novel nonlinear response theory that overcomes the constraints of polynomial response theory of any order. We illustrate our findings in a class of sinusoidally driven damped nonlinear oscillators.

DY 18.3 Tue 10:30 ZEU 147

Pseudo-laminar chaos from on-off intermittency — •David Müller-Bender[1], Rahil N. Valani[2], and Günter Radons[1,3] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]School of Mathematical Sciences, University of Adelaide, Adelaide, South Australia 5005, Australia — [3]ICM - Institute for Mechanical and Industrial Engineering, 09117 Chemnitz, Germany

In finite-dimensional, chaotic, Lorenz-like wave-particle dynamical systems one can find diffusive trajectories, which share their appearance with that of laminar chaotic diffusion [Phys. Rev. Lett. 128, 074101 (2022)] known from delay systems with lag-time modulation. Applying, however, to such systems a test for laminar chaos, as proposed in [Phys. Rev. E 101, 032213 (2020)], these signals fail such test, thus leading to the notion of pseudo-laminar chaos. The latter can be interpreted as integrated periodically driven on-off intermittency. We demonstrate that, on a signal level, true laminar and pseudo-laminar chaos are hardly distinguishable in systems with and without dynamical noise. However, very pronounced differences become apparent when correlations of signals and increments are considered. We compare and contrast these properties of pseudo-laminar chaos with true laminar chaos.

Details can be found in the preprint [arXiv:2211.01278 (2022)].

DY 18.4 Tue 10:45 ZEU 147

Power-flow-based circuit synthesis of neuronal dynamics — •Karlheinz Ochs[1], Sebastian Jenderny[1], and Philipp Hövel[2] — [1]Ruhr-Universität Bochum, Germany — [2]Christians-Albrechts-Universität zu Kiel, Germany

We present a modeling framework to study neuronal dynamics based on power-flow considerations. This is inspired by a circuit synthesis and analog electronics. Exemplified by the Hindmarsh-Rose model, we demonstrate that the proposed framework reproduces key characteristics of the dynamical model, including spiking and bursting behavior. This approach is a stepping stone towards the emulation of neuronal behavior on larger networks by means of analog circuits.

15 min. break

DY 18.5 Tue 11:15 ZEU 147

On the Correlation of Functionality and Lyapunov Stability in Oscillator-based Ising machines — •Bakr Al Beattie[1], Maximiliane Noll[2], Hermann Kohlstedt[2], and Karlheinz Ochs[1] — [1]Ruhr-Universität Bochum, Lehrstuhl für digitale Kommunikationssysteme, Bochum, Deutschland — [2]Christian-Albrechts-Universität zu Kiel, Lehrstuhl für Nanoelektronik, Kiel, Deutschland

Oscillator-based Ising machines are a promising analog approach for dealing with combinatorial optimization problems that are classified as NP (nondeterministic polynomial). The idea is to mimic the Ising model by coupling electrical oscillators that behave like the spins of the Ising model. Here, the coupling should somehow map the Ising Hamiltonian onto the energy of electrical system. With this contribution, we demonstrate numerical evidence demonstrating the correlation between the Ising machine*s functionality and stability. We make use of the well-known Kuramoto model to describe a coupled oscillator network and show stability to be the key property that makes an Ising machine solve optimization problems. Furthermore, we give an answer to the question: when has an Ising machine finished solving a mapped problem?

DY 18.6 Tue 11:30 ZEU 147

Manifolds of equilibrium states in ensembles of globally coupled oscillators — •Michael Zaks — Humboldt Universität zu Berlin, Berlin, Germany

Global fields generated by ensembles of coupled oscillators are responsible for many unusual kinds of collective behavior. Among their most striking effects are existence of numerous constants of motion and a drastic reduction in the number of degrees of freedom. Here, we offer a simpler approach, restricted to the widespread situations in which the number of parameters defining the action of the global fields is smaller than the overall number of elements in the ensemble. In the phase space of such ensembles, high-dimensional manifolds composed of the equilibrium states can generically arise. Existence of these manifolds

is not related to symmetries. In the simplest cases, such continua of steady states are attracting or repelling as a whole; in general, however, their stability with respect to transversal perturbations varies in the course of the motion along the manifold. Remarkably, the suggested mechanism does not require that all oscillators are identical: the sufficiently strong global field is able to counteract diversity among the ensemble units and halt the temporal evolution.

DY 18.7 Tue 11:45 ZEU 147

X-ray imaging of the sonoluminescent cavitation bubble collapse with single XFEL pulses — •Hannes Paul Hoeppe[1], Atiyeh Aghelmaleki[2], Juan Manuel Rosselló[3], Malte Vassholz[1], Markus Osterhoff[1], Daniel Schwarz[4], Johannes Hagemann[4], Robert Mettin[2], Anders Madsen[5], and Tim Salditt[1] — [1]Institute for X-ray Physics, Georg-August-University, Göttingen, Germany — [2]Third Institute of Physics, Georg-August-University, Göttingen, Germany — [3]Faculty of Mechanical Engineering, University of Ljubljana, Ljubljana, Slovenia — [4]Center for X-ray and Nano Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [5]European X-Ray Free-Electron Laser Facility, Schenefeld, Germany

We study the dynamics and in particular the collapse of a single cavitation bubble in water. A cavitation bubble is trapped and driven by an ultrasonic field leading to nonlinear radial oscillations. During its periodic collapses, extreme pressure and temperature is reached which can lead to the formation of a plasma core and the emission of light. The fast evolving pressure, density and temperature distribution and the shape of the bubble during its collapse has so far only been accessible by simulations. Full-field X-ray phase contrast imaging provides quantitative information of the density distribution of the sample. Implemented at X-ray free-electron lasers, this enables the investigation of fast processes and extreme states of matter with a unique contrast. We present the evolution of the bubble's density profile during the sonoluminescent collapse and the current state of analysis.

DY 18.8 Tue 12:00 ZEU 147

Quantum synchronization in a network of dissipatively coupled linear oscillators — •Juan Moreno[1], Christopher W Wächtler[2], and Alexander Eisfeld[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Department of Physics,University of California Berkeley, CA, 94720-7300

Synchronization in classical systems has a long history and by now is a very well understood phenomenon. However, the question whether the classical notions of synchronization can be extended to the quantum regime has only recently been addressed in investigations of classically inspired models like quantum Van der Pol oscillators as well as models without classical analog. Inspired by the theoretical prediction that two-level atoms are able to synchronize even without interacting directly [1], we investigate a network of dissipatively coupled quantum harmonic oscillators. Within a mean-field approximation we find that the network is able to synchronize. For the fully quantum system described in terms of a Lindblad master equation we analyze various measures that have been proposed in the literature. Additionally, we investigate the Liouvillian spectrum in order to draw connections between the spectrum and the synchronization measures.

[1] PRA 101, 042121 (2020)

DY 19: Physics of Contagion Processes II (joint session SOE/DY)

Time: Tuesday 10:00–10:45 Location: ZEU 260

DY 19.1 Tue 10:00 ZEU 260

Explosive Epidemics — •Georg Börner[1], Malte Schröder[1], Davide Scarselli[2], Nazmi Burak Budanur[2,3], Björn Hof[2], and Marc Timme[1,4,5] — [1]Chair for Network Dynamics, Center for Advancing Electronics Dresden (cfaed) and Institute of Theoretical Physics, Technische Universität Dresden, Dresden 01062, Germany — [2]Institute of Science and Technology Austria, Klosterneuburg, Austria — [3]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [4]Cluster of Excellence Physics of Life, Technische Universität Dresden, Dresden 01062 Germany — [5]Lakeside Labs, Lakeside B04b, 9020 Klagenfurt, Austria

Standard epidemic models exhibit one continuous, second order phase transition to macroscopic outbreaks. However, interventions to control outbreaks may fundamentally alter epidemic dynamics. We reveal how such interventions modify the type of phase transition. In particular, we uncover three distinct types of explosive phase transitions for epidemic dynamics with capacity-limited interventions. Depending on the capacity limit, interventions may (i) leave the standard second-order phase transition unchanged but exponentially suppress the probability of large outbreaks, (ii) induce a first-order discontinuous transition to macroscopic outbreaks, or (iii) cause a secondary explosive yet continuous third-order transition. These insights highlight inherent limitations in predicting and containing epidemic outbreaks. More generally our study offers a cornerstone example of a third-order explosive phase transition in complex systems.

DY 19.2 Tue 10:15 ZEU 260

Large-deviations of the SIR model under the influence of Lockdowns — Leo Patrick Mulholland[1], •Yannick Feld[2], and Alexander K. Hartmann[2] — [1]Queen's University Belfast, United Kingdom — [2]Institute of Physics, Carl von Ossietzky University, Oldenburg, Germany

Due to the high real-wold impact of diseases, the modelling of its dynamics has long since become an important aspect of various disciplines. Statistical physics is one of them as it gives us the tools investigate the fundamental processes through which a disease spreads throughout a population.

The transmission of a disease is affected by a lot of different factors. For example in response to the SARS-CoV 2 pandemic many governmental bodies imposed interventions to impede the spread of disease. One of the earliest non-pharmaceutical interventions (NPIs) that most countries used were lockdowns.

Motivated by that, we numerically [1] study the dynamics of the susceptible-infected-recovered (SIR) model with lockdowns on small-world networks by using a large-deviation approach, which was previously used to study the case of an unimpeded spread [2]. This allows us to obtain the probability density function of the cumulative fraction of infected nodes down to very small probabilities like 10^{-55}. The density exhibits remarkable discontinuties of the first derivative.

[1] A.K. Hartmann, *Big Practical Guide to Computer Simulations* (World Scientific, 2015)
[2] Y. Feld, A. K. Hartmann, Phys. Rev. E **105** 17 (2022)

DY 19.3 Tue 10:30 ZEU 260

Short messages spread wider in online social networks — Patryk A. Bojarski, •Krzysztof Suchecki, and Janusz A. Holyst — Faculty of Physics, Warsaw University of Technology, Warsaw, 00-662 Poland

We explore the behavior of an online message spreading model, that includes mutable message content, user opinions and limited processing capacities. The model shows robust power-law distribution of the number of shares for different messages and that the tail of the distribution is composed almost entirely of very short messages. The possibility to modify message content by spreaders makes already popular, short messages even more popular if the users are selective about what content they spread, but not too much. The distribution of message variants is also a power-law, in agreement with real message spreading in Facebook. The behavior of the model is robust against model parameters and network topology variations and offers an explanation as to why services focused on short messages, such as Twitter, are popular.

DY 20: Networks: From Topology to Dynamics I (joint session SOE/DY)

Time: Tuesday 11:00–12:15 Location: ZEU 260

DY 20.1 Tue 11:00 ZEU 260

Modelling the perception of music in brain network dynamics — •Jakub Sawicki[1,2,3,4], Lenz Hartmann[5], Rolf Bader[5], and Eckehard Schöll[1,4,6] — [1]Potsdam Institute for Climate Impact Research — [2]Institut für Musikpädagogik, Universität der Künste Berlin — [3]Fachhochschule Nordwestschweiz FHNW, Basel, Switzerland — [4]Institut für Theoretische Physik, TU Berlin — [5]Institute of Systematic Musicology, University of Hamburg — [6]Bernstein Center for Computational Neuroscience Berlin

We analyze the influence of music in a network of FitzHugh-Nagumo oscillators with empirical structural connectivity measured in healthy human subjects [1]. We report an increase of coherence between the global dynamics in our network and the input signal induced by a specific music song. We show that the level of coherence depends crucially on the frequency band. We compare our results with experimental data, which also describe global neural synchronization between different brain regions in the gamma-band range and its increase just before transitions between different parts of the musical form (musical high-level events). The results also suggest a separation in musical form-related brain synchronization between high brain frequencies, associated with neocortical activity, and low frequencies in the range of dance movements, associated with interactivity between cortical and subcortical regions. [1] Sawicki, J., Hartmann, L., Bader, R., Schöll, E., Front. Netw. Physiol. 2, 910920 (2022).

DY 20.2 Tue 11:15 ZEU 260

Order-disorder transition in the zero-temperature Ising model on random graphs — Armin Pournaki[1,2], Eckehard Olbrich[2], Sven Banisch[3], and •Konstantin Klemm[4] — [1]Laboratoire Lattice, CNRS & ENS-PSL, Paris — [2]Max Planck Institute for Mathematics in the Sciences, Leipzig — [3]Karlsruhe Institute for Technology — [4]IFISC (UIB-CSIC), Palma de Mallorca, Spain

The zero-temperature Ising model is known to reach a fully ordered ground state in sufficiently dense graphs. In sparse random graphs, the dynamics gets absorbed in disordered local minima at magnetization close to zero. Here we find that the non-equilibrium transition between the ordered and the disordered regime occurs at an average degree that slowly grows with the system size. The system shows bistability: the distribution of the absolute magnetization in the absorbing state reached is bimodal with peaks only at zero and unity. For fixed system size, the average time to absorption behaves non-monotonically as a function of average degree. The peak value of the average absorption time grows as a power law of system size. These findings have relevance for community detection, opinion dynamics and games on networks. Full manuscript available at https://arxiv.org/abs/2209.09325

DY 20.3 Tue 11:30 ZEU 260

Analytical methods to stochastic binary-state dynamics on networks. — •Antonio Fernandez Peralta[1] and Raul Toral[2] — [1]Central European University, Vienna, Austria — [2]IFISC (Instituto de Física Interdisciplinar y Sistemas Complejos), Palma de Mallorca, Spain

Recently, there has been a lot of effort in the development of highly accurate mathematical descriptions of the dynamics of binary-state models defined on complex networks. There are two main approaches: (i) individual based-approaches where the variables are the state of each node, and (ii) compartmental approaches where nodes are aggregated based on some topological property such as, for example, the number of neighbors in the network. Except in a few cases where stochastic effects are taken into account at some extent, the approaches are usually followed by a deterministic description, neglecting the stochastic nature of the models defined by the individual transitions rates. Stochastic effects may become relevant even for extremely large system sizes, specially if the system is close to a critical point, or the network has high degree heterogeneity. Besides, there are some models where the deterministic approach does not provide the relevant information sought. For instance, the noisy-voter (Kirman) model, the contact process or the Threshold model, are examples of relevance in which the stochastic effects greatly dominate the dynamics. The main aim of this work is to give a general theoretical approach to binary-state models on complex networks that takes into account stochastic effects, going beyond incomplete deterministic approaches.

DY 20.4 Tue 11:45 ZEU 260

Infinite sequence of explosive transitions in network robustness — •Laura Barth[1,2,3] and Thilo Gross[1,2,3] — [1]Helmholtz Institute for Functional Marine Biodiversity (HIFMB), Oldenburg, Germany — [2]Alfred-Wegener Institute (AWI), Helmholtz Center for Polar and Marine Research, Bremerhaven, Germany — [3]Institute for Chemistry and Biology of the Marine Environment (ICBM), Carl-von-Ossietzky University, Oldenburg, Germany

Explosive transitions in networks have recently received much attention. Here we show that such transitions also appear in one of the most fundamental problems in network science if it is considered from a certain angle. This problem is the fragmentation of networks under node or link removal, which has been studied extensively in the context of social networks. One key property in this context is v, the probability that a random link of a random node does not connect to the giant component. Now suppose we are constructing a random graph with a prescribed mean degree. How would we choose the degree distribution such that v is minimal after the attack? We show that the optimal degree distributions undergo an infinite sequence of discontinuous transitions as the size of the attack is changed.

DY 20.5 Tue 12:00 ZEU 260

Information parity to measure the consonance of influence in complex networks — Aline Viol[1] and •Philipp Hövel[2] — [1]Scuola Internazionale Superiore di Studi Avanzati, Italy — [2]Christians-Albrechts-Universität zu Kiel, Germany

We discuss a new analytical tool to quantify the consonance of influence between nodes with respect to the whole network architecture: information parity. Unlike traditional approaches to quantitative network analysis that consider only local or global scales, information parity instead quantifies pairwise statistical similarities over the entire network structure. Based on information theory and using the statistics of geodesic distances, information parity assesses how similarly a pair of nodes can influence and be influenced by the network. This allows us to quantify the access of information gathered by the nodes. To demonstrate the method's potential, we evaluate a social network and human brain networks. Our results indicate that emerging phenomena like an ideological orientation of nodes in social networks can be shaped by their information parities. We also show the potential of information parity to identify central network regions in structural brain networks placed near the mid-sagittal plane. We find that functional networks have, on average, greater information parity for inter-hemispheric homologous regions in comparison to the whole network. Finally, we explore functional brain networks under influence of a psychedelic substance.

DY 21: Quantum Chaos and Coherent Dynamics

Time: Tuesday 14:00–15:15 Location: MOL 213

DY 21.1 Tue 14:00 MOL 213

Bit-Flipping based on Stability Transition of Coupled Spins — •Maximilian F. I. Kieler and Arnd Bäcker — TU Dresden, Institut für Theoretische Physik, Dresden, Germany

A bipartite spin system is proposed for which a bit-flipping mechanism between two states is possible when the coupling is varied. The states correspond in the semiclassical limit to equilibrium points showing a stability transition from elliptic-elliptic stability to complex instability. Based on the classical system we find a universal scaling for the transfer time, which even applies in the deep quantum regime.

DY 21.2 Tue 14:15 MOL 213

New type of scarring in quantum chaotic scattering — •Jan Robert Schmidt and Roland Ketzmerick — TU Dresden, Institut für Theoretische Physik, Dresden, Germany

We study the three-disk scattering system, which is a paradigmatic example for quantum chaotic scattering. It is shown that any resonance state can be described by a product of a multifractal pattern of classical origin and universal, exponentially distributed fluctuations, as found for optical microcavities [1]. The first factor is determined by averaging resonance states with similar lifetime and is compared to an approximate conditionally-invariant measure from open chaotic maps [2]. A new type of scarring along ray segments, unrelated to periodic-orbit scarring, was recently observed in (partially open) optical microcavities [1]. Ray-segment scarring is just as well observed in the (fully open) three-disk system and has been overlooked for 30 years.

[1] R. Ketzmerick, K. Clauß, F. Fritzsch, and A. Bäcker, Phys. Rev. Lett. **129**, 193901 (2022).

[2] K. Clauß, M. J. Körber, A. Bäcker, and R. Ketzmerick, Phys. Rev. Lett. **121**, 074101 (2018).

DY 21.3 Tue 14:30 MOL 213

Manipulating light inside a microcavity with phase-space tailoring — Yan-Jun Qian[1], Hui Liu[1], Qi-Tao Cao[1], •Julius Kullig[2], Kexiu Rong[1], Cheng-Wei Qiu[3], Jan Wiersig[2], Qihuang Gong[1,4], Jianjun Chen[5], and Yun-Feng Xiao[1,4] — [1]Peking University, Beijing, China — [2]Otto-von-Guericke-University Magdeburg, Magdeburg, Germany — [3]National University of Singapore, Singapore, Singapor — [4]Shanxi University, Taiyuan, China — [5]Beijing Normal University, Beijing, China

We report on a novel powerful method for purposely manipulating light inside an optical microcavity. Via small absorptive, reflective or refractive elements embedded in the interrior of the microcavity the photon transport is controlled in the phase space. Thus, phase-space tailoring allows for a spactial and tempral control of the light confinement enabling a manipulation of the far-field emisson pattern or the quality-factor.

DY 21.4 Tue 14:45 MOL 213

A spectral duality in graphs and microwave networks — •Tobias Hofmann[1], Junjie Lu[2], Ulrich Kuhl[1,2], and Hans-Jürgen Stöckmann[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Institut de Physique de Nice, CNRS, Université Côte d'Azur, 06108 Nice, France

Quantum graphs and their experimental counterparts, microwave networks, are ideally suited to study the spectral statistics of chaotic systems. The graph spectrum is obtained from the zeros of a secular determinant derived from energy and charge conservation. Depending on the boundary conditions at the vertices, there are Neumann and Dirichlet graphs. The first ones are realized in experiments, since the standard junctions connecting the bonds obey Neumann boundary conditions due to current conservation. On average, the corresponding Neumann and Dirichlet eigenvalues alternate as a function of the wave number, with the consequence that the Neumann spectrum is described by random matrix theory only locally, but adopts features of the interlacing Dirichlet spectrum for long-range correlations. Another spectral interlacing is found for the Green's function, which in contrast to the secular determinant is experimentally accessible. This is illustrated by microwave studies and numerics.

DY 21.5 Tue 15:00 MOL 213

Quantum Coherent Spin-Bath Dynamics and The Impact of Interactions on Quantum Memory Effects — •Tobias Boorman and Bernd Braunecker — University of St Andrews, St Andrews, United Kingdom

Using a robust theoretical framework, we systematically extract the joint-coherent dynamics of an impurity spin coupled to a strongly correlated material as the central process of a magnetic resonance. This framework enables a complete dynamical picture, extending beyond the usual high-temperature approximation that underpins the contemporary understanding of spin-bath decoherence, and allowing one to probe even further to the sub-thermal time regime, where quantum memory effects are the dominant feature. As a theoretically and experimentally accessible model of a strongly correlated conductor, we take the Luttinger liquid as a prototype to study how interactions alter the response of the bath to the impurity. Taken under the lens of the framework, we find that the joint quantum-coherent dynamics manifests itself as a rapid and seemingly instantaneous initial slip prior to the spin decoherence, whilst interactions within the bath play a role in modulating the amplitude and rate of this feature. We fit this understanding into a wider picture of magnetic resonance in interacting systems at intermediate temperatures, improving upon the known interaction-induced modifications of high-temperature approximations.

DY 22: Machine Learning in Dynamics and Statistical Physics II

Time: Tuesday 14:00–15:15 Location: ZEU 160

DY 22.1 Tue 14:00 ZEU 160

Reservoir Computing using Quantum Dot Lasers — •Huifang Dong, Lina Jaurigue, and Kathy Lüdge — Institute of Physik, Technische Universität Ilmenau, Weimarer Str. 32, 98684 Ilmenau, Germany.

Time-multiplexed reservoir computing is a machine-learning approach which is well suited for implementation using semiconductor lasers subject to optical feedback. In such a delay-based setup the feedback has two important roles; it directly influences the memory of the system and it generates the high dimensional transient dynamics needed for good computational performance [1]. However, commonly used and commercially available quantum well semiconductor lasers are dynamically very sensitive to optical feedback, which can make the implementation of such systems difficult. Implementation and on-chip integration of optical reservoir computing become feasible with quantum dot lasers, as they emit at the telecommunication wavelength and are less sensitive to unwanted reflections [2]. Using typical benchmark tasks for time series prediction we show that quantum dot lasers show good computing performance that can be further optimized by proper delay time tuning.

[1] T. Hülser, et al., Opt. Mater. Express 12, 3, 1214 (2022).
[2] C. Otto, et al., Int. J. Bifurc. Chaos 22, 10, 1250246 (2012).

DY 22.2 Tue 14:15 ZEU 160

Studying sequence property relationships with neural networks — •Huzaifa Shabbir[1], Jens Uwe Sommer[1,2], and Marco Werner[1] — [1]Leibniz Institute for Polymer Research Dresden, Germany. — [2]Technische Universität Dresden

In this work, we investigate the relationships between chemical sequence and property space for various sequence lengths with the help of neural networks (NN). Two different systems are investigated for this purpose: system I comprises copolymer sequences and their free energy of interaction with a lipid bilayer membrane. System II consists of metallic nanoparticle sequences and their plasmonic spectrum. We compare the performance of different neural network architectures such as feed-forward NNs and gated recurrent unit (GRU) networks in terms of their interpolation and extrapolation capacity between different sequence lengths. We show that the GRU is particularly suitable to transfer the learned patterns from smaller sequence lengths to enhance significantly the learning result for larger sequence lengths.

DY 22.3 Tue 14:30 ZEU 160

Modelling dynamic 3D-heat transfer for laser material processing using physics-informed neural networks (PINNs) — •Michael Moeckel and Jorrit Voigt — TH Aschaffenburg, Würzburger Str. 45, 63743 Aschaffenburg

Machine learning (ML) algorithms are increasingly applied to fit complex models to empirical data and to predict on dynamical system behaviour. However, such models are not intrinsically protected from violating causality or other, well-understood physical laws. Black-box ML models offer limited interpretability. Extending ML models by including physical knowledge in the optimization procedure is known as physics-based and data-driven modelling. A promising recent development are physics informed neural networks (PINN), which ensure consistency to physical laws and measured data via appropriately designed optimization routines. Here we model the 3D time-dependent temperature profile following the passage of a laser focus at the surface of some material using PINNs. In this setting, we discuss aspects of numerically efficient training for PINNs, e.g. on a set of varying collocation points. The results from the PINN agree with finite element simulations, proving the suitability of the approach. The proposed models can be smoothly integrated in monitoring systems and naturally extend to the joint analysis of measurement data and dynamical behaviour encoded in governing equations.

DY 22.4 Tue 14:45 ZEU 160

Optical convolutional neural network with atomic nonlinearity — •Mingwei Yang[1,2], Elizabeth Robertson[1,2], Luisa Esguerra[1,2], Kurt Busch[3,4], and Janik Wolters[1,2] — [1]Deutsches Zentrum für Luft- und Raumfahrt, Institute of Optical Sensor Systems, Berlin, Germany. — [2]Technische Universität Berlin, Berlin, Germany. — [3]Humboldt-Universität zu Berlin, Institut für Physik, AG Theoretische Optik & Photonik, Berlin, Germany. — [4]Max-Born-Institut, Berlin, Germany.

Due to their inherent parallelism, fast processing speeds and low energy consumption, free-space-optics implementations have been identified as an attractive possibility for analog computations of convolutions [1,2]. However, the efficient implementation of optical nonlinearities for such neural networks still remains challenging. In this work, we report on the realization and characterization of a three-layer optical convolutional neural network where the linear part is based on a 4f-imaging system and the optical nonlinearity is realized via the absorption profile of a cesium atomic vapor cell. This system classifies the handwritten digital dataset MNIST with 83.96% accuracy, which agrees well with corresponding simulations. [1] H. J. Caulfield and S. Dolev, *Why future supercomputing requires optics,* Nat. Photonics 4, 261*263 (2010). [2] M. Miscuglio, Z. Hu, S. Li, J. K. George, R. Capanna, H. Dalir, P. M. Bardet, P. Gupta, and V. J. Sorger, *Massively parallel amplitude-only fourier neural network,* Optica 7, 1812*1819 (2020).

DY 22.5 Tue 15:00 ZEU 160

Phase Diagram of the J_1-J_2 Ising Model from Unsupervised Learning: Neural Networks vs Image Comparison — •Burak Çivitcioğlu[1], Andreas Honecker[1], and Rudolf A. Römer[2] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, CY Cergy Paris Université, Cergy-Pontoise, France — [2]Department of Physics, University of Warwick, Coventry, CV4 7AL, United Kingdom

Machine learning methods have been shown to be one of the novel approaches in identifying the phases and phase transitions in models of statistical physics. Here, we study the performance of unsupervised learning in the J_1-J_2 Ising model. We benchmark the results for phase diagram reconstruction using variational autoencoders (VAEs) against straightforward image comparison. We show that such image comparison can result in accuracies that are akin to that of VAEs.

DY 23: Statistical Physics: General II

Time: Tuesday 14:00–15:15 Location: ZEU 250

DY 23.1 Tue 14:00 ZEU 250

Microscopic theory for the shear-induced structure distortion in concentrated suspensions of spherical colloids — •Carmine Anzivino[1], Francesco Leone[1], Luca Banetta[2], Michael S. Murillo[3], and Alessio Zaccone[1] — [1]Department of Physics "A. Pontremoli", University of Milan, via Celoria 16, 20133 Milan, Italy — [2]Department of Applied Science and Technology, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129, Turin, Italy — [3]Department of Computational Mathematics, Science and Engineering, Michigan State University, East Lansing, Michigan 48824, USA

We combine an analytical solution of the Smoluchowski convection-diffusion equation that fully takes into account the boundary-layer structure, with generalized integral equations of the liquid state. We investigate the shear-induced structural distortion in suspensions of spherical colloids, in concentrated regimes of packing fraction so far explored only by means of numerical simulations [1].

For hard spheres, our findings are in very good parameter-free agreement with numerical data from literature [2]. In addition, our scheme predicts (for the first time) a consistent enhancement of the structure factor S(k) at vanishing k, upon increasing the shear rate, which we argue may signal the onset of a shear-induced phase transition from the isotropic phase to a non-uniform one.

[1] L. Banetta, F. Leone, C. Anzivino, M.S. Murillo and A. Zaccone, Phys. Rev. E 106, 044610 (2022). [2] J.F. Morris and B. Katyal, Physics of Fludis 14, 1920 (2002).

DY 23.2 Tue 14:15 ZEU 250

Coupling of a particle-based solver to a fluctuating hydrodynamic reservoir through an adaptive resolution simulation approach — •Abbas Gholami[2], Rupert Klein[1], and Luigi Delle Site[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany

Adaptive Resolution Simulation (AdResS) is a multi-resolution approach for coupling different particle-based regions. In AdResS, a fully atomistic subregion (open system) is in contact with reservoirs of non-interacting particles through a small buffer region. In this approach, a thermostat and an external (thermodynamic) force are applied in the reservoir and buffer regions to ensure the same behaviour as the reference simulation. Coupling a particle-based domain with a continuum reservoir will significantly reduce computational costs while preserving satisfactory precision in different regions.

This work uses a novel algorithm to couple the AdResS particle-based simulator to a Navier-Stokes Landau-Lifshitz solver. The coupling algorithm suggests that the proper thermodynamic force for the AdResS simulation will be interpolated among a set of pre-calculated thermodynamic forces based on the resulting continuum state at the interface region. On the other hand, to pass the information from the particle side to the continuum reservoir, the result of the AdResS simulation will apply to the corresponding continuum cells with proper interface values. The accuracy of this coupling algorithm is demonstrated through various numerical scenarios with different initial conditions.

DY 23.3 Tue 14:30 ZEU 250

The orientation field generated by a moving defect: multivalued solutions of the diffusion equation — •Jacopo Romano, Benoit Mahault, and Ramin Golestanian — Max Planck Institute for Dynamics and Self-Organization

Point-like topological defects are singular configurations that occur in a variety of in and out of equilibrium systems with two-dimensional orientational order. As they are associated with a nonzero circuitation condition, the presence of defects induces a long-range perturbation of the orientation landscape around them. Their effective dynamics is thus generally described in terms of quasi-particles interacting through the orientation field they produce, which in the simplest setting is described by the diffusion equation. Due to the multivaluedness of the orientation field, its expression for a defect moving with an arbitrary trajectory cannot be obtained via simple techniques and is often approximated by that of a static defect. Here, we propose a solution to this problem that relies on particular gauge invariance properties of the proper multivalued field derivatives. Our approach allows to derive the exact expression for the orientation created by multiple moving defects, which we find to depend on their past trajectories and thus to be nonlocal in time. Performing various expansions in relevant regimes, we show how improved approximations with respect to the static defect solution can be obtained. Moreover, our results lead to so far unnoticed structures in the orientation field of moving defects which we discuss in light of existing experimental results.

DY 23.4 Tue 14:45 ZEU 250

Perturbative and Semiclassical Expansions in Quantum Thermodynamics Using a Modified Keldysh Contour — •Sadeq S. Kadijani, Vasco Cavina, Massimiliano Esposito, and Thomas L. Schmidt — Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg

Modified Keldysh contours are a versatile tool for calculating moment generating functions (MGFs) in the context of quantum thermodynamics and quantum transport theory, and are the backbone of both Green's functions (GFs) and path integral approaches to open quantum systems. By using a different modification of the Keldysh contour, we will construct a perturbation expansion of the MGFs and discuss its semi-classical expansion. Using the symmetry property of the modified contour, we prove that the perturbative expansion obtained in this way satisfies the fluctuation theorem (FT) in every order of perturbation theory. We show that the contribution of the different diagrams can be added to obtain a general expression of the work statistics in terms of a sum of independent Poisson processes.

To further investigate the work MGF we apply the Feynman path integral techniques to the modified contour. In this way, the MGF can be written in terms of the action, which depends on the fields running on the modified contour. The action can be used to obtain a semiclassical expansion of the MGF, which is then used to compute explicitly the zeroth (classical) and the first quantum correction to the work MGF.

DY 23.5 Tue 15:00 ZEU 250

Effect of Frequency-Dependent Viscosity on Molecular Friction in Liquids — •Henrik Kiefer[1], Domenico Vitali[2], Benjamin Dalton[3], Laura Scalfi[4], and Roland Netz[5] — [1]Freie Universität Berlin, Department of Physics, Berlin, Germany — [2]Freie Universität Berlin, Department of Physics, Berlin, Germany — [3]Freie Universität Berlin, Department of Physics, Berlin, Germany — [4]Freie Universität Berlin, Department of Physics, Berlin, Germany — [5]Freie Universität Berlin, Department of Physics, Berlin, Germany

A fundamental problem in molecular dynamics is the relation between the frequency-dependent friction of a molecule in a liquid and the hydrodynamic properties of the liquid. We investigate this connection in the case of a water molecule moving in liquid water using all-atomistic molecular dynamics simulations and linear hydrodynamic theory. For this, we analytically calculate the frequency-dependent friction of a sphere with finite surface slip moving in a non-Newtonian compressible fluid by solving the linear transient Stokes equation, including frequency-dependent shear and volume viscosities, which are both determined from MD simulations of bulk liquid water. By fitting the effective sphere radius and the slip length, the frequency-dependent friction and velocity autocorrelation function from the transient Stokes equation and simulations quantitatively agree with the frequency-dependent friction of a single water molecule moving in liquid water, as defined by the generalized Langevin equation from MD simulation trajectories, provided accurate frequency-dependent viscosities are used.

DY 24: Glasses and Glass Transition (joint session DY/CPP)

Time: Tuesday 14:00–15:00 Location: ZEU 147

DY 24.1 Tue 14:00 ZEU 147

Dynamical phase transitions in trap models and universality classes of aging — •Diego Tapias[1] and Peter Sollich[1,2] — [1]Institute for Theoretical Physics, University of Göttingen, Germany — [2]Department of Mathematics, King's College London, London, UK

We investigate how aging and driving by trajectory biasing interact in two mean field models of glassy dynamics, widely known as trap models. We show that similarly to kinetically constrained models, the equilibrium state of the unbiased system above the glass transition temperature is located at the coexistence of two dynamical phases (active and inactive). In contrast, below this temperature, we find two different nonequilibrium scenarios: energetic (or activated) aging that is destroyed by any dynamical bias towards low activity, which we call "fragile aging", and entropic aging that is stable against the existence of such a dynamical bias, which we refer to as "robust aging". We conjecture that these categories have broader relevance as universality classes for aging dynamics in glassy systems.

DY 24.2 Tue 14:15 ZEU 147

Fragile to strong crossover as general glassy feature — •Anshul Deep Singh Parmar and Andreas Heuer — Institute of Physical Chemistry, University of Münster, Corrensstrasse 28/30, 48149 Münster, Germany

As a liquid is cooled below the melting temperature, the dynamics become increasingly sluggish with the degree of supercooling, known as fragility. The fundamental question is whether the liquid ceases to flow at some finite temperature, the material undergoing the glass transition, or dynamics diverge smoothly to zero temperature. This is a central question of pivotal importance for unraveling the nature of glass and theoretical understanding, concealing with astronomical long observation times.

We circumvent this infeasibility by taking advantage of swap Monte Carlo with multi-billion speedups for equilibration well beyond the glass transition. Our investigation of a wide range of system sizes and temperatures across the experimental glass transition unveils the nature of the energy landscape. We observe a notable deviation from the Gaussian nature of the potential-energy landscape. Rapid depletion of states is associated with the glassy bottom of the landscape, unveiling the fragile to strong crossover is the general glassy behavior. Our result ultimately rules out the finite-temperature divergence and establishes the conceptualized Arrhenius description of the dynamics at low temperatures. Our findings are critical in advancing the investigation of glass in an experimental and theoretical framework.

DY 24.3 Tue 14:30 ZEU 147

A solution to the plasticity of glasses based on topological physics — •Alessio Zaccone — Department of Physics, University of Milan, 20133 Milano, Italy

I will start by reviewing the microscopic theory of linear elasticity in amorphous solids which, from first-principles consideration of non-centrosymmetry in the particle contact environment, leads to mathematical predictions of elastic moduli in quantitative parameter-free agreement with numerical simulations of random jammed packings [1]. This theory fully accounts for the extra non-affine displacements which arise due to the lack of centrosymmetry in disordered solids. I will then show that non-affinity of particle motions gives rise to well-defined topological defects (dislocation-like topological defects, DTDs) which have recently been discovered in the displacement field of glasses [1] and later confirmed in [2]. The norm of the associated Burgers vector of these defects can be used as an accurate predictor of the onset of plastic flow and yielding of glasses, and, in combination with Schmid's law, it can explain the phenomenon of shear banding via self-organization of DTDs in slip systems at 45 degrees with respect to flow direction [4]. Broader implications of a unifying topological field theory of liquids and the glass transition will also be mentioned. [1] A. Zaccone and E. Scossa-Romano, Phys. Rev. B 83, 184205 (2011) [2] Z. W. Wu, Y. Chen, W.-H. Wang, W. Kob, L. Xu, arXiv:2209.02937 (2022)

DY 24.4 Tue 14:45 ZEU 147

Confinement induced relaxations and phase behavior of a nanoconfined ionic liquid crystal — •Mohamed Aejaz Kolmangadi[1], Andreas Schönhals[1], Li Zhuoqing[2], and Patrick Huber[2] — [1]Bundesantalt für Materialforschung und -prüfung (BAM), Berlin, Germany — [2]Technical Univeristy Hamburg TUHH and DESY

We investigate the molecular dynamics and electrical conductivity of a linear shaped guanidinium based ILC confined in self-ordered nano porous alumina oxide membranes of pore size ranging from 180nm down to 25nm by employing broadband dielectric spectroscopy (BDS) and calorimetry. Calorimetric investigation reveals a complete suppression of the columnar - isotropic transition, while the plastic crystalline - columnar transition temperature decreases with inverse pore size and deviates from the Gibbs - Thomson equation. For the bulk case, BDS detects two relaxation modes in the crystalline phase, the gamma relaxation and the α1 relaxation, and two relaxation modes in the columnar phase, the α2 and α3 relaxation. For the confined case, all relaxation modes slow down compared to the bulk. However, for the least pore size (25 nm), the α2 relaxation is absent. We discuss the possible molecular origins of the different relaxation modes observed. For the bulk ILC, a clear jump of 4 orders of magnitude in the absolute values of DC conductivity occurs at the transition from the plastic crystalline to hexagonal columnar phase, for the confined ILC, this transition is smooth. DC conductivity is reduced for the confined case, except for the 25nm, where the values is similar to the bulk.

DY 25: Many-Body Quantum Dynamics (joint session DY/TT)

Time: Wednesday 9:30–13:00 Location: MOL 213

Invited Talk DY 25.1 Wed 9:30 MOL 213

Many-body localization from Hilbert- and real-space points of view — •Ivan Khaymovich[1], Giuseppe De Tomasi[2], Frank Pollmann[3], and Simone Warzel[3] — [1]Nordic Institute for Theoretical Physics, Stockholm, Sweden — [2]University of Illinois Urbana-Champaign, USA — [3]Technical University Munich, Germany

Many-body localization (MBL), known as a generic mechanism to break quantum ergodicity, has been recently shown to be not the Hilbert-space Anderson localization. Instead, the MBL eigenstate occupies a fractal support [1-2], with extensive number of configurations. On the other hand, the well-established and accepted by the community picture of an emergent set of local integrals of motion [3] provides the structure of the MBL in the real space.

In this talk, I will provide the observable (later measured in the experiment [4]) which combines the fractality in the Hilbert space with the presence of local integrals of motion [2]. This observable, being the radial profile of the eigenstate over the Hamming distance, keeps the information about both the Hilbert-space fractal dimensions and the real-space localization lengths and uncovers the structure of these measures across the MBL transition. Phenomenological picture behind this behavior is consistent with the Kosterlitz-Thouless scenario of the MBL transition, suggested in the literature.

Literature: [1] N. Macé et al., PRL 123, 180601 (2019). [2] G. De Tomasi, I. M. Khaymovich et al. PRB 104, 024202 (2021). [3] Abanin et al., RMP 91, 021001 (2019). [4] Y. Yao et al arXiv:2211.05803.

DY 25.2 Wed 10:00 MOL 213

Bridging classical and quantum many-body information dynamics — •Andrea Pizzi[1,2], Daniel Malz[3,4], Andreas Nunnenkamp[5], and Johannes Knolle[6,4,7] — [1]Department of Physics, Harvard University, Cambridge 02138, Massachusetts, USA — [2]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom — [3]Max-Planck-Institute of Quantum Optics, Hans-Kopfermann-Str. 1, 85748 Garching, Germany — [4]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany — [5]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1190 Vienna, Austria — [6]Department of Physics, Technische Universität München, James-Franck-Stra. 1, 85748 Garching, Germany — [7]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

The fundamental question of how information spreads in closed quantum many-body systems is often addressed through the lens of the bipartite entanglement entropy. Among its most striking features are unbounded linear growth in the thermodynamic limit, asymptotic extensivity in finite-size systems, and measurement-induced phase transitions. Here, we show that these key qualitative features emerge naturally also for the classical bipartite mutual information, the natural classical analogue of the quantum entanglement entropy. Key for this observation is treating the classical many-body problem on par with the quantum one, that is, explicitly accounting for the exponentially large probability distribution. Our analysis is supported by extensive numerics on prototypical cellular automata and Hamiltonian systems.

DY 25.3 Wed 10:15 MOL 213

Performance boost of a collective qutrit refrigerator — •Dmytro Kolisnyk[1] and Gernot Schaller[2] — [1]Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany

A single qutrit with transitions selectively driven by weakly-coupled reservoirs can implement one of the world's smallest refrigerators. We analyze the performance of N such fridges that are collectively coupled to the reservoirs. We observe a quantum boost, manifest in a quadratic scaling of the steady-state cooling current with N. As N grows further, the scaling reduces to linear, since the transitions responsible for the quantum boost become energetically unfavorable. Fine-tuned inter-qutrit interactions may be used to maintain the quantum boost for all N and also for not-perfectly collective scenarios.

[1] D. Kolisnyk and G. Schaller, Performance boost of a collective qutrit refrigerator, arXiv:2210.07844.

[2] M. Kloc, K. Meier, K. Hadjikyriakos, and G. Schaller, Superradiant Many-Qubit Absorption Refrigerator, Phys. Rev. Applied 16, 044061 (2021).

[3] N. Linden, S. Popescu, and P. Skrzypczyk. How small can thermal machines be? The smallest possible refrigerator. Phys. Rev. Lett. 105:130401, 2010.

DY 25.4 Wed 10:30 MOL 213

Hidden Phase of the Spin-Boson Model — •Florian Otterpohl[1,2], Peter Nalbach[3], and Michael Thorwart[2,4] — [1]Center for Computational Quantum Physics, Flatiron Institute, New York, New York 10010, USA — [2]I. Institut für Theoretische Physik, Universität Hamburg, Notkestraße 9, 22607 Hamburg, Germany — [3]Fachbereich Wirtschaft und Informationstechnik, Westfälische Hochschule, Münsterstraße 265 46397 Bocholt, Germany — [4]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

A quantum two-level system immersed in a sub-Ohmic bath experiences enhanced low-frequency quantum statistical fluctuations which render the nonequilibrium quantum dynamics highly non-Markovian. Upon using the numerically exact time-evolving matrix product operator approach, we investigate the phase diagram of the polarization dynamics. In addition to the known phases of damped coherent oscillatory dynamics and overdamped decay, we identify a new third region in the phase diagram for strong coupling showing an aperiodic behavior. We determine the corresponding phase boundaries. The dynamics of the quantum two-state system herein is not coherent by itself but slaved to the oscillatory bath dynamics.

DY 25.5 Wed 10:45 MOL 213

Exploring anomalies by many-body correlations — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN, Campus Universitário Lagoa nova,59078-970 Natal, Brazil

The quantum anomaly can be written alternatively into a form violating conservation laws or as non-gauge invariant currents seen explicitly on the example of chiral anomaly. By reinterpreting the many-body averaging, the connection to Pauli-Villars regularization is established which gives the anomalous term a new interpretation as arising from quantum fluctuations by many-body correlations at short distances. This is exemplified by using an effective many-body quantum potential which realizes quantum Slater sums by classical calculations. It is shown that these quantum potentials avoid the quantum anomaly but approaches the same anomalous result by many-body correlations. A measure for the quality of quantum potentials is suggested to describe these quantum fluctuations in the mean energy. Consequently quantum anomalies might be a short-cut way of single-particle field theory to account for many-body effects. This conjecture is also supported since the chiral anomaly can be derived by a completely conserving quantum kinetic theory. [Eur. Phys. J. B 92 (2019) 176, Phys. Lett. A 383 (2019) 1362, Phys. Status Solidi B (2021) 2100316]

DY 25.6 Wed 11:00 MOL 213

Non-Markovian Stochastic Schrödinger Equation: Matrix Product State Approach to the Hierarchy of Pure States — Xing Gao[1], Jiajun Ren[2], Zhigang Shuai[2], and •Alexander Eisfeld[3] — [1]Sun Yat-sen University, Shenzhen, Guangdong, China — [2]Tsinghua University, Beijing, China — [3]MPI-PKS, Dresden

We derive a stochastic hierarchy of matrix product states (HOMPS) for non-Markovian dynamics in open quantum system at finite temperature, which is numerically exact and efficient. HOMPS is obtained from the stochastic hierarchy of pure states (HOPS) by expressing HOPS in terms of formal creation and annihilation operators. The resulting stochastic first order differential equation is then formulated in terms of matrix product states and matrix product operators. In this way the exponential complexity of HOPS can be reduced to scale polynomial with the number of particles. The validity and efficiency of HOMPS is demonstrated for the spin-boson model and long chains where each site is coupled to a structured, strongly non-Markovian environment.

[1] X. Gao, J. Ren, A. Eisfeld, Z. Shuai, *Phys. Rev. A* 105, L030202 (2022)

DY 25.7 Wed 11:15 MOL 213

ultrafast gap dynamics near the zone boundary in a cuprate superconductor — •Qinda Guo, Maciej Dendzik, Magnus Berntsen, Cong Li, Wanyu Chen, Yang Wang, Dibya Phuyal, and Oscar Tjernberg — Department of Applied Physics, KTH Royal Institute of Technology, Hannes Alfvéns väg 12, 114 19 Stockholm, Sweden

The time- and angle- resolved photoemission spectroscopy (tr-ARPES) is a powerful technique to directly probe the ultrafast electron dynamics in the momentum space. Our recently developed narrow-bandwidth tr-ARPES setup enabled us to access the ultrafast dynamics of the quasiparticle population as well as the superconducting gap, in the whole surface Brillouin zone of the photoexcited cuprate superconductor (Bi2212). The results show non-trivial dynamics at the d-wave antinode and provide new insights into the enigma of the Cooper-pair formation process and condensation that takes place in the high-temperature cuprate superconductor.

15 min. break

DY 25.8 Wed 11:45 MOL 213

Controlling Many-Body Quantum Chaos — •Lukas Beringer[1], Steven Tomsovic[1,2], Juan Diego Urbina[1], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Department of Physics and Astronomy, Washington State University, Pullman, WA USA

Targeting in classical chaos control problems makes optimal use of the system's exponential instabilities to direct a given initial state to a predetermined final target state. A generalization to chaotic quantum systems in the semiclassical regime is possible [1], but also requires controlling an initially localized evolving quantum state's spreading. A coherent procedure of this kind enables directing highly excited, far-out-of-equilibrium states from an initial to some final target quantum state. Such methods have been successfully developed and applied to initially minimum uncertainty wave packets in a quantum kicked rotor system. The aim of our work is to extend those procedures to bosonic many-body systems. More specifically, we demonstrate how to make a localized quantum initial state follow special chaotic mean-field solutions of a Bose-Hubbard system toward an arbitrary localized target final state.

[1] S. Tomsovic, J. D. Urbina, and Klaus Richter, Controlling Quantum Chaos: Optimal Coherent Targeting, arXiv:2211.07408

DY 25.9 Wed 12:00 MOL 213

Environment-induced decay dynamics of antiferromagnetic order in Mott-Hubbard systems — •Gernot Schaller[1], Friedemann Queisser[1,2], Nikodem Szpak[3], Jürgen König[3], and Ralf Schützhold[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [3]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany

We study the dissipative Fermi-Hubbard model in the limit of weak tunneling and strong repulsive interactions, where each lattice site is tunnel-coupled to a Markovian fermionic bath. For cold baths at intermediate chemical potentials, the Mott insulator property remains stable and we find a fast relaxation of the particle number towards half filling. On longer time scales, we find that the antiferromagnetic order of the Mott-Néel ground state on bipartite lattices decays, even at zero temperature. For zero and nonzero temperatures, we quantify the different relaxation time scales by means of waiting time distributions, which can be derived from an effective (non-Hermitian) Hamiltonian and obtain fully analytic expressions for the Fermi-Hubbard model on a tetramer ring.

[1] G. Schaller *et al.*, Phys. Rev. B **105**, 115139 (2022).

DY 25.10 Wed 12:15 MOL 213

Arrow of time concept based on properties of Lanczos coefficients — •Christian Bartsch, Mats H. Lamann, Robin Heveling, Lars Knipschild, Jiaozi Wang, Robin Steinigeweg, and Jochen Gemmer — Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, DE-49076 Osnabrück

We introduce an arrow of time concept based on a specifically defined class of arrow of time functions (ATF) consisting of a limited number of Krylov space generating observables. These ATF'S are found to be essentially monotonously decaying in time which is measured by some quantifying parameter. The ATF's are constructed to be upper bounds for pertinent autocorrelation functions. Employing certain features of the Lanczos coefficients and the wave package-like excitation moving on the Krylov chain, we find reasonable agreement with corresponding numerics.

DY 25.11 Wed 12:30 MOL 213

Fast Time-Evolution of Matrix-Product States using the QR decomposition — •Jakob Unfried[1,2], Johannes Hauschild[1], and Frank Pollmann[1,2] — [1]Department of Physics, TFK, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany

Numerical simulations of quantum many-body dynamics in and out of equilibrium is essential for the understanding of a wide range of physical phenomena. Efficient matrix product state simulation techniques, such as time evolution block decimation (TEBD), are widely successful in extracting experimentally relevant signatures, such as dynamical correlation functions. We propose and benchmark a modified TEBD algorithm that uses a truncation scheme based on the QR decomposition instead of the singular value decomposition (SVD). The modification reduces the scaling with the dimension of the physical Hilbert space d from d^3 down to d^2. Unlike the SVD, the QR decomposition allows for highly efficient implementations on GPU hardware. In a benchmark simulation of a global quench in a quantum clock model, we observe a speedup of orders of magnitude comparing the QR based scheme on a GPU to the SVD based TEBD on CPU.

DY 25.12 Wed 12:45 MOL 213

Simulating infinite temperature spin dynamics by a dynamic mean-field theory — •Timo Grässer[1], Kristine Rezai[2], Alexander O. Sushkov[2], and Götz S. Uhrig[1] — [1]Condensed Matter Theory, TU Dortmund University, Otto-Hahn Straße 4, 44221 Dortmund, Germany — [2]Department of Physics, Boston University, Boston, MA 02215, USA

We develop a dynamic mean-field theory for spin systems at infinite temperature (spinDMFT) [1]. The idea is to replace the large environment of a spin by a dynamic mean-field which displays a random Gaussian temporal evolution. Its autocorrelations are self-consistently linked to the quantum mechanic expectation values of spin-spin correlations. This approach becomes exact in the limit of large lattice coordination numbers. We improve the approach by considering spin clusters quantum-mechanically (cluster spinDMFT). The extended model is able to describe dynamic spin correlations measured in recent experiments [2] where an inhomogeneous spin-$\frac{1}{2}$ ensemble on a diamond surface is probed using nitrogen-vacancy centers as sensors.

[1] T. Gräßer et al., Phys. Rev. Research **3**, 043168 (2021).

[2] K. Rezai et al., arXiv:2207.10688 (2022).

DY 26: Focus Session: From Inter-individual Variability to Heterogeneous Group Dynamics and Disorder in Active Matter (joint session DY/BP/CPP)

The study of active particle dynamics has developed into a vibrant field of multidisciplinary research, including such diverse systems as bacterial colonies, cellular self-organization, synthetic colloids and microrobots as well as macroscopic systems like locusts, flocks of birds, schools of fish or pedestrians. Whereas many studies in the past focused either on the random transport of individual particles or on the interplay of temporal fluctuations (noise) and interactions (velocity alignment or attraction/repulsion), there is now an increasing interest in the question how structural disorder and inter-individual variability, i.e., different motility characteristics of individuals, shape the active particle dynamics and emergent pattern formation of groups. The presence of structural or quenched disorder raises furthermore the immediate question how to bridge data and models based on (short time) tracking data, given the simultaneous presence of temporal fluctuations. With this focus session, we aim at bringing researchers from statistical physics and biophysics together to discuss this interdisciplinary topic and exchange ideas on common challenges arising in different application areas.

Organized by Robert Großmann (Potsdam)

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

Invited Talk DY 26.1 Wed 9:30 ZEU 160

More is different: High-throughput 3D tracking reveals bacterial navigation strategies — •Katja Taute — Rowland Institute at Harvard, Harvard University, Cambridge, MA, USA — Department of Biology, Microbiology, LMU München, 82152 Martinsried, Germany

How microbes navigate environmental chemical gradients has implications that range from health to climate. The behavioral mechanisms underlying chemotaxis are unknown for most species because of a lack of techniques capable of bridging scales from individual navigation behavior to the resulting population-level performance. We present a multiscale 3D chemotaxis assay that combines high-throughput 3D bacterial tracking with microfluidically created chemical gradients. Large datasets of 3D trajectories yield the statistical power required to assess chemotactic performance at the population scale, while simultaneously resolving the underlying 3D navigation behavior for every individual. Applying this technique to the well-studied model bacterium Escherichia coli, we uncover dramatic, previously unknown heterogeneity in chemotactic performance. We investigate the underlying behavioral mechanisms and discuss potential implications at the population level.

Invited Talk DY 26.2 Wed 10:00 ZEU 160

Variability and heterogeneity in natural swarms — •Gil Ariel — Bar Ilan University, Ramat Gan, Israel

Collective motion of large-scale natural swarms, such as moving animal groups or expanding bacterial colonies, have been described as self-organized phenomena. Thus, it is clear that the observed macroscopic, coarse-grained swarm dynamics depend on the properties of the individuals of which it is composed. In nature, individuals are never identical, and may differ in practically every parameter. Hence, intra-group variability and its effect on the ability to form coordinated motion is of interest, both from theoretical and a biological points of view. In this talk, I will review and examine some of the fundamental properties of heterogeneous collectives in nature, with an emphasis on two widely-used model organisms - swarming bacteria and locusts. Theoretical attempts to explain the observed phenomena will be discussed in view of laboratory experiments, highlighting their successes and failures. While heterogeneity typically discourages collectivity, there are several natural examples where it has an opposite effect.

DY 26.3 Wed 10:30 ZEU 160

Effect of individual differences on the jamming transition in traffic flow — •Yi-Chieh Lai and Kuo-An Wu — Department of Physics, National Tsing Hua University, 30013 Hsinchu, Taiwan

The individual difference, particularly in drivers' distance perception, is introduced in the microscopic one-dimensional optimal velocity model to investigate its effect on the onset of the jamming instability seen in traffic systems. We show analytically and numerically that the individual difference helps to inhibit the traffic jam at high vehicle densities while it promotes jamming transition at low vehicle densities. In addition, the jamming mechanism is further investigated by tracking how the spatial disturbance travels through traffics. We find that the jamming instability is uniquely determined by the overall distribution of drivers' distance perception rather than the spatial ordering of vehicles. Finally, a generalized form of the optimal velocity function is considered to show the universality of the effect of the individual difference.

DY 26.4 Wed 10:45 ZEU 160

Distinct impacts of polar and nematic self-propulsion on active unjamming — Varun Venkatesh[1], •Chandana Mondal[2], and Amin Doostmohammadi[1] — [1]Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, 2100 Copenhagen, Denmark — [2]UGC-DAE CSR, University Campus, Khandwa Road, Indore 452017, India

We explore, by MD simulations, the jamming-unjamming transition in a dense system of active semiflexible filaments. In particular, we characterize the distinct impact of polar vs nematic driving for different filament rigidities and at varying densities. Our results show that high densities of dynamic active filaments can be achieved by only changing the nature of the active force, nematic or polar. Interestingly, while polar driving is more effective at unjamming the system at high densities below confluency, we find that at even higher densities, nematic driving enhances unjamming compared to its polar counterpart. The effect of varying the rigidity of filaments is also significantly different in the two cases: While for nematic driving, lowering the bending rigidity unjams the system, we find an intriguing reentrant jamming-unjamming-jamming transition for polar driving as the filament rigidity is lowered. While the first transition (unjamming) is driven by softening due to reduced rigidity, the second transition (jamming) is a cooperative effect of ordering and coincides with the emergence of nematic order in the system. Together, through a generic model of self-propelled flexible filaments, our results demonstrate how tuning the nature of self-propulsion and flexibility can be employed by active materials to achieve high densities without getting jammed.

15 min. break

Invited Talk DY 26.5 Wed 11:15 ZEU 160

Superstatistical Analysis and Modelling of Complex Dynamical Systems — •Claus Metzner[1,2], Christoph Mark[2], Ben Fabry[2], Patrick Krauss[1], Achim Schilling[1], Maximilian Traxdorf[3], and Holger Schulze[1] — [1]Neuroscience Lab, University Hospital Erlangen, Germany — [2]Biophysics Lab, Friedrich-Alexander Universität Erlangen-Nürnberg — [3]Department of Otorhinolaryngology, Head and Neck Surgery, Paracelsus Medical University, Nuremberg, Germany

On longer time scales, complex systems often pass through different dynamical attractors and thus produce 'anomalous' distributions and correlations when analyzed with conventional statistical tools. We argue that the most appropriate way of describing such systems is by hierarchical multilevel models, in which the lowest level is a relatively simple random walk model that can generate the observed time series on short time scales, but which depends on latent hyper-parameters that are themselves time-dependent and controlled by the higher levels of the model. First, our Bayesian method is introduced for the sequen-

tial inference of those gradual or abrupt parameter changes. We then review possible applications of the superstatistical framework in such diverse fields as biophysics, neuroscience, finance, or policy assessment. Finally, we discuss more recent extensions of the method for model selection and the use of machine learning models for estimating complex likelihood functions.

DY 26.6 Wed 11:45 ZEU 160

How to infer parameter distributions in heterogeneous populations of active particles — •Jan Albrecht[1], Robert Grossmann[1], and Manfred Opper[2,3] — [1]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [2]TU Berlin, Fakultät IV-MAR 4-2, Marchstraße 23, 10587 Berlin, Germany — [3]Centre for Systems Modelling and Quantitative Biomedicine, University of Birmingham, B15 2TT, United Kingdom

Experiments with active particles, e.g., motile microorganisms like bacteria or amebae, provide information about their position at discrete points in time. However, most active particle models, like active Ornstein-Uhlenbeck particles for example, are commonly described by first order stochastic differential equations for the velocity or force. This leads to a second order model in position posing challenges for parameter inference, because there is no general way to obtain a closed form expression for the likelihood of the parameters in terms of those time-sampled trajectories. This would be needed to apply efficient Bayesian parameter estimation techniques. In this talk, we propose a filtering-like sequential method to address this problem. The likelihood is first expressed in terms of integrals over transition probabilities. Approximating the transition probability for small times makes these integrals analytically feasible, leading to a likelihood approximation that allows consistent parameter inference. Using a Bayesian approach, we furthermore show how to extend this framework to estimate the entire distribution of motility parameters in heterogeneous populations of particles efficiently.

DY 26.7 Wed 12:00 ZEU 160

Derivation and analysis of a phase field crystal model for a mixture of active and passive particles[⋆] — •Michael te Vrugt[1,2], Max Philipp Holl[1], Aron Koch[1], Raphael Wittkowski[1,2,3], and Uwe Thiele[1,3,4] — [1]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Center for Soft Nanoscience — [3]Center for Nonlinear Science — [4]Center for Multiscale Theory and Computation

We discuss an active phase field crystal (PFC) model that describes a mixture of active and passive particles [1]. First, a microscopic derivation from dynamical density functional theory is presented that includes a systematic treatment of the relevant orientational degrees of freedom. Of particular interest is the construction of the nonlinear and coupling terms. This allows for interesting insights into the microscopic justification of phenomenological constructions used in PFC models, the approximations required for obtaining them, and possible generalizations. Second, the derived model is investigated using linear stability analysis and nonlinear methods. It is found that the model allows for a rich nonlinear behavior with states ranging from steady periodic and localized states to various time-periodic states. The latter include standing, traveling, and modulated waves corresponding to spatially periodic and localized traveling, wiggling, and alternating peak patterns and their combinations.

[1] MtV et al., Modelling Simul. Mater. Sci. Eng. 30, 084001 (2022)

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

DY 26.8 Wed 12:15 ZEU 160

Active Brownian Particles in a disordered motility environment — Gianni Jacucci[1], •Davide Breoni[2], Sandrine Heijnen[3], Hartmut Löwen[2], Giorgio Volpe[3], and Sylvain Gigan[1] — [1]Laboratoire Kastler-Brossel, Paris, France — [2]HHU Universität, Düsseldorf, Germany — [3]University College London, London, United Kingdom

The study of active matter, i.e. matter that consumes energy to perform actions, is fundamental to deepen the knowledge of living systems, as for example bacterial colonies or flocks of birds, and their collective behaviors. Complex environments, like the internal structure of a cell or a blood vessel, are of particular relevance in this field, as they provide a better description of the real-life settings typical of living matter.

In this work we study the effects of a disordered motility field on active Brownian particles, both in experiments and simulations. Experimentally, the motility field is generated by applying a speckle light field to thermophoretic Janus particles, in our case silica colloids half-coated with a carbon layer, suspended in a critical mixture of water and 2,6-lutidine. We focus on the differences between the effects of respectively a homogeneous and a disordered motility field on the dynamics of the particles.

DY 26.9 Wed 12:30 ZEU 160

Characterization of spatial heterogeneities as influencing factors on the dynamics of confluent endothelial cell migration — •Anselm Hohlstamm, Andreas Deussen, Stephan Speier, and Peter Dieterich — Institut für Physiologie, TU Dresden

Confluent endothelial cells are in perpetual movement. Their collective dynamics arises from the interplay of self-propelled motility and various distance-related cell interactions. However, an understanding of collective cell dynamics is complicated by large spatial heterogeneities and local cluster formations. It is the aim of this work to quantify and characterize their influence on the dynamics of cell migration. We used human umbilical vein endothelial cells, which were stained with a fluorescent dye and observed for 48 hours via time-lapse microscopy. With automated image segmentation we could track several 10.000 cells. Cell densities and mean squared velocities showed a heterogeneous spatial distribution with an inverse relation to each other. Higher cell densities also affected the strength of the velocity autocorrelation, whereas correlation times remained mostly stable during experiments. However, cell division increased the mean squared velocity without changing temporal correlations. In parallel, the mean squared displacement characterized regions with short superdiffusive phases in an aging, highly non-stationary system. In addition, local dynamics are coupled by long range spatial correlations. In summary, the dynamics of an entire endothelial layer is influenced by interactions of small heterogenous regions. Next, we will use this approach to compare different endothelial cells.

DY 26.10 Wed 12:45 ZEU 160

Exploiting the unknown - Smart nutrient collection surpassing the run and tumble strategy — •Mahdi Nasiri, Edwin Loran, and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

Throughout evolution, microorganisms have developed efficient strategies for locating nutrients and avoiding toxins in complex environments. Understanding their adaptive policies can provide new key insights for the development of smart artificial active particles. In this talk, we will present a novel method that uses deep reinforcement learning (DRL) to develop smart nutrient collection strategies for chemotactic active particles. Our method is complementary to our previous work which used DRL to explore optimal navigation [1] and is able to devise efficient survival strategies inside unknown and complex environments while only having access to local sensory data. We were also able to extract an interpretable model from the learned strategies which resemble striking similarities with the classical run and tumble motion.

[1] M. Nasiri, B. Liebchen, New J. Phys. 24, 073042 (2022).

DY 27: Statistical Physics: Far From Equilibrium I

Time: Wednesday 9:30–13:00 Location: ZEU 250

Invited Talk DY 27.1 Wed 9:30 ZEU 250

Evolution in changing environments and driven disordered systems — •Joachim Krug, Suman Das, and Muhittin Mungan — Institute for Biological Physics, University of Cologne, Köln, Germany

Biological evolution is governed by the fitness landscape, a map from the genetic sequence of an organism to its fitness. A fitness landscape depends on the organism's environment, and evolution in changing environments is still poorly understood. After introducing the concept of fitness landscapes and their mathematical description, the talk will focus on a particular model of antibiotic resistance evolution in bacteria [1]. Tradeoffs between adaptation to low and high concentration lead to a rugged landscape with an exponentially large number of fitness peaks. With evolutionary dynamics that follow fitness gradients, resistance evolution under slowly changing antibiotic concentration maps to the zero temperature dynamics of a disordered spin system [2]. Specifically, the set of genetic sequences that form a fitness peak at some concentration maps exactly to the metastable states in an equivalent Preisach system, a paradigmatic model of hysteresis in random magnets. Making use of the conceptual tool of state transition graphs developed in the context of driven disordered systems, we quantify the degree of genotypic and phenotypic reversibility in the response of the population to antibiotic concentration cycling.

[1] S.G. Das, S.O.L. Direito, B. Waclaw, R.J. Allen, J. Krug, eLife 9:e55155 (2020)

[2] S.G. Das, J. Krug, M. Mungan, Phys. Rev. X 12:031040 (2022)

DY 27.2 Wed 10:00 ZEU 250

Anomalous relaxation of density waves in a ring-exchange system — •Pranay Patil[1,2], Markus Heyl[1,3], and Fabien Alet[2] — [1]Max-Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Laboratoire de Physique Theorique, Universite de Toulouse, CNRS, UPS, France — [3]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

We present the analysis of the slowing down exhibited by stochastic dynamics of a ring-exchange model on a square lattice, by means of numerical simulations. We find the preservation of coarse-grained memory of initial state of density-wave types for unexpectedly long times. This behavior is inconsistent with the prediction from a low frequency continuum theory developed by assuming a mean field solution. Through a detailed analysis of correlation functions of the dynamically active regions, we exhibit an unconventional transient long ranged structure formation in a direction which is featureless for the initial condition, and argue that its slow melting plays a crucial role in the slowing-down mechanism. We expect our results to be relevant also for the dynamics of quantum ring-exchange dynamics of hard-core bosons.

DY 27.3 Wed 10:15 ZEU 250

Colloidal monolayers: bridging the gap between two and three spatial dimensions — Johannes Bleibel[2], •Alvaro Domínguez[1], and Martin Oettel[2] — [1]Univ. Sevilla, Spain — [2]Univ. Tübingen

It is well established that, unlike for a three-dimensional fluid, particle interactions prevent the hydrodynamic transport coefficients from being defined for a two-dimensional fluid due to the notorious "long-time tail" feature of the velocity autocorrelation.

A colloidal monolayer formed at a fluid interface builds a bridge between these two limiting cases, and it provides insight on the transition from three down to two spatial dimensions: the particle positions are constrained to a plane and the colloid thus resembles a two-dimensional fluid. But the exchange of particle momentum takes place in three-dimensional space through hydrodynamic interactions in the ambient fluid.

Here we study the colloidal diffusivity starting from the Smoluchowski equation. We show that the diffusivity exhibits an intermediate behavior between purely two-dimensional and fully three-dimensional fluid: on the one hand, Fick's law, which pertains to *collective diffusion*, breaks down altogether, as confirmed experimentally. On the other hand, the coefficient of *self-diffusion* is finite, but the transitional nature of the monolayer shows up in a non-analytic dependence on the colloidal packing fraction, at odds with the case of a fully three-dimensional colloid.

DY 27.4 Wed 10:30 ZEU 250

Nonequilibrium mixture dynamics: A model for mobilities and its consequences — Maryam Akaberian, •Filipe Thewes, Peter Sollich, and Matthias Krüger — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany

Extending the famous Model B for the time evolution of a liquid mixture, we develop an approximate approach for the mobility matrix that couples the different mixture components. This approach is based on a single component fluid with particles that are artificially grouped into colors and the relevant parameters can be determined from experiments or numerical simulations. We identify two distinct regimes, corresponding to collective motion and inter-diffusion, respectively, and show how they emerge from the microscopic properties of the fluid. As a test scenario, we study the dynamics after a thermal quench, providing a number insights from a Gaussian theory. Specifically, for systems with two or three components, analytical results for the time evolution of the equal time correlation function compare well to results of Monte Carlo simulations of a lattice gas. A rich behavior is observed, including the possibility of fractionation.

DY 27.5 Wed 10:45 ZEU 250

Dynamical Renormalization Group Theory for Driven Systems — •Nikos Papanikolaou and Thomas Speck — Institute of Theoretical Physics 4, University of Stuttgart, Stuttgart, Germany

Active matter describes nonequilibrium systems that are self-driven due to their microscopic dynamics. These systems pose a fundamental physics challenge by unveiling new phenomena, not present in equilibrium systems, such as the Motility Induced Phase Separation; formation of clusters in the absence of any attractive interactions. To study analytically nonequilibrium complex systems, the Renormalization Group (RG) theory has been successfully used to extract the phase diagram, to study its qualitative behavior, and to explore the critical properties in the different phases. In this project, we explore a variation of RG called Dynamical RG to study self-driven systems by directly applying the RG to dynamical field equations such as the KPZ equation or the Active Model B+ which describe the stochastic evolution of systems like the population of bacteria, interfaces, and neural networks.

DY 27.6 Wed 11:00 ZEU 250

Metastability as a Mechanism for Yielding in Amorphous Solids under Cyclic Shear — •Muhittin Mungan[1] and Srikanth Sastry[2] — [1]Institute of Biological Physics, University of Cologne, Cologne, Germany — [2]Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru, India

We consider the yielding behavior of amorphous solids under cyclic shear deformation and show that it can be mapped into a random walk in a confining potential with an absorbing boundary. The resulting dynamics is governed by the first passage time into the absorbing state and suffices to capture the essential qualitative features recently observed in atomistic simulations of amorphous solids. Our results provide insight into the mechanism underlying yielding and its robustness. When the possibility of activated escape from absorbing states is added, it leads to a unique determination of a threshold energy and yield strain, suggesting thereby an appealing approach to understanding fatigue failure [1].

[1] M. Mungan and S. Sastry, Phys. Rev. Lett. 127 (2021) 248002

15 min. break

DY 27.7 Wed 11:30 ZEU 250

Tunable Brownian magneto heat pump — •Iman Abdoli[1], René Wittmann[2], Joseph Brader[3], Jens-Uwe Sommer[1], Hartmut Löwen[2], and Abhinav Sharma[1] — [1]Leibniz-Institut für Polymerforschung Dresden, 01069 Dresden, Germany — [2]Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany — [3]Université de Fribourg, CH-1700 Fribourg, Switzerland

We propose a mesoscopic Brownian magneto heat pump made of a single charged Brownian particle that is steered by an external magnetic

field. The particle is subjected to two thermal noises from two different heat sources. When confined, the particle performs gyrating motion around a potential energy minimum. We show that such a magneto-gyrator can be operated as both a heat engine and a refrigerator. The maximum power delivered by the engine and the performance of the refrigerator, namely the rate of heat transferred per unit external work, can be tuned and optimised by the applied magnetic field. Further tunability of the key properties of the engine, such as the direction of gyration and the torque exerted by the engine on the confining potential, is obtained by varying the strength and direction of the applied magnetic field. In principle, our predictions can be tested by experiments with colloidal particles and complex plasmas.

DY 27.8 Wed 11:45 ZEU 250

Work fluctuations in the harmonic Active Ornstein-Uhlenbeck particle model — •Giuseppe Gonnella — Università degli Studi di Bari, Bari, Italy — Istituto Nazionale di Fisica Nucleare, sezione di Bari

Over the past few years great interest arose in providing a thermodynamic description of Active Matter Systems and an important emphasis was put on the Active Work study. The distribution of such an observable has been object of recent research[1] as possible singularities signal the occurrence of Dynamical Phase Transitions (DPTs)[2,3], in turn related to peculiar trajectory realisations.

Here we focus on a single harmonically trapped Active Ornstein-Uhlenbeck Particle and provide the analytic expression for the scaled cumulant generating function (SCGF) of the Active Work. Interestingly, we find the SCGF to be non-steep in many physical situations and we provide insight on the effect of relevant system parameters, such as the Peclet number, on the SCGF steepness trough a phase diagram in the system parameter space. Through Legendre-Fenchel transform, the SCGF steepness is shown to lead to singular rate functions with linear tails, and ultimately to the occurrence of DPTs also in this system. We also investigate on the role of initial and final condition in producing the consequent anomalous trajectories.

[1] Semeraro M. et al, J Stat Mech, 2021
[2] Cagnetta F. et al., PRL, 2017
[3] Keta YE. et al., PRE, 2021

DY 27.9 Wed 12:00 ZEU 250

Non-thermal fixed points of universal sine-Gordon coarsening dynamics — Philipp Heinen[1], Aleksandr N. Mikheev[1,2], Christian-Marcel Schmied[1], and •Thomas Gasenzer[1,2] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg — [2]Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 16, 69120 Heidelberg

We examine coarsening of field-excitation patterns of the sine-Gordon (SG) model, in two and three spatial dimensions, identifying it as universal dynamics near non-thermal fixed points. The focus is set on the non-relativistic limit, governed by a Schrödinger-type equation with Bessel-function nonlinearity. The results of our classical statistical simulations suggest that, in contrast to wave turbulent cascades, in which the transport is local in momentum space, the coarsening is dominated by rather non-local processes corresponding to a spatial containment in position space. The scaling analysis of a kinetic equation obtained with path-integral techniques corroborates this numerical observation and suggests that the non-locality is directly related to the slowness of the scaling in space and time. Our methods, which we expect to be applicable to more general types of models, could open a long-sought path to analytically describing universality classes behind domain coarsening and phase-ordering kinetics from first principles, which are usually modelled in a near-equilibrium setting by a phenomenological diffusion-type equation in combination with conservation laws.

DY 27.10 Wed 12:15 ZEU 250

Nonequilibrium probability currents in optically-driven colloidal suspensions — •Samudrajit Thapa[1,2], Daniel Zaretzky[3], Grzegorz Gradziuk[4], Chase Broedersz[4,5], Yair Shokef[1,2,6], and Yael Roichman[3,6,7] — [1]School of Mechanical Engineering, Tel Aviv University, Tel Aviv 69978, Israel — [2]Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv 69978, Israel — [3]School of Chemistry, Tel Aviv University, Tel Aviv 69978, Israel — [4]Arnold Sommerfeld Center for Theoretical Physics, Ludwig Maximilians Universitaet Muenchen, Theresienstr. 37, 80333 Munich, Germany — [5]Department of Physics and Astronomy, Vrije Universiteit Amsterdam, 1081 HV Amsterdam, The Netherlands — [6]Center for the Physics and Chemistry of Living Systems, Tel Aviv University, 69978, Tel Aviv, Israel — [7]School of Physics & Astronomy, Tel Aviv University, Tel Aviv 69978, Israel

In the absence of visible currents and prior knowledge, it is often hard to recognize athermal fluctuations. Probability currents provide such a measure in terms of the rate at which they enclose area in phase space. We measure this area enclosing rate for trapped colloidal particles, where only one particle is driven, and they interact hydrodynamically. By combining experiment, theory and simulation, we identify an optimal measurement protocol in terms of the relations between the different time scales in the system. Furthermore, we find that hydrodynamic interactions render the effect of athermal agitation more local than that of elastic interactions. This may have significant implications for the interpretation of fluctuations in biological systems.

DY 27.11 Wed 12:30 ZEU 250

A nonlinear fluctuation-dissipation theorem for Markovian systems — •Benjamin Lindner[1,2], Kirsten Engbring[2], Dima Boriskovsky[3], and Yael Roichman[3] — [1]Bernstein Center for Computational Neuroscience Berlin, Philippstr.\ 13, Haus 2, 10115 Berlin, Germany — [2]Physics Department of Humboldt University Berlin, Newtonstr.\ 15, 12489 Berlin, Germany — [3]The Raymond and Beverley School of Physics \& Astronomy and The Raymond and Beverley School of Chemistry, Tel Aviv University, Tel Aviv 6997801, Israel

Fluctuation-Dissipation-Theorems (FDT) connect the internal spontaneous fluctuations of a system with its response to an external perturbation. In this work we propose a new nonlinear fluctuation-dissipation theorem as a test for Markovianity. Previously suggested FDTs are based on linear response and require a significant amount of measurements. However, the nonlinear relation holds for systems out of equilibrium, and for strong perturbations requiring significantly less data than the standard linear relation. We verify the nonlinear theorem for two theoretical model systems: a Brownian particle in a tilted periodic potential, and a harmonically bound particle. In addition, we apply our formalism and test for Markovianity in an inherently out of equilibrium experimental system, based on self-propelled agents.

DY 27.12 Wed 12:45 ZEU 250

Heat capacity for a driven array of semiclassical dots — •Pritha Dolai and Christian Maes — Instituut voor Theoretische Fysica, KU Leuven, Belgium

We analyze thermal properties for particle transport along an array of two-level systems. More specifically, we obtain analytic and numerical results for the heat capacity of a system of particles subject to mutual exclusion and to birth and death, driven around a ring by an external field. We find a zero-temperature phase transition as a function of the chemical potential of the environment, as shown by the divergence of the heat capacity at zero temperature. The non-vanishing of the heat capacity at absolute zero, violating the extended Third Law, is caused by a localization and corresponding delay in relaxation of excess heat. We also derive a regime of negative heat capacity indicating an anticorrelation between the temperature-dependence of the stationary occupation and the excess heat.

DY 28: Focus Session: Critical Transitions in Society, Economy, and Nature (joint session SOE/DY)

Organizers: Fakhteh Ghanbarnejad (Robert Koch-Institut), Diego Rybski (Potsdam Institute for Climate Impact Research)

Time: Wednesday 9:30–11:45 Location: ZEU 260

Topical Talk DY 28.1 Wed 9:30 ZEU 260

Many universality classes in an interface model restricted to non-negative heights — •Peter Grassberger[1], Deepak Dhar[2], and Pradeep Mohanty[3] — [1]JSC, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Indian Institute of Science Education and Research, Pune, 411 008, India — [3]Indian Institute of Science Education and Research - Kolkata Mohanpur, 741 246, India

We present a simple 1-d stochastic model with two control parameters and a rich zoo of phase transitions. At each (discrete) site x and time t, there is an integer $n(x,t)$ that satisfies a linear interface equation with added random noise. Depending on the control parameters, this noise may or may not satisfy detailed balance, so that the model is – for suitable initial conditions – in the Edwards-Wilkinson (EW) or in the Kardar-Parisi-Zhang (KPZ) universality class. But in contrast to these, there is also a constraint $n(x,t) \geq 0$. Points x where $n > 0$ on one side and $n = 0$ on the other are called "fronts". These fronts can be "pushed" or "pulled", depending on the control parameters. For pulled fronts, the lateral spreading is in the directed percolation (DP) universality class, while it is of a novel type for pushed fronts, with yet another novel behavior in between. In the DP case, the activity at each active site can in general be arbitrarily large, in contrast to previous realizations of DP. Finally, we find two different types of transitions when the interface detaches from the line $n = 0$ (with $\langle n(x,t)\rangle \to const$ on one side, and $\to \infty$ on the other), again with new universality classes. We also discuss a mapping of this model onto a directed Oslo rice pile model in specially prepared backgrounds.

Topical Talk DY 28.2 Wed 10:00 ZEU 260

Nonequilibrium phase transitions and critical behavior in networks — •Eckehard Schöll — Institut für Theoretische Physik, TU Berlin — Potsdam Institute for Climate Impact Research — Bernstein Center for Computational Neuroscience Berlin

Phase transitions in nonlinear dynamical systems far from thermodynamic equilibrium have been investigated since the 1970s and 1980s, and concepts from thermodynamics and statistical physics have been applied to describe self-organization, spatio-temporal pattern formation, phase coexistence, critical phenomena, and first and second order nonequilibrium phase transitions. Much more recently, phase transitions and critical phenomena have been studied in dynamical networks, where synchronization transitions may arise, giving birth to a plethora of partial synchronization patterns and complex collective behavior, with applications to many natural, socioeconomic, and technological systems. We review these developments, and draw some connections of tipping transitions, explosive synchronization, nucleation, critical slowing down, critical exponents, etc. with nonequilibrium thermodynamics. [1] Tumash, L., Olmi, S. and Schöll, E., Effect of disorder and noise in shaping the dynamics of power grids, Europhys. Lett. 123, 20001 (2018). [2] Berner, R., Sawicki, J., Thiele, M., Löser, T. and Schöll, E., Critical parameters in dynamic network modeling of sepsis, Front. Netw. Physiol. 2, 904480 (2022). [3] Fialkowski, J., Yanchuk, S., Sokolov, I. M. , Schöll, E., Gottwald, G. A. and Berner, R., Heterogeneous nucleation in finite size adaptive dynamical networks, arXiv:2207.02939 (2022).

15 min. break

Topical Talk DY 28.3 Wed 10:45 ZEU 260

Critical transition to monsoon: statistical physics principles of monsoon forecasting — •Elena Surovyatkina — Potsdam Institute for Climate Impact Research (PIK), Potsdam, Germany — Space Research Institute of the Russian Academy of Sciences (IKI), Moscow, Russia

Numerical weather models are limited to forecasting the weather for up to 5 days in the future. A fundamental problem lies in the chaotic nature of the spatial differential equations used to simulate the atmosphere. The limitations of current prediction models prevent further progress.

I present a recently developed approach fundamentally different from the numerical weather and climate models. It is based on statistical physics principles and recently discovered spatial-temporal regularities (or teleconnections between Tipping Elements) in a monsoon system.

First, I begin with evidence in observational data that the transition from pre-monsoon to monsoon is a critical transition. Second, I show how to detect the Tipping elements in the spatial organization of monsoon using the phenomenon of critical growth of fluctuations. Third, I explain how the regularities between the Tipping Elements allow predicting the upcoming monsoon onset and withdrawal for 40 and 70 days in advance, respectively.

Furthermore, I present the results of retrospective tests from 1951 to 2015, which show 73 % success for monsoon onset and 84 % for a withdrawal date. Remarkably, that forecasts of future monsoons showed to be successful already seven years in a row, 2016-2022.

DY 28.4 Wed 11:15 ZEU 260

Synchronization-desynchronization transitions in neural networks — •Anna Zakharova — BCCN Berlin, Germany

Synchronization of neurons is believed to play a crucial role in the brain under normal conditions, for instance, in the context of cognition and learning, and under pathological conditions such as Parkinson's disease or epileptic seizures. In the latter case, when synchronization represents an undesired state, understanding the mechanisms of desynchronization is of particular importance. In other words, the possible transitions from synchronized to desynchronized regimes and vice versa should be investigated. It is known that such dynamical transitions involve the formation of partial synchronization patterns, where only one part of the network is synchronized. The most prominent example is given by chimera states [1]. In the present talk, we discuss an alternative scenario. We show how the so-called solitary states in networks of coupled FitzHugh-Nagumo neurons can lead to the emergence of chimera states. By performing bifurcation analysis of a suitable reduced system in the thermodynamic limit we demonstrate how solitary states, after emerging from the synchronous state, become chaotic in a classical period-doubling cascade [2].

[1] A. Zakharova, Chimera Patterns in Networks: Interplay between Dynamics, Structure, Noise, and Delay, Understanding Complex Systems (Springer, Cham, 2020) doi: 10.1007/978-3-030-21714-3

[2] L. Schülen, A. Gerdes, M. Wolfrum, A. Zakharova, Solitary routes to chimera states, Phys. Rev. E Letter 106, L042203 (2022) doi: 10.1103/physreve.106.l042203

DY 28.5 Wed 11:30 ZEU 260

The war in Ukraine, a statistical analysis — •Juergen Mimkes — Physics Department, Paderborn University

War is a serious disruption of normal social order and may be analyzed by statistics. In homogeneous systems the Lagrange function depends on two Lagrange factors: L (λ, p). In physics, they are mean energy or temperature (λ) and pressure (p). In politics, they are mean capital or standard of living (λ) and military pressure (p). The factors (λ),(p) determine the state or phases of a system. In materials we have solid, liquid, gas, in politics autocratic, democratic, global. Different phases can only coexist at equilibrium in the phase diagram. Outside of equilibrium water and ice cannot coexist in close contact, water is melting ice (climate crisis). Outside of equilibrium democracy and autocracy cannot coexist in close contact, democracy is *melting* autocracy since the Marshall plan in 1947. Accordingly, there has been an aggressive reaction by the autocracy: DDR 1953, Hungary 1956, CSR 1968, Ukraine 2014. There is no chance for peace, unless one party vanishes. The only solution to keep hot and cold together is a thermos, and to keep democracy and autocracy side by side is a new iron curtain like in Korea or Europe (1961 to 1989).

DY 29: Wetting, Droplets and Microfluidics (joint session DY/CPP)

Time: Wednesday 10:00–13:00 Location: ZEU 147

DY 29.1 Wed 10:00 ZEU 147

Crises and chaotic scattering in hydrodynamic pilot-wave experiments — George Choueiri[1,2], Balachandra Suri[1,3], Jack Merrin[1], Maksym Serbyn[1], Björn Hof[1], and •Nazmi Burak Budanur[1,4] — [1]Institute of Science and Technology Austria, 3400 Klosterneuburg, Austria — [2]MIME Department, University of Toledo, Toledo, Ohio 43606, USA — [3]Department of Mechanical Engineering, Indian Institute of Science, Bengaluru 560012, India — [4]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Theoretical foundations of chaos have been predominantly laid out for finite-dimensional dynamical systems, such as the three-body problem in classical mechanics and the Lorenz model in dissipative systems. In contrast, many real-world chaotic phenomena, e.g., weather, arise in systems with many (formally infinite) degrees of freedom, which limits direct quantitative analysis of such systems using chaos theory. In the present work, we demonstrate that the hydrodynamic pilot-wave systems offer a bridge between low- and high-dimensional chaotic phenomena by allowing for a systematic study of how the former connects to the latter. Specifically, we present experimental results, which show the formation of low-dimensional chaotic attractors upon destabilization of regular dynamics and a final transition to high-dimensional chaos via the merging of distinct chaotic regions through a crisis bifurcation. Moreover, we show that the post-crisis dynamics of the system can be rationalized as consecutive scatterings from the nonattracting chaotic sets with lifetimes following exponential distributions.

DY 29.2 Wed 10:15 ZEU 147

Chemically Active Wetting — •Susanne Liese[1], Xueping Zhao[2], Frank Jülicher[3], and Christoph Weber[1] — [1]Universität Augsburg, Augsburg, Germany — [2]Xiamen University, Xiamen, China — [3]MPI/PKS, Dresden, Germany

In living cells, wetting of condensed phases on membrane surfaces provides a mechanism for positioning biomolecules. Biomolecules are also able to bind to such membrane surfaces. In living cells, this binding is often chemically active as it is kept out of equilibrium by the supply of energy and matter. Here, we investigate how active binding on membranes affects the wetting of condensates. To this end, we derive the non-equilibrium thermodynamic theory of active wetting. We find that active binding significantly alters the wetting behavior leading to non-equilibrium steady states with condensate shapes reminiscent of a fried egg or a mushroom. We further show that such condensate shapes are determined by the strength of active binding in the dense and dilute phases, respectively. Strikingly, such condensate shapes can be explained by an electrostatic analogy where binding sinks and sources correspond to electrostatic dipoles along the triple line. Through this analogy, we can understand how fluxes at the triple line control the three-dimensional shape of condensates.

DY 29.3 Wed 10:30 ZEU 147

Stimuli-responsive high aspect ratio surfaces for wetting studies — •Gissela Constante[1], Indra Apsite[1], Paul Auerbach[2], Sebastian Aland[2], Dennis Schönfeld[3], Thorsten Pretsch[3], Pavel Milkin[1], and Leonid Ionov[1,4] — [1]Uni Bayreuth, Bayreuth, Germany — [2]HTW Dresden, Dresden, Germany — [3]Fraunhofer IAP, Postdam, Germany — [4]Bavarian Polymer Institute, Bayreuth, Germany

The fabrication of switchable surfaces has been of interest in different fields such as biotechnology, industry, robotics, and others. The fabrication of these shape-changing bioinspired surfaces is a challenge due to the limited availability of materials and methods. In this research, an exceptional high aspect ratio lamellar surface topography was fabricated by melt-electrowriting of microfibers of a shape-memory thermo-responsive polyurethane. Two different types of stimuli: temperature and light exposition were applied to modify the mechanical properties and by it the deformation and recovery of the original surface. Wetting studies showed that the deformation of the high aspect ratio lamellar surface can be tunned not only manually, but as well by a liquid droplet. This behavior is controlled by variation of temperature conducted by direct heating/cooling or by exposure to light when the lamellae were stained with black ink. The liquid in combination with thermo-responsive topography presents a new type of wetting behavior. This feature opens the possibility to apply such topographies for the design of smart elements for microfluidic devices, for example, smart valves.

DY 29.4 Wed 10:45 ZEU 147

A Study about Shock-Induced Spallation in Mono- and Nanocrystalline High-Entropy Alloys — •Daniel Thürmer[1], Nina Merkert née Gunkelmann[1], Shiteng Zhao[2], Orlando Deluigi[3], Camelia Stan[4], Iyad Alhafez[5], Herbert Urbassek[5], Marc Meyers[6], and Eduardo Bringa[3,7] — [1]Institute of Applied Mechanics, Clausthal University of Applied Technology, Arnold-Sommerfeld-Stra*e, D-38678 Clausthal-Zellerfeld, Germany — [2]School of Material Science and Engineering, Beihang University, 37 Xueyuan Rd, Haidian District, Beijing, China, 100191 — [3]CONICET and Faculty of Engineering, University of Mendoza, Mendoza, 5500, Argentina — [4]Advanced Light Source Facility, Lawrence Berkeley National Laboratory, One Cyclotron Road, Berkeley, CA 94720, United States — [5]Physics Department and Research Center OPTIMAS, University Kaiserslautern, Erwin-Schr*odinger-Stra*e, D-67663 Kaiserslautern, Germany — [6]Mechanical and Aerospace Department, Univ. of California San Diego, La Jolla, CA 92093, United States — [7]Centro de Nanotecnología Aplicada, Universidad Mayor, Santiago, Chile

High-entropy alloys are highly attractive for future applications in the technical field thanks to their incredible potential regarding mechanical properties. Although they are increasingly sparking interest for future usage, their general understanding is not yet complete. To further understand high-entropy alloys and their capabilites, we studied the influence of shock-induced spallation on mono- and nanocrystalline high-entropy alloys with varying grain sizes.

DY 29.5 Wed 11:00 ZEU 147

Instability of Active Fluid Interfaces in Microfluidics — •Kuntal Patel and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

In recent years, microfluidic lab-on-a-chip devices have emerged as efficient miniaturized flow control platforms. Specifically, the advent of nonlinear microfluidics has opened a new avenue for chemical and biomedical applications such as droplet formation and cell sorting. In this work, we integrate ideas from active matter into a microfluidic setting and try to understand the mechanism and practical relevance of resulting microfluidic flows.

The present setup consists of two vertically stacked fluid layers with identical densities but different viscosities, sandwiched between the walls of a microfluidic channel. The interface separating both fluids is initialized with uniformly distributed active particles, which induce force dipoles that generate flows in the adjacent fluids.

Our hybrid lattice-Boltzmann finite-difference simulations reveal that when we perturb the fluid interface covered with extensile force dipoles $\updownarrow$, it eventually returns to its flat state irrespective of the strength of interfacial tension. In contrast, contractile force dipoles $\downarrow\uparrow$ lead to activity-driven interfacial instability. However, such instability emerges only above a critical value of the activity, which is proportional to the interfacial tension. We further examine the mechanism of instability and quantify the effect of viscosity contrast and perturbation wavelength. Lastly, we demonstrate the systematic formation of droplets using the present interfacial instability.

DY 29.6 Wed 11:15 ZEU 147

Optically controlled micro-transport with reduced heating impact — •Antonio Minopoli, Elena Erben, Susan Wagner, and Moritz Kreysing — Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Recently it was demonstrated that thermoviscous flows can be used to move the cytoplasm of cells and developing embryos. These laser-induced intracellular flows (aka FLUCS), reach velocities comparable with those occurring during early stages of embryogenesis. As a side effect, the laser scanning may also cause temperature gradients across the sample (1-3 Kelvins) that could give rise to out-of-equilibrium phenomena. Here, we demonstrate that exploiting symmetry relations during the laser scan, we disentangle heating and flows. Specifically, since the flow speeds depend on the repetition frequency rather than on the beam velocity, it is possible to accelerate the scanning of the

primary scan pattern, effectively compressing the scan signal to occupy only a fraction of the original period, and allowing to complement the flow stimuli by flow-invariant heat stimuli. We introduce strategies to complement even complex primary scan patterns by secondary heating stimuli thereby yielding a near isothermal temperature distribution and still generating significant net flows. As we experimentally show, the resulting temperature distributions are near homogenous across the sample (standard deviations 5-10 times lower than those measured with standard FLUCS) and can therefore be better compensated for by ambient cooling. In the next future, ISO-FLUCS may become the new standard for optofluidic manipulations within biological systems.

15 min. break

DY 29.7 Wed 11:45 ZEU 147

3D passive non-mechanical microfluidic valves fabricated using grayscale lithography — •Sebastian Bohm[1,3], Hai Binh Phi[2,3], Erich Runge[1], Lars Dittrich[3], and Steffen Strehle[2] — [1]TU Ilmenau, FG Theoretische Physik I — [2]TU Ilmenau, FG Mikrosystemtechnik — [3]5microns GmbH, 98693 Ilmenau

Passive non-mechanical valves represent a promising method for rectifying flows in micro- or nanofluidic systems [1]. They are very robust due to the absence of mechanical parts, easy to fabricate, and allow the implementation of efficient microfluidic systems such as micropumps [2,3]. However, with existing methods, the fabrication of fully three dimensional (3D) structured geometries is very hard to achieve. Here, a new and easy to implement method for the fabrication of three-dimensional valves is presented: Grayscale lithography followed by a proportional transfer with reactive ion etching is utilized to create 3D diffuser valves in silicon and glass substrates. We show that higher diodicities were achieved with 3D diffuser valves compared to conventional diffuser valves. These experimental findings correspond fit very well to the predictions of our numerical simulations. In combination with highly efficient optimization methods for two-dimensional Tesla valves, the fabrication of even more efficient 3D Tesla valves is hence now within reach.

[1] Bohm, S. et al.; npg Microsystems & Nanoengineering (8), 97 (2022)
[2] Bohm, S. et al.; COMSOL Conference 2020 Europe, 14-15. Oct. 2020 online
[3] Hoffmann, M. et al.; German patent DE112011104467 (2017)

DY 29.8 Wed 12:00 ZEU 147

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

Coalescence of droplets is ubiquitous in nature and modern technology. Various experimental and theoretical studies explored droplet dynamics in three dimensions (3D) and on two-dimensional (2D) solid or liquid substrates, e.g. [1-4]. Here, we demonstrate coalescence experiments of isotropic and nematic droplets in quasi-2D liquids, viz. overheated smectic A freely suspended films. We investigated their dynamics experimentally and measured the shape deformation during the entire merging process using high-speed imaging and interferometry. This system is a unique example where the lubrication approximation can be directly applied, and the smectic membrane plays the role of a precursor film. Our studies reveal the scaling laws of the coalescence time depending on the droplet size and the material parameters. We also compared the dynamics of isotropic and nematic droplets and additionally analyzed the results based on an existing model for liquid lens coalescence on liquid and solid surfaces [4].

This study was supported by DLR with project 50WM2054 and by DFG with project STA 425/40.

References:
[1] J. D. Paulsen et al., Nat. Commun., 5, 3182 (2014) [2] D. G. A. L. Aarts et al., Phys. Rev. Lett., 95, 164503 (2005). [3] M. A. Hack et al., Phys. Rev. Lett. 124, 194502 [4] N. S. Shuravin et al., Phys. Rev. E, 99, 062702 (2019) [5] C. Klopp et al., Langmuir, 36, 10615 (2020)

DY 29.9 Wed 12:15 ZEU 147

effect of deposition method on the static contact angle of nanodroplets measured by AFM — •mohammadali hormozi and regine von klitzing — soft matter at interface, tu darmstadt, darmstadt, Germany

The wetting properties of substrates are often described by the static contact angle of a particular liquid. The contact angle depends on many parameters like substrate chemistry, liquid properties, and environment condition. In this study, we show that the method of depositing the liquid phase on the solid phase can play an important role for the static contact angle. For this purpose, microscale droplets of non-volatile liquids including Polyethylene Glycol (PEG200) and Squalane are deposited on the silanized substrate using four different methods. These methods are either based on nucleation (condensation and solvent exchange) or printing (inkjet and microcontact printing) of droplets. The contact angle of the microdroplets is scanned with an AFM and allows detailed analysis of the three phase contact line on a nm scale. The final static contact angle of the microdroplets is compared with the macroscopic contact angle determined by optical methods. Droplets formed via nucleation show smaller contact angle than printed ones. The latter ones were closer to the macroscopic contact angle. We will discuss this phenomenon.

DY 29.10 Wed 12:30 ZEU 147

Fingering contact propagation between a droplet and a thin liquid film — •Kirsten Harth — Fachbereich Technik, TH Brandenburg — MRTM und MARS, Otto von Guericke Universität Magdeburg

When impacting droplets approach a hard plane substrate slowly, so that the Weber number is below approximately 5, a contact-less rebound will occur due to the entrainment of ambient gas. On slightly deformable and smooth spin-coated liquid films upon a rigid solid, this effect is more robust and may occur until slightly higher Weber numbers. Deformation of the thin film is usually ignored while it is proven to be present. The deformation amplitude depends on the impact dynamics as well as the thickness and viscosity of the surficial oil layer. At slightly higher impact velocities, i.e. slightly higher Weber numbers, delayed contact formation between the film liquid and the droplet occurs. Depending on the layer properties, interestingly, the contact line may be unstable displaying a fingering texture. Instability occurs independently of whether the drop and film liquid differ or not. We present and analyze this phenomenon.

DY 29.11 Wed 12:45 ZEU 147

Universality in One-Dimensional Breath Figures — •Daniel Dernbach, Adrian Häussler-Möhring, M Muhammad, and Jürgen Vollmer — Institut für Theoretische Physik, Universität Leipzig, Brüderstr. 16, D-04103 Leipzig, Germany

Patterns of droplets which condense upon substrates reveal self-similar features. They are described by a scaling theory with a non-trivial exponent that has been related to the fractal dimension of the scaling of the free area ("porosity") in between droplets. There is no agreement if this exponent is universal or affected by the dynamics. Here, we present numerical data that address the dependence of the asymptotic scaling of the porosity for hyper-spherical droplets growing on one-dimensional substrates. We vary the droplet dimension and interactions. For a given dimension the exponent is universal up to a critical range of interaction. For longer-ranged interactions the scaling depends on the dynamics.

DY 30: Nonequilibrium Quantum Many-Body Systems II (joint session TT/DY)

Time: Wednesday 15:00–18:30 Location: HSZ 204

DY 30.1 Wed 15:00 HSZ 204

Hilbert space fragmentation in open quantum systems — •Yahui Li, Pablo Sala, and Frank Pollmann — Department of Physics, TFK, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany

Several mechanisms have been identified that can lead to a breakdown of thermalization in closed quantum systems-including integrability and many-body localization. Recently, a novel mechanism for ergodicity breaking has been discovered in systems with certain dynamical constraints, where the Hilbert space fragments into exponentially many disconnected subspaces. An open question is how such systems evolve when they are coupled to a dissipative bath.

We find that the Hilbert space fragmentation can be utilized to preserve coherence in the presence of dissipation. We study a quantum fragmented model, which fragments in an entangled basis due to unconventional non-Abelian symmetries. We investigate the Lindblad dynamics under two different couplings, which either preserves or destroys the quantum fragmentation structure. At sufficiently large couplings, the operator space entanglement is suppressed, which allows for an efficient numerical simulation using tensor networks. Surprisingly, under the structure-preserving noise, we observe finite Renyi negativity, indicating non-vanishing quantum correlations. Using an analytic approach, we derive the stationary states under both couplings, which explains the long-time behaviors observed in numerical simulations.

DY 30.2 Wed 15:15 HSZ 204

Hilbert space fragmentation and interaction-induced localization in the extended Fermi-Hubbard model — •Philipp Frey, Lucas Hackl, and Stephan Rachel — University of Melbourne

We study Hilbert space fragmentation in the extended Fermi-Hubbard model with nearest and next-nearest neighbor interactions. Using a generalized spin/mover picture and saddle point methods, we derive lower bounds for the scaling of the number of frozen states and for the size of the largest block preserved under the dynamics. We find fragmentation for strong nearest and next-nearest neighbor repulsions as well as for the combined case. Our results suggest that the involvement of next-nearest neighbor repulsions leads to an increased tendency for localization. We then model the dynamics for larger systems using Markov simulations to test these findings and unveil in which interaction regimes the dynamics becomes spatially localized. In particular, we show that for strong nearest and next-nearest neighbor interactions random initial states will localize provided that the density of initial movers is sufficiently low.

[1] arXiv:2209.11777 (accepted for publication in PRB Letter)

DY 30.3 Wed 15:30 HSZ 204

Rate functions and the approach to adiabaticity in quantum many body systems — •Vibhu Mishra, Salvatore Manmana, and Stefan Kehrein — Institute for Theoretical Physics, Georg-August-Universität Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen

The quantum adiabatic theorem is a fundamental result in quantum mechanics with applications ranging from quantum adiabatic computation to topological systems, while also serving as a theoretical foundation to many body perturbation theory via the Gell-Mann Low theorem.

We establish an inherent competition between ramp times T for an adiabatic process vs the system size N, in the behavior of relevant many body overlaps. We study this interplay between T and N by analyzing the properties of rate functions which are defined to be intensive quantities that give us a quantitative measure of the deviation from adiabaticity in the thermodynamic limit.

We analyze the Transverse Field Ising Model and the XXZ chain in $1D$ using exact diagonalization. We find that the rate functions show algebraic decay with increasing ramp time T. The decay exponent of the rate function for ramps within the gapped phase is 2, for ramps across Ising critical point it is 0.5 and within the Luttinger Liquid phase it is 1. The immediate implication is that the many body adiabatic time scales grow unavoidably with system size, namely as the $\sqrt{N}$ for ramps within the gapped phase, and with N within the Luttinger Liquid phase.

DY 30.4 Wed 15:45 HSZ 204

Classical route to ergodicity and scarring phenomena in a two-component Bose-Josephson junction — Debabrata Mondal[1], Sudip Sinha[1], •Sayak Ray[2], Johann Kroha[2], and Subhasis Sinha[1] — [1]Indian Institute of Science Education and Research Kolkata, Mohanpur, Nadia 741246, India — [2]Physikalisches Institut, Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 12, 53115 Bonn, Germany

We consider a Bose-Josephson junction (BJJ) formed by the binary mixture of ultracold atoms to investigate the manifestation of coherent collective dynamics on ergodicity and quantum scars, unfolding the connection between them. By tuning the inter and intra-species interaction, we demonstrate a rich variety of Josephson dynamics and transitions between them, which plays a crucial role in controlling the overall ergodic behaviour. The signature of underlying classicality is revealed from the entanglement spectrum, which also elucidates the formation of quantum scars of unstable steady states and of periodic orbits leading to athermal behaviour in a reduced Hilbert space. We show how the degree of ergodicity across the energy band and the scarring phenomena can be probed from the auto-correlation function as well from the phase fluctuation of the condensates, which has relevance in cold atom experiments. The model can also be realized in spin systems with application to information processing and lattice-gauge simulation.

[1] D. Mondal, S. Sinha, S. Ray, J. Kroha, and S. Sinha, Phys. Rev. A **106**, 043321 (2022)

DY 30.5 Wed 16:00 HSZ 204

Ultrafast dynamics of cold Fermi gas after a local quench — Nikolay Gnezdilov[1], •Andrei Pavlov[2,3], Vladimir Ohanesjan[4], Yevheniia Cheipesh[4], and Koenraad Schalm[4] — [1]Department of Physics, University of Florida, Gainesville, USA — [2]The Abdus Salam International Centre for Theoretical Physics (ICTP) Strada Costiera 11, Trieste, Italy — [3]Institut für QuantenMaterialien und Technologien, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen, Germany — [4]Instituut-Lorentz, Universiteit Leiden, Leiden, The Netherlands

We consider energy dynamics of two initially independent reservoirs A and B filled with a cold Fermi gas coupled and decoupled by two quantum quenches following one another. The energy change in the system adds up the heat transferred between A and B and the work done by the quench to uncouple the reservoirs. In case when A and B interact for a short time, we find an energy increase in both reservoirs upon decoupling. This energy gain results from the quenches' work and does not depend on the initial temperature imbalance between the reservoirs. We relate the quenches' work to the mutual correlations of A and B expressed through their von Neumann entropies. Utilizing this relation, we show that once A and B become coupled, their von Neumann entropies grow (on a timescale of the Fermi time) faster than thermal transport within the system. For a metallic setup, this implies the characteristic timescale of correlations' growth to be in the femtosecond range, while for the ultracold atoms, we expect it to be in the millisecond range.

DY 30.6 Wed 16:15 HSZ 204

A conjecture regarding the overlap of different ground states within the same phase — •Sarah Damerow and Stefan Kehrein — Georg-August Universität Göttingen

An extension of the adiabatic theorem to quantum quenches, i.e. non-adiabatic changes, is presented. Using exact diagonalisation, we numerically study the Transverse Field Ising Model (TFIM) and the Axial Next Nearest Neighbour Ising Model (ANNNI). We numerically test the following conjecture: Within the same phase, the overlap between the initial ground state and the ground state of the quenched Hamiltonian is the largest possible eigenstate overlap. In the TFIM, this conjecture is confirmed for both the paramagnetic (PM) and the ferromagnetic (FM) phases. In the ANNNI model results are ambiguous in some phases, due to both numerical errors and finite size effects.

15 min. break

DY 30.7 Wed 16:45 HSZ 204

Charge, spin, and heat shot noises in the absence of average currents — •Ludovico Tesser, Matteo Acciai, Christian Spånslätt, Juliette Monsel, and Janine Splettstoesser — Chalmers University of Technology, Gothenburg, Sweden

Shot noise in electronic conductors occurs when the system is brought out of equilibrium, e.g., by a stationary bias. However, nonequilibrium does not imply that an average current flows. Indeed, the situation where selected currents are suppressed is of interest in fields like thermoelectrics and spintronics, raising the question of how the related noises behave.

I will present results on zero-current charge, spin, and heat noises in two-terminal mesoscopic conductors induced by voltage, spin and temperature biases. The nonequilibrium shot noises can be arbitrarily large, even if the respective average currents vanish. However, as soon as a temperature bias is present, additional equilibrium (thermal-like) noise necessarily occurs. This equilibrium noise sets an upper bound on the zero-current nonequilibrium charge and spin shot noise [1,2]. We have shown that the bound on the charge noise for strictly two-terminal conductors even extends into the finite-frequency regime. By contrast, these bounds can be overcome for heat transport by breaking the spin and electron-hole symmetries, respectively.

[1] J. Eriksson, M. Acciai, L. Tesser, J. Splettstoesser, Phys. Rev. Lett. 127, 136801 (2021)
[2] L. Tesser, M. Acciai, C. Spånslätt, J. Monsel, J. Splettstoesser, arXiv:2210.06051 [cond-mat.mes-hall] (2022)

DY 30.8 Wed 17:00 HSZ 204

Maximally chaotic to Fermi liquid crossover in a generalized SYK model — •Nick von Selzam and Stefan Kehrein — Institute for Theoretical Physics, University of Göttingen, Germany

We consider a generalized Sachdev-Ye-Kitaev (SYK) model: Majorana fermions on $\mathcal{N}$ sites with random $\frac{q}{2}$-body all to all interactions plus a kinetic energy term.

The SYK model can be seen as a toy model for quantum chaos and does not allow for a quasiparticle description. We discuss the continuous crossover between the Fermi liquid regime, dominated by the kinetic term, and the maximally chaotic regime, dominated by the SYK interaction, by studying the quantum Lyapunov exponents.

For fixed interaction strength there exists a crossover temperature for which the Lyapunov exponent becomes maximal. For lower temperatures the Lyapunov exponent is exponentially small. For larger temperatures the behaviour is close to indistinguishable from the pure SYK term.

DY 30.9 Wed 17:15 HSZ 204

Vibrationally-coupled electron transport in a quantum shuttle: A study using the hierarchical equations of motion approach — •Salvatore Gatto, Christoph Kaspar, and Michael Thoss — Institute of Physics, Albert-Ludwigs-Universität Freiburg

A quantum shuttle is an archetypical nanoelectromechanical device, in which the coupling of electronic and mechanical degrees of freedom is crucial [1]. In this contribution, we investigate transport properties of quantum shuttles, with a particular focus to the so-called shuttling regime, in which the transport of electrons is synchronized with the mechanical motion. The transport characteristics are strongly influenced by the interplay of electronic and vibrational degrees of freedom, which manifests itself in step structures of the current-voltage characteristics. An effective molecule-lead coupling results in an increase of the current with respect to the tunneling regime. The study uses the hierarchical equations of motion approach, which allows a numerically exact simulation of nonequilibrium transport in general open quantum systems involving multiple bosonic and fermionic environments [2].

[1] Novotný et al., Phys. Rev. Lett. 92, 248302 (2004)
[2] J. Bätge, Y. Ke, C. Kaspar, and M. Thoss, Phys. Rev. B 103, 235413 (2021)

DY 30.10 Wed 17:30 HSZ 204

Effective form factors for finite temperature correlation functions — •Oleksandr Gamayun — University of Warsaw, ul. Pasteura 5, 02-093 Warsaw, Poland

The behavior of dynamical correlation functions in one-dimensional quantum systems at zero temperature is now very well understood in terms of linear and non-linear Luttinger models. The "microscopic" justification of these models consists in exactly accounting for the soft-mode excitations around the vacuum state and at most few high-energy excitations. At finite temperature, or more generically for finite entropy states, this direct approach is not strictly applicable due to the different structure of soft excitations. To address these issues we study the asymptotic behavior of correlation functions in one-dimensional free fermion models. On the one hand, we obtain exact answers in terms of Fredholm determinants. On the other hand, based on "microscopic" resummations, we develop a phenomenological approach that introduces the effective form factors and reduces the problem to the zero temperature case. The information about the initial state is transferred into the scattering phase of the effective fermions. I will demonstrate how this works for correlation functions in the XY model, mobile impurity, and the sine-kernel Fredholm determinants.

DY 30.11 Wed 17:45 HSZ 204

Transfer-matrix summation of path integrals for transport through nanostructures — Simon Mundinar, •Alexander Hahn, Jürgen König, and Alfred Hucht — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

On the basis of the method of iterative summation of path integrals (ISPI), we develop a numerically exact transfer-matrix method to describe the nonequilibrium properties of interacting quantum-dot systems. For this, we map the ISPI scheme to a transfer-matrix approach [1], which is more accessible to physical interpretation, allows for a more transparent formulation of the theory, and substantially improves the efficiency. In particular, the stationary limit is directly implemented, without the need of extrapolation. The resulting new method, referred to as "Transfer-matrix Summation of Path Integrals" (TraSPI), is then applied to resonant electronic transport through a single-level quantum dot [2].

[1] S. Mundinar, P. Stegmann, J. König, and S. Weiss, Phys. Rev. B **99**, 195457 (2019)
[2] S. Mundinar, A. Hahn, J. König, and A. Hucht, Phys. Rev. B **106**, 165427 (2022)

DY 30.12 Wed 18:00 HSZ 204

Quasi-particle excitations at Mott-metal interfaces — •Jan Verlage[1], Friedemann Queisser[2,3], Peter Kratzer[1], and Ralf Schützhold[2,3] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Institut für Theoretische Physik, Helmholtz-Zentrum Dresden-Rossendorf — [3]Institut für Theoretische Physik, Technische Universität Dresden

We investigate excitations at the interface between a metallic bulk and a strongly correlated Mott insulator. Employing a hierarchy of correlations we identify effective quasi-particle and hole excitations in the heterostructure. To leading order in the hierarchy, the modes satisfy an effective two-component evolution equation. This allows the investigation of evanescent modes at the interface and tunneling through a Mott insulating layer.

The project is funded by the DFG, grant # 278162697 (CRC 1242).

DY 30.13 Wed 18:15 HSZ 204

Configuration interaction based nonequilibrium steady state impurity solver — •Daniel Werner, Jan Lotze, and Enrico Arrigoni — ITPCP, Graz, Austria

We present a solver for correlated impurity problems out of equilibrium based on a combination of the so-called auxiliary master equation approach (AMEA) and the configuration interaction (CI) expansion. Within AMEA one maps the original impurity model onto an auxiliary open quantum system with a restricted number of bath sites which can be addressed by numerical many-body approaches such as ED or MPS. While the mapping becomes exponentially more accurate with increasing number of bath sites, ED implementations are severely limited due to the fast increase of the Hilbert space dimension for open systems, and the MPS solver typically requires rather long runtimes. Here, we propose to adopt a CI approach to solve numerically the correlated auxiliary open quantum system. This allows access to a larger number of bath sites at lower computational costs than for ED. We benchmark the approach with NRG results in equilibrium and with MPS out of equilibrium. We evaluate the current, the conductance as well as the Kondo peak and its splitting. We obtain a rather accurate scaling of the conductance as a function of the bias voltage and temperature rescaled by TK for moderate to strong interactions in a wide range of parameters. The approach combines the fast runtime of ED with an accuracy close to the one achieved by MPS making it an attractive solver for nonequilibrium DMFT. (arXiv: 2210.09623)

DY 31: Microswimmers and Fluid Physics of Life (joint session DY/CPP)

Time: Wednesday 15:00–18:15 Location: MOL 213

DY 31.1 Wed 15:00 MOL 213

Physics of gut motility governs digestion and bacterial growth — •Agnese Codutti[1], Jonas Cremer[2], and Karen Alim[1] — [1]School of Natural Sciences, Technical University of Munich, Germany — [2]Biology Department, Stanford University, USA

Malfunctioning of the small intestine contractility and the ensuing bacterial population therein are linked to a plethora of diseases. We, here, study how the small intestine's variety of contractility patterns impacts nutrient uptake and bacterial population [1]. Our analytical derivations in agreement with simulations identify flow velocity as the key control parameter of the nutrients uptake efficiency and bacterial growth, independently of the specifics of contractility patterns. Self-regulating flow velocity in response to the number of nutrients and bacteria in the gut allows for achieving 100% efficiency in nutrient uptake. Instead of the specifics of intestine contractility, our work points to the flow velocity and its variation in time within the intestine to prevent malfunctioning.

[1] Codutti A., Cremer J., Alim K., "Changing Flows Balance Nutrient Absorption and Bacterial Growth along the Gut" PRL 129, 138101 (2022)

DY 31.2 Wed 15:15 MOL 213

Turbulence induces clustering and arrested phase separation in polar active fluids — Vasco Worlitzer[1,2], Gil Ariel[2], Avraham Beer[3], Holger Stark[4], •Markus Bär[1,4], and Sebastian Heidenreich[1] — [1]Physikalisch-Technische Bundesanstalt, Berlin — [2]Bar-Ilan University, Ramat Gan, Israel — [3]Ben-Gurion University, Beer Sheva, Israel — [4]Technische Universität Berlin

We study a novel phase of active polar fluids, which is characterized by the continuous creation and destruction of dense clusters due to self-sustained turbulence. This state arises due to the interplay between self-advection of the aligned swimmers and their defect topology. The typical cluster size is determined by the characteristic vortex size. Our results are obtained by investigating a continuum model of compressible polar active fluids [1], which incorporates typical experimental observations in bacterial suspensions [2], in particular a non-monotone dependence of speed on density.

[1] V. Worlitzer et al., Soft Matter 17, 10447-10457 (2021)
[2] A. Beer et al., Communications Physics 3, 66 (2020)

DY 31.3 Wed 15:30 MOL 213

Bacterial spreading in complex environments — •Agniva Datta, Sönke Beier, Veronika Pfeifer, Robert Grossmann, and Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany

Elucidating the principles of bacterial motility and navigation is key to understand many important phenomena such as the spreading of infectious diseases and the formation of biofilms. A prime challenge of swimming bacteria is to navigate in their habitat purposefully and efficiently, e.g., in the soil, which is a complex, structured environment. In this talk, we address the question of how bacterial navigation at the microscale relates to their large-scale spreading in heterogeneous environments. We combine experiments with the soil bacterium *Pseudomonas putida* with active particle modeling. In particular, the motility pattern of these bacteria in agar will be discussed with a focus on anomalous transport properties in disordered environments. In contrast to *E. coli*, our analysis reveals transient subdiffusion of bacteria in agar due to intermittent trapping, giving rise to a hop-and-trap dynamics with power-law distributed trap times.

DY 31.4 Wed 15:45 MOL 213

Minimum Entropy Production by Microswimmers with Internal Dissipation — •Andrej Vilfan, Abdallah Daddi-Moussa-Ider, Babak Nasouri, and Ramin Golestanian — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Microswimmers are natural or artificial self-propelled microscale objects moving through a fluid at low Reynolds numbers. The entropy production of microswimmers, related to their dissipated power, consists of two contributions. The external dissipation takes place in the viscous fluid surrounding the microswimmer. Internal dissipation takes place in the propulsive layer on the swimmer's surface. We have previously shown that a lower bound on the external dissipation can be derived with the knowledge of drag coefficients of two bodies of the same shape, one with a no-slip and one with a perfect slip boundary condition [1]. Here, we show that our approach can be generalized to take into account the internal dissipation, which is often the dominant contribution. By combining the Helmholtz minimum dissipation theorem and the principle of linear superposition, we solve the combined minimum dissipation problem for different classes of swimmers including surface-driven viscous droplets, swimmers driven by tangential forces and swimmers driven by normal forces. We show that the minimum entropy production in suspensions of active microswimmers differs fundamentally from particles driven by external forces.

[1] B. Nasouri, A. Vilfan and R. Golestanian, Phys. Rev. Lett., 126, 034503 (2021).

DY 31.5 Wed 16:00 MOL 213

Synchronization of model cilia by time-dependent elasto-hydrodynamics — •Albert von Kenne[1], Holger Stark[2], and Markus Bär[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), 10587 Berlin — [2]Technische Universität Berlin, 10623 Berlin

Collections of hair-like micro actuators known as cilia are employed in biology to pump extra cellular fluids at low Reynolds number conditions. Their collective dynamics exhibit synchronization and a large scale coordinated motion called metachronal waves. Typically, simple models that characterize the self-organization among hydrodynamically interacting cilia neglect the inertial forces in the fluid against the viscous forces. In this case, the mutual flows are determined instantaneously through the forces exerted by cilia. Consequentially synchronization requires a symmetry breaking external to hydrodynamics, that can come from elastic responses to flow perturbations (*T. Niedermayer et al., Chaos 2008*). Meanwhile, experiments show that inertial forces are significant in microscopic flow at the relevant scales (*D. Wei et al. Phys. Rev. Lett. 2019*). In this situation, the fluid response is explicitly time-dependent and hydrodynamic correlations can lead to synchronization (*M. Theers and R. Winkler, Phys. Rev. 2013*). We derived a simplified phase-oscillator model that describes the leading order coupling between cilia by elastic responses and hydrodynamic correlations. We show that its interrelations don't change the collective state qualitatively. However, the strength of coupling is always increased.

DY 31.6 Wed 16:15 MOL 213

Microswimming near a wedge — •Alexander R. Sprenger and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany

Artificial and living microswimmer encounter a large variety of geometric confinements and surfaces in the biological world which alter their motion when nearby. Here, we study the low-Reynolds-number dynamics of a microswimmer enclosed by a wedge-shaped free-slip interface. For various opening angles of the wedge, we derive an exact solution for flow and pressure fields using the method of images. The active swimmer is represented in terms of a superposition of Stokes singularities. In this way, the hydrodynamic interactions between the swimmer and the confining interfaces are examined. In particular, we find attraction or repulsion by the wedge depending on the propulsion mechanism (pusher- or puller-type swimming strokes) and the opening angle of the wedge. For the dynamics of a microswimmer inside the wedge, we present a minimal model in terms of coupled Langevin equations for position and orientation. Our analytic results are evaluated for parameters inspired by common self-propelling microorganisms like *Escherichia coli*.

15 min. break

DY 31.7 Wed 16:45 MOL 213

Role of cohesion in the flow of active particles through bottlenecks — •Timo Knippenberg[1], Anton Lüders[1], Celia Lozano[2], Peter Nielaba[1], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, Germany — [2]Bosonit, AI Department, La Rioja, Spain

Recently, many studies examined the intermittent flow of granular

particles through bottleneck-shaped apertures. A common framework which describes the occurring flow statistics was empirically found for a wide range of such systems reaching from microscopic colloids and macroscopic grains up to sheep herds. However, similar studies with active matter are scarce and do merely consider steric agent interactions. Here, we experimentally and numerically study the flow of programmable, colloidal active Janus swimmers through bottlenecks. Our results confirm the applicability of the above-mentioned statistical framework of granular intermittent flow also on complex-interacting active microswimmers. Moreover, upon increasing the strength of interparticle cohesion, we find a transition from an arch-dominated clogging regime to a cohesion-dominated regime where droplets form at the outlet. The flow-rate only weakly depends on the cohesion strength in the arch-dominated regime, which suggests that cohesion needs not necessarily to hinder particle flow through geometric constrictions or pores.

DY 31.8 Wed 17:00 MOL 213

Self-assembling meso-machines along liquid-air interfaces — •Nicolas Vandewalle, Megan Delens, and Ylona Collard — GRASP, University of Liege, B4000 Liege, Belgium

Magnetocapillary driven self-assembly allows us to create complex structures floating along a liquid-air interface. We show how these structures can be elaborated and how they can be triggered for locomotion. First, the pairwise capillary and magnetic interactions between floating objects are experimentally studied and rationalized through analogies with electrostatics. Then, the combination of capillary attraction and magnetic repulsion will lead to the spontaneous formation of a rich variety of floating structures. Placed in processing magnetic fields, those structures may behave like swimming ciliate organisms and start to move along the liquid-air interface. The conditions to obtain this magnetic powered locomotion are emphasized.

DY 31.9 Wed 17:15 MOL 213

Induced capillary dipoles in floating particle assemblies — •Megan Delens, Ylona Collard, and Nicolas Vandewalle — GRASP, Institut de Physique B5a, Université de Liège, Liège, BE

Capillary-driven self-assembly is a common fabrication method that consists in placing floating particles onto a liquid-air interface. The attractive capillary interaction between particles is due to the local deformations of the interface which can be described via so-called capillary charges. When the particles are spherical and far from each other, the menisci are planar circles and can be described by monopolar capillary charges. The capillary interaction is then approximately found by assuming that the charges carried by individual spheres may be linearly superposed. However, when particles are close together, we experimentally observed that the attraction is enhanced and becomes far more complex. Indeed, the contact lines start to tilt and the superposition principle no longer holds. For these situations, we propose to additionally consider induced capillary dipoles to describe the menisci, therefore, providing an extra attraction between particles at short distances. This effect is enhanced when particles have different sizes such that binary self-assemblies may reveal unusual local ordering.

DY 31.10 Wed 17:30 MOL 213

A Versatile Swarm of Individually Controlled Microparticles for Object Manipulation and Transport — •Veit-Lorenz Heuthe[1], Emanuele Panizon[2], and Clemens Bechinger[1] — [1]Universität Konstanz, Konstanz, Germany — [2]International Centre for Theoretical Physics, Trieste, Italy

Some tasks for robotic systems require many robots to cooperate, similar to ants that join their forces to carry large objects. On a macroscopic scale, many examples for such collective tasks exist, like robot swarms that can assemble objects. However, future potential applications like minimally invasive medicine call for miniaturization of such concepts. On the microscopic scale, one major challenge is the strong thermal noise, that demands for much more robust control. We use a reinforcement learning algorithm to individually steer microswimmers in a swarm that can manipulate and transport a large object. Due to decentralized control, our multi robot system is highly flexible, scalable and robust. With this demonstration we take micro-robot swarms one step further on their way to become tools for manipulating microscopic objects.

DY 31.11 Wed 17:45 MOL 213

New insights into the mechanism of self-phoresis — •Alvaro Domínguez[1], Mihail Popescu[1], and Siegfried Dietrich[2] — [1]Univ. Sevilla, Spain — [2]MPI für Intelligente Systeme, Stuttgart

Chemophoresis describes the displacement of a particle in an ambient fluid due to a gradient in chemical composition. Classic phoresis can be understood through linear–response theory: in the presence of a sufficiently small gradient $(\nabla n)_{\rm ext}$ in concentration, the phoretic velocity of the particle is $\mathbf{V} = \mathcal{L}_{\rm lin}(\nabla n)_{\rm ext}$, in terms of the phoretic coefficient $\mathcal{L}_{\rm lin}$ given by a Green–Kubo expression.

Self-phoretic particles induce a composition gradient $(\nabla n)_{\rm act}$ through catalytic activity and provide a physical realization of artificial swimmers. Experimental observations are then customarily addressed as another instance of classic phoresis, $\mathbf{V} = \mathcal{L}_{\rm lin}(\nabla n)_{\rm act}$.

However, an additional role of the particle's chemical activity has been recently identified [1,2], namely, as responsible for a specific activity–induced response $\mathcal{L}_{\rm act}$, so that one has to write

$$\mathbf{V} = (\mathcal{L}_{\rm lin} + \mathcal{L}_{\rm act})\,[(\nabla n)_{\rm ext} + (\nabla n)_{\rm act}]$$

in the more general scenario. This would mean a change in paradigm as it disproves the claim that "self-phoresis is phoresis in a self-induced gradient".

[1] A. Domínguez, M. Popescu, C. Rohwer, S. Dietrich, Physical Review Letters, **125**, 268002 (2020).
[2] A. Domínguez, M. Popescu, Current Opinion in Colloid & Interface Science, **61**, 101610 (2022).

DY 31.12 Wed 18:00 MOL 213

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

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

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

DY 32: Focus Session: Physics of Fluctuating Paths (joint session DY/CPP)

State-of-the-art experiments probe physical observables, such as heat, work or entropy production, empirical densities and currents, on the level of individual, stochastic paths. Such experiments are typically analysed by averaging along a limited number of individual realisations, which leads to substantial uncertainties in estimates. The systematic sample-to-sample fluctuations of such path-observables encode important information about the underlying, microscopic dynamical processes and are therefore a frontier of experimental, theoretical, and computational physics. Recently there has been a surge in the development and applications of path-based concepts across many fields of physics. This focus session complements a symposium and contains contributed talks.

Organized by Aljaz Godec, Udo Seifert, and Peter Sollich

Time: Wednesday 15:00–18:15 Location: ZEU 160

DY 32.1 Wed 15:00 ZEU 160

Towards a stochastic thermodynamics of fields and tracers — •Sarah A.M. Loos[1], Davide Venturelli[2], Benjamin Walter[3], Edgar Roldan[4], and Andrea Gambassi[2] — [1]DAMTP, University of Cambridge, Cambridge, UK — [2]SISSA, Trieste, Italy — [3]Imperial College London, UK — [4]ICTP, Trieste, Italy

Many results of stochastic thermodynamics, including the close connection between entropy production and stochastic heat dissipation, rely on physical assumptions, e.g., break down if there is no clear separation into "fast equilibrium bath degrees of freedom" and "slow nonequilibrium degrees of freedom". In this talk, I will discuss some insights into thermodynamic notions of nonequilibrium systems that do not fall into the usual paradigm of stochastic thermodynamics. In particular, we develop a thermodynamic description for systems consisting of tracer particles coupled to correlated scalar fields with thermal fluctuations in terms of trajectory-wise energy flows of the particle and the field, as well as the joint entropy production rate measured by path-probability ratios. As an illustration, we consider the case in which the particle is dragged by a harmonic trap through a complex medium described by a fluctuating Gaussian field. Using a perturbative approach, we uncover three dynamical regimes with distinct scaling behavior of the power and discuss the heat dissipation occurring within the field.

DY 32.2 Wed 15:15 ZEU 160

Fluctuation theorem for time reversal markers — •Gabriel Knotz, Till M. Muenker, Timo Betz, and Matthias Krüger — Fakultät für Physik, Georg-August-Universität, Göttingen, Germany

The analysis of particle trajectories is of high theoretical and experimental interest. Especially if hidden degrees are present, detecting broken detailed balance is a challenging task. We introduce and analyze a class of observables with certain symmetry properties under time reversal of trajectories that detect the breakage of detailed balance. Further, these observables fulfill a new form of fluctuation theorem and, under certain conditions, this fluctuation theorem provides bounds and relations for the total change in entropy. These findings are not limited to Markov or overdamped dynamics.

DY 32.3 Wed 15:30 ZEU 160

Necessity for Coarse Graining Empirical Densities and Currents in Continuous Space — •Cai Dieball and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Goettingen, Germany

We present general results on fluctuations and spatial correlations of the coarse-grained empirical density and current of diffusion in equilibrium or non-equilibrium steady states on all time scales. The time averaging and coarse graining hardwired in the definition of the functionals under consideration give rise to experimentally relevant but highly non-trivial statistics. We unravel a deep connection between current fluctuations and generalized time-reversal symmetry. We highlight the essential role of coarse graining in space from mathematical, thermodynamical, and experimental points of view. Spatial coarse graining is required to uncover salient features of currents that break detailed balance, and a thermodynamically "optimal" coarse graining ensures the most precise inference of dissipation. Defined without coarse graining, the fluctuations of empirical density and current are proven to diverge on all time scales in dimensions higher than one, which has far-reaching consequences for large-deviation limits in continuous space and for continuum limits of Markov-jump processes. Our findings provide new intuition about time-averaged observables and allow for a more efficient analysis of single-molecule experiments.

References: Phys. Rev. Lett. 129, 140601 (2022) and Phys. Rev. Research 4, 033243 (2022)

DY 32.4 Wed 15:45 ZEU 160

How Stickiness Can Speed Up Diffusion in Confined Systems — Arthur Alexandre[1], Matthieu Mangeat[2], •Thomas Guérin[1], and David Dean[1] — [1]Laboratoire Ondes et matière d'Aquitaine, CNRS/University of Bordeaux, F-33400 Talence, France — [2]Center for Biophysics and Department for Theoretical Physics, Saarland University, D-66123 Saarbrücken, Germany

The paradigmatic model for heterogeneous media used in diffusion studies is built from reflecting obstacles and surfaces. It is well known that the crowding effect produced by these reflecting surfaces slows the dispersion of Brownian tracers. In this talk, using a general adsorption desorption model with surface diffusion, we present an analytical theory showing that making surfaces or obstacles attractive can accelerate dispersion. In particular, we show that this enhancement of diffusion can exist even when the surface diffusion constant is smaller than that in the bulk. Even more remarkably, this enhancement effect occurs when the effective diffusion constant, when restricted to surfaces only, is lower than the effective diffusivity with purely reflecting boundaries. We give analytical formulas for this intriguing effect in periodic arrays of spheres as well as undulating microchannels. Our results are confirmed by numerical calculations and Monte Carlo simulations. [Ref: How Stickiness Can Speed Up Diffusion in Confined Systems, Phys Rev Lett 128 210601 (2022)]

DY 32.5 Wed 16:00 ZEU 160

From trajectories to models: data-driven approaches to decipher the stochastic dynamics of living systems — •Pierre Ronceray — Turing Centre for Living Systems, CINaM, CNRS, Aix-Marseille University, France

Stochastic differential equations are often used to model the dynamics of living systems, from Brownian motion at the molecular scale to the dynamics of cells and animals. How does one learn such models from experimental data? This task faces multiple challenges, from information-theoretical limitations to practical considerations. I will present a recent and ongoing effort to develop new methods to reconstruct such stochastic dynamical models from experimental data, with a focus on robustness and data efficiency. This provides a generic means to quantify complex behavior and unfold the underlying mechanisms of an apparently erratic trajectory.

DY 32.6 Wed 16:15 ZEU 160

Entropons as vibrational excitations in active solids — •Lorenzo Caprini[1], Umberto Marini Bettolo Marconi[2], Andrea Puglisi[3], and Hartmut Löwen[1] — [1]Heinrich-Heine-Universität Düsseldorf — [2]Scuola di Scienze e Tecnologie, University of Camerino — [3]Istituto dei Sistemi Complessi, CNR

We study the vibrational properties of non-equilibrium active crystals, i.e. solids formed by active particles, that are intrinsically out of equilibrium and governed by entropy production. As known in solid-state physics, equilibrium crystals are characterized by basic collective excitations with thermal origins that are named phonons. In this talk, I will show that active crystals are described by additional vibrational excitations that we called 'entropons' because each of them represents a mode of spectral entropy production. Entropons coexist with phonons and dominate over them for large activity, i.e. when the solid is far from equilibrium, while they vanish in equilibrium conditions. Their existence can be verified in experiments on dense self-propelled col-

loidal Janus particles and granular active matter, as well as in living systems such as dense cell monolayers.

15 min. break

DY 32.7 Wed 16:45 ZEU 160

Inferring Fractional Processes Using Path Integrals — •Johannes A. Kassel[1], Benjamin Walter[2], and Holger Kantz[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Imperial College London, London, UK

We present a method for inferring overdamped nonlinear Langevin equations driven by multiplicative fractional Gaussian noise from single-trajectory time series. Constructing a maximum-likelihood estimator, we simultaneously infer the nonlinear deterministic force term and the space-dependent diffusion term. We illustrate our method using artificial time series. We observe that Markovian modeling of long-range correlated data leads to a substantial underestimation of the deterministic force term while for anti-correlated data it leads to an overestimation of the force term.

DY 32.8 Wed 17:00 ZEU 160

Kinetics of Imperfect Reactions for non-Markovian Random Walks — •Toni Vieira Mendes and Thomas Guérin — Laboratoire Ondes et Matière d'Aquitaine, Université de Bordeaux

Most transport influenced reactions between two random walkers are usually imperfect, i.e., they do not occur at first contact between the reactants. For such imperfect reactions, recent work has been made to determine the statistics of first reaction time for Markovian random walkers in confinement. However, a lot of physical random walks are actually non-Markovian, i.e., their movement in the future depend on the trajectory they have followed up to then, thus displaying memory effects. These memory effects can be seen, for example, for beads moving inside complex fluids where the force fields do not equilibrate instantly. In this contribution, we describe an analytical theory giving access to the mean reaction time for imperfect reactions for random walkers with memory in confinement. Our theory clearly shows that, contrary to the Markovian case, the reaction time is not the sum of the mean first passage time and the time to react once within reactive distance. We show that the results of our theory match the results of simulations for both one and two dimensions. Then, the equations are analytically solved in the limit of weakly non-Markovian processes. Remarkably, in the limit of weakly reactive targets for fractional Brownian Motion, we find that the mean reaction time displays a non-trivial scaling as a function of the reactivity.

DY 32.9 Wed 17:15 ZEU 160

Instantons and the Path to Intermittency in Turbulent Flows — •André Fuchs[1], Corentin Herbert[2], Joran Rolland[3], Matthias Wächter[1], Freddy Bouchet[2], and Joachim Peinke[1] — [1]Institute of Physics and ForWind, University of Oldenburg, Küpkersweg 70, 26129 Oldenburg, Germany — [2]Université de Lyon, Ens de Lyon, Université Claude Bernard, CNRS, Laboratoire de Physique, F-69364 Lyon, France — [3]Université de Lille, CNRS, ONERA, Arts et Métiers Institute of Technology, Centrale Lille, UMR 9014 - LMFL - Laboratoire de Mécanique des fluides de Lille - Kampé de Fériet, F-59000 Lille, France

Processes leading to anomalous fluctuations in turbulent flows, referred to as intermittency, are still challenging. We consider cascade trajectories through scales as realizations of a stochastic Langevin process for which multiplicative noise is an intrinsic feature of the turbulent state. The trajectories are conditioned on their entropy exchange. Such selected trajectories concentrate around an optimal path, called instanton, which is the minimum of an effective action. The action is derived from the Langevin equation, estimated from measured data. In particular instantons with negative entropy pinpoint the trajectories responsible for the emergence of non-Gaussian statistics at small-scales.

DY 32.10 Wed 17:30 ZEU 160

A nonadiabatic generalized-dividing-surface instanton rate theory — •Rhiannon A. Zarotiadis, Joseph E. Lawrence, and Jeremy O. Richardson — Lab. für Physikalische Chemie, ETH Zürich, Zürich, Switzerland.

The accurate prediction of quantum rate processes is fundamental to our understanding of chemical reactions, but exact calculations are extremely costly. To make them tractable many chemical processes are described within the Born-Oppenheimer (BO) approximation, which assumes strong coupling between the diabatic states, and BO instanton theory is known to capture nuclear quantum effects for these systems well [1]. Alternatively, some systems are better captured by Fermi's golden rule, which is appropriate in the opposite limit of weak coupling.

Nevertheless, many reactions are in neither of these two limits, and so a universal rate theory is desirable. We introduce a new nonadiabatic generalized-dividing-surface instanton approach rigorously derived from the flux-flux correlation function. Our new theory correctly recovers the weak- and strong-coupling limits and goes beyond existing, ad hoc attempts to describe general, nonadiabatic rate processes.

Instanton rate theories [1] have already resolved many longstanding discrepancies between experiment and theory [2] and this new rate theory will be key to address processes beyond their scope such as proton-coupled electron transfer reactions.

[1] Richardson, J. O., Int. Rev. Phys. Chem., 2018, 37:2, 171-216.
[2] Zarotiadis, R. A., Fang, W., Richardson, J. O., Phys. Chem. Chem. Phys., 2020, 22, 10687.

DY 32.11 Wed 17:45 ZEU 160

Sojourn probabilities for diffusive dynamics with state-dependent friction: Theory and experiment — Alice Thorneywork[1,2], Jannes Gladrow[2,3], Ulrich F. Keyser[2], Ronojoy Adhikari[4], and •Julian Kappler[4,5] — [1]Department of Chemistry, University of Oxford, Oxford, United Kingdom — [2]Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom — [3]Microsoft Research, Cambridge, United Kingdom — [4]Department of Applied Mathematics and Theoretical Physics, Cambridge University, Cambridge, United Kingdom — [5]Fakultät für Physik, Ludwig-Maximilians-Universität, München, Germany

The trajectories of diffusion processes are continuous but nondifferentiable, and each occurs with vanishing probability. This introduces a gap between theory, where path probabilities are used in many contexts, and experiment, where only events with nonzero probability are measurable. We bridge this gap by considering the sojourn probability, i.e. the probability for diffusive trajectories to remain within a tube of small but finite radius around a smooth path. For systems with state-dependent diffusivity, we show that the sojourn probability is characterized by a functional that is different from all previously reported multiplicative-noise stochastic actions. We corroborate our theoretical results by comparison to experimentally measured sojourn probabilities for a colloidal particle in a corrugated microchannel. Our work directly connects the discussion of path probabilities for diffusive dynamics with state-dependent friction to physical observables.

DY 32.12 Wed 18:00 ZEU 160

Optimality of non-conservative driving in discrete systems — •Jonas Fritz and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

A fundamental problem in stochastic thermodynamics is that of optimal driving. The goal is to drive a system from some specified initial state to a specified final state, while minimizing entropy production (or work performed) along the trajectory. As shown recently [1], the optimal protocol in a cyclical Markov network has a non-conservative force, i.e. non-zero cycle affinity, which is in contrast to continuous systems. However, the reduction in entropy production from such a non-conservative force has been numerically found to be at most on the order of 10^{-2} for the case of the three state cycle. We investigate why this is the case, by systematically varying step size and initial conditions numerically for the simple case of the three state cycle. Further, we try to maximize the improvement in entropy production through the non-conservative force. By increasing the number of states in the cycle, we find a possible improvement which is an order of magnitude larger than the previously known one. We attempt to find a lower bound for the possible improvement through non-conservative driving, by analyzing the scaling behavior of the underlying quantities.

[1] Benedikt Remlein and Udo Seifert, Phys. Rev. E 103, L050105

DY 33: Biologically Inspired Statistical Physics (joint session DY/BP)

Time: Wednesday 15:00–16:30 Location: ZEU 250

DY 33.1 Wed 15:00 ZEU 250

Comparison of fitting strategies to extract the diffusion coefficient in microrheological experiments — •Sten Leipnitz, Christian Wagner, and Thomas John — Experimental Physics, Saarland University, Saarbrücken

Tracking of small particles undergoing a Brownian motion in liquids is a widespread method in passive microrheology to extract the diffusion coefficient D, the viscosity of the sample respectively. The mean-squared displacement (MSD) is determined from particle positions as a function of the timelag $MSD(\tau) = \sigma_0^2 + 2nD\tau + v_{\text{drift}}^2\tau^2$, where v_{drift} is a possible drift velocity and σ_0 is an offset due to position detection noise in experiments. We present: the extracted parameters depend strongly on the used number of fitting points in the MSD-relation. Surprisingly, considering only the beginning of the MSD-relation in the fitting procedure leads to the best expectation value of the diffusion coefficient. This is shown by numerical simulations of the Brownian motion as well as from experimental data.

DY 33.2 Wed 15:15 ZEU 250

Non-monotonic behavior of timescales of passage in heterogeneous media: Dependence on the nature of barriers — Moumita Dasgupta[1], •Sougata Guha[2], Leon Armbruster[1], Dibyendu Das[2], and Mithun K. Mitra[2] — [1]Department of Physics, Augsburg University, USA — [2]Department of Physics, IIT Bombay, India

Usually time of passage across a region may be expected to increase with the number of barriers along the path. Can this intuition fail depending on the special nature of the barrier? We study experimentally the transport of a robotic bug which navigates through a spatially patterned array of obstacles. Depending on the nature of the obstacles we call them either entropic or energetic barriers. For energetic barriers we find that the timescales of first passage vary non-monotonically with the number of barriers, while for entropic barriers first passage times increase monotonically. We perform an exact analytic calculation to derive closed form solutions for the mean first passage time for different theoretical models of diffusion. Our analytic results capture this counter-intuitive non-monotonic behaviour for energetic barriers. We also show non-monotonic effective diffusivity in the case of energetic barriers. Finally, using numerical simulations, we show this non-monotonic behaviour for energetic barriers continues to hold true for super-diffusive transport. These results may be relevant for timescales of intra-cellular biological processes.

DY 33.3 Wed 15:30 ZEU 250

Phase behavior and finite-size effects in biology — •Felix Hermann, Burkhard Duenweg, and Martin Girard — Max-Planck Institut fuer Polymerforschung (MPI-P), Mainz, Germany

Phase behavior observed in biology remains puzzling. For instance, the plasma membrane of cells exhibits signs of criticality, as it is controlled to remain near a demixing point. This membrane contains thousand of components, and it is largely unclear how its composition is controlled. Beyond this, one can ask whether cells should obey the traditional thermodynamic picture, given their small size, large number of components and the presence of non-equilibrium processes.

Here, we study toy systems, lattice models containing many (>30) components. We show that these systems exhibit strong finite-size effects. These manifest as behavior that appears similar to traditional critical behavior, but vanish logarithmically with system size. We examine scaling laws, and whether traditional paradigms from macroscopic thermodynamics can be broken in such systems.

DY 33.4 Wed 15:45 ZEU 250

Hierarchical interactions in complex ecosystems — •Lyle Poley[1], Joseph W. Baron[3], and Tobias Galla[1,2] — [1]Theoretical Physics, Department of Physics and Astronomy, School of Natural Sciences, The University of Manchester, Manchester M13 9PL, UK — [2]Instituto de Física Interdisciplinar y Sistemas Complejos IFISC (CSIC-UIB), 07122 Palma de Mallorca, Spain — [3]Laboratoire de Physique Statistique, École Normale Supérieure (ENS), Paris Sciences et Lettres (PSL) Research University, Sorbonne Université, 75005 Paris, France

In the analysis of complex ecosystems it is common to use random interaction coefficients, often assumed to be such that all species are statistically equivalent. We relax this assumption by imposing hierarchical inter-species interactions, which we incorporate into a generalised Lotka-Volterra dynamical system. These interactions impose a hierarchy in the community. Species benefit more, on average, from interactions with species below them in the hierarchy than from interactions with those above.

Using analytical tools from the theory of disordered systems, most notably path-integrals and dynamic mean-field theory, we demonstrate that a stronger hierarchy stabilises the community by reducing the number of species in the surviving community. We will also show that the probability of survival for a given species is dependent on its position in the hierarchy.

Reference: Poley L, Baron J W and Galla T Generalised Lotka-Volterra model with hierarchical interactions 2022 arXiv:2208.01569

DY 33.5 Wed 16:00 ZEU 250

Quantifying information content in continuous attractor networks — •Tobias Kühn[1,2] and Rémi Monasson[1] — [1]Laboratoire de Physique de l'Ecole Normale Supérieure, ENS, Université PSL, CNRS, Sorbonne Université, Université Paris Cité, F-75005 Paris — [2]Institut de la Vision, Sorbonne Université, INSERM, CNRS, F-75012 Paris

Attractor networks are a theme with long tradition to model information storage in the brain. Continuous attractor neural networks (CANN), in particular, have been employed to describe the storage of information about space and orientation. However, it stays controversial how useful this paradigm really is to explain actual processes, for example the representation of space in grid and place cells in the entorhinal cortex and the hippocampus, respectively.

A common criticism is that the disorder present in the connections might deteriorate the system's capability to reliably preserve the information of a certain pattern. In order to investigate if this criticism is valid, a measure is needed to objectively quantify the information content of a given neural network. Using the replica-trick, we compute the Fisher information for a network receiving space-dependent input whose connections are composed of a distance-dependent and a disordered component. We observe that the decay of the Fisher information is slow for not too large disorder strength, indicating that CANNs have a regime in which the advantageous effects of connectivity on information storage outweigh the detrimental ones.

DY 33.6 Wed 16:15 ZEU 250

Gift of gab: Probing the limits of dynamic concentration-sensing across a network of communicating cells — •Mohammadreza Bahadorian[1,2], Christoph Zechner[1,2,3], and Carl D. Modes[1,2,3] — [1]Max Planck Institut for Molecular Cell Biology and Genetics (MPI-CBG), 01307 Dresden, Germany — [2]Center for Systems Biology Dresden (CSBD), 01307 Dresden, Germany — [3]Cluster of Excellence Physics of Life, TU Dresden, 01069 Dresden, Germany

Many systems in biology and other sciences employ collaborative, collective communication strategies for improved efficiency and adaptive benefit. One such paradigm of particular interest is the community estimation of a dynamic signal, when, for example, an epithelial tissue of cells must decide whether to react to a given dynamic external concentration of stress-signaling molecules. At the level of dynamic cellular communication, however, it remains unknown what effect, if any, arises from communication beyond the mean field level. What are the limits and benefits to communication across a network of neighbor interactions? What is the role of Poissonian versus super-Poissonian dynamics in such a setting? How does the particular topology of connections impact the collective estimation and that of the individual participating cells? In this article we construct a robust and general framework of signal estimation over continuous-time Markov chains in order to address and answer these questions.

DY 34: Statistical Physics: Far From Equilibrium II

Time: Wednesday 16:45–18:15 Location: ZEU 250

DY 34.1 Wed 16:45 ZEU 250

Lane formation of colloidal particles driven by gravity — •Marc Isele, Kay Hofmann, and Peter Nielaba — Physics Department, University of Konstanz, Konstanz, Germany

Systems of particles that move with differing relative speeds as a counterpart to the movements of pedestrians and crowds have been shown to form a so-called lane structure. We simulate a quasi two dimensional system of two spherical particle types of different sizes driven by gravity. The particles are confined by hard walls orthogonal to the driving force and we employed Brownian Dynamics simulations (without hydrodynamic interactions). We found that the particles formed the well-known lane structure rather quickly. In this formation process the particles form slanted boundaries between the soon to be lanes which leads to regions of high and low densities. In the steady state we further found that the lanes closest to the hard walls were always occupied by the smaller particles (via something we call a funneling process). We also analyzed a wide variety of parameters giving us an optimized system for lane formation. Our work shows that the lane formation of driven particles is a phenomenon with a lot of different aspects that can depend heavily on the chosen system.

DY 34.2 Wed 17:00 ZEU 250

Time-reversal symmetries and equilibrium-like Langevin equations — •Lokrshi Prawar Dadhichi and Klaus Kroy — ITP, Leipzig University, Brüderstraße 15, 04103, Leipzig

Graham has shown in Z. Physik B 26, 397-405 (1977) that a fluctuation-dissipation relation can be imposed on a class of nonequilibrium Markovian Langevin equations that admit a stationary solution of the corresponding Fokker-Planck equation. Here we show that the resulting equilibrium form of the Langevin equation is associated with a nonequilibrium Hamiltonian and ask how precisely the broken equilibrium condition manifests itself therein. We find that this Hamiltonian need not be time reversal invariant and that the "reactive" and "dissipative" fluxes loose their distinct time reversal symmetries. The antisymmetric coupling matrix between forces and fluxes no longer originates from Poisson brackets and the "reactive" fluxes contribute to the ("housekeeping") entropy production, in the steady state. The time-reversal even and odd parts of the nonequilibrium Hamiltonian contribute in qualitatively different but physically instructive ways to the entropy. Finally, this structure gives rise to a new, physically pertinent instance of frenesy.

DY 34.3 Wed 17:15 ZEU 250

Quantum and classical contributions to entropy production in fermionic and bosonic Gaussian systems — •Krzysztof Ptaszyński[1,2] and Massimiliano Esposito[2] — [1]Institute of Molecular Physics, Polish Academy of Sciences, Mariana Smoluchowskiego 17, 60-179 Poznań, Poland — [2]Complex Systems and Statistical Mechanics, Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg, Luxembourg

As previously demonstrated, the entropy production – a key quantity characterizing the irreversibility of thermodynamic processes – is related to generation of correlations between degrees of freedom of the system and its thermal environment. The natural question appears whether such correlations are of a classical or a quantum nature, namely, whether they are accessible through measurements. We deal with this problem by investigating fermionic and bosonic Gaussian systems. It is shown that for fermions the entropy production is mostly quantum due to parity superselection rule which restricts the set of physically allowed measurements to projections on the Fock states, which significantly limits the amount of classically accessible correlations. In contrast, in bosonic systems a much larger amount of correlations can be accessed through Gaussian measurements. Specifically, while quantum contribution may be important at low temperatures, in the high temperature limit the entropy production corresponds to purely classical position-momentum correlations.

DY 34.4 Wed 17:30 ZEU 250

Optimal power extraction from active particles with hidden states — •Luca Cocconi[1,2], Jacob Knight[2], and Connor Roberts[2] — [1]The Francis Crick Institute, London — [2]Imperial College, London

We identify generic protocols achieving optimal power extraction from a single active particle subject to continuous feedback control under the assumption that the instantaneous velocity, but not the fluctuating self-propulsion velocity, is accessible to direct observation. Our Bayesian approach draws on the Onsager-Machlup path integral formalism and is exemplified in the cases of free run-and-tumble and active Ornstein-Uhlenbeck dynamics in one dimension. Such optimal protocols extract positive work even in models characterised by time-symmetric positional trajectories and thus vanishing informational entropy production rates. We argue that the theoretical bounds derived in this work are those against which the performance of realistic active matter engines should be compared.

DY 34.5 Wed 17:45 ZEU 250

Driving a first-order phase transformation by quenching the density: Unleashing hidden states — •Miriam Klopotek[1], Martin Oettel[2], and Hans Joachim Schöpe[2] — [1]University of Stuttgart, SimTech Cluster of Excellence EXC 2075, Stuttgart, Germany — [2]University of Tübingen, Institute for Applied Physics, Tübingen, Germany

Abruptly increasing the number density, the primary order parameter of a many-particle system, is a basic mechanism to drive a first-order phase transition – elementary for athermal systems and thus for the solidification process from a fluid. A better-known experiment on thermal systems is quenching the temperature down to below the critical point, suddenly 'freezing out' the original degrees of freedom, whereafter the system densifies locally upon response. A density quench, in turn, intervenes directly and globally on the order parameter. A manifest example is thin film growth. As dynamical arrest is imminent, 'hidden' metastable states appear. We employ kinetic Monte Carlo simulations of a simple lattice model of sticky hard rods under quasi-2D confinement, gradually growing a full monolayer under different quench (growth) rates. The phenomenology is extremely rich: At least five distinct, non-classical phase transformation pathways are identified in this most simple model. They 'tile' a corresponding dynamical control diagram.

DY 34.6 Wed 18:00 ZEU 250

New phases and peculiar fluctuations in nonreciprocal systems — •Sarah Loos — DAMTP, University of Cambridge, UK

Nonreciprocal interactions, i.e., interactions that violate the *actio=reactio* principle, occur in various biological and artificial nonequilibrium systems on a wide range of scales. For example, a bird in a flock may react to the movements of the bird in front of it, while the reverse interaction is zero, simply due to missing visual information. Recent research shows that the occurrence of such nonreciprocal interactions can have a dramatic impact on the self-organization of many-body systems [1], and on their thermodynamic properties [2]. In this talk, we will consider a nonequilibrium lattice model with vision cone interactions [3], and show how the presence of nonreciprocal interactions can lead to the emergence of new phases and peculiar fluctuations.

[1] Fruchart, Non-reciprocal phase transitions, Nature (2021).
[2] S.A.M. Loos and S.H.L. Klapp, NJP 22, 123051 (2020).
[3] S.A.M. Loos, S.H.L. Klapp, and T. Martynec, ArXiv:2206.10519 (2022).

DY 35: Statistical Physics of Biological Systems I (joint session BP/DY)

Time: Thursday 9:30–13:00 Location: TOE 317

DY 35.1 Thu 9:30 TOE 317

Reduced stochastic models of drifting assemblies in plastic neuronal networks — •Sven Goedeke, Christian Klos, Yaroslav Felipe Kalle Kossio, and Raoul-Martin Memmesheimer — University of Bonn, Bonn, Germany

In a standard model, associative memories are represented by assemblies of strongly interconnected neurons. It has recently been proposed that these assemblies are not static but drift freely in neural circuits. On the level of single neurons, assembly drift is reflected by characteristic dynamics: relatively long times of stable assembly membership interspersed with fast transitions. How can we mechanistically understand these dynamics? Here we answer this question by proposing simplified, reduced models. We first construct a random walk model for neuron transitions between assemblies based on the statistics of synaptic weight changes measured in simulations of spiking neural networks exhibiting assembly drift. It shows that neuron transitions between assemblies can be understood as noise-activated switching between metastable states. The random walk's potential landscape and inhomogeneous noise strength induce metastability and thus support assembly maintenance in the presence of ongoing fluctuations. In a second step, we derive an effective random walk model from first principles. In this model, a neuron spikes at a fixed background rate and with an input weight-dependent probability when its current or another assembly reactivates. The approach can be applied generally to networks of drifting assemblies, irrespective of the employed neuron and plasticity models.

DY 35.2 Thu 9:45 TOE 317

Fluctuation-dissipation relations for spiking neurons — •Benjamin Lindner — Bernstein Center for Computational Neuroscience Berlin, Philippstr. 13, Haus 2, 10115 Berlin, Germany — Physics Department of Humboldt University Berlin, Newtonstr. 15, 12489 Berlin, Germany

Spontaneous fluctuations and stimulus response are essential features of neural functioning but how they are connected is poorly understood. I derive fluctuation-dissipation relations (FDR) between the spontaneous spike and voltage correlations and the firing rate susceptibility for i) the leaky integrate-and-fire (IF) model with white noise; ii) an IF model with arbitrary voltage dependence, an adaptation current, and correlated noise. The FDRs can be used to derive thus far unknown statistics analytically [model (i)] or the otherwise inaccessible intrinsic noise statistics [model (ii)].

DY 35.3 Thu 10:00 TOE 317

Current fluctuations in nanopores: origin and breakdown of 1/f noise — •Paul Robin, Mathieu Lizee, Alessandro Siria, and Lydéric Bocquet — ENS, Université PSL, CNRS, Sorbonne Université, Université Paris-Cité, Paris, France

Ion transport through nanometric pores is key to many biological processes, from osmoregulation to neurotransmission, yet this process is known to occur under strong fluctuations. The power spectrum of this current noise is known to scale like 1/f at low frequency, according to the long-standing yet empirical Hooge law. Modelling attempts generally rely on complex assumptions such as self-organized criticality or microscopic disorder - in contrast with the apparent universality of 1/f pink noise. In this talk, I will present a simple theoretical model accounting for the presence of 1/f fluctuations in ionic currents through nanopores regardless of their microscopic structure. In particular, I will show how pink noise can emerge from diffusive processes alone, rather than necessitating complex conductance switching mechanisms. This prediction also explains why pink noise can be observed for frequencies much lower than that of microscopic processes. Lastly, I will discuss under which conditions this description is expected to break down. Notably, chemical processes on the pore's walls can alter ion dynamics and slow down diffusion, leading to memory effects and deviations to Hooge's law. I will compare these predictions to experimental data on artificial nanofluidic pores with various surface properties and reactivities.

DY 35.4 Thu 10:15 TOE 317

Selective alignment force in schooling fish linked to leader-follower interactions given by relative speeds of neighbours — •Andreu Puy[1], Palina Bartashevich[2,3], and Pawel Romanczuk[2,3] — [1]Departament de Física, Universitat Politècnica de Catalunya, Barcelona, Spain — [2]Institute for Theoretical Biology, Humboldt-Universität zu Berlin, Germany — [3]Excellence Cluster Science of Intelligence, Technische Universität Berlin, Germany

Collective motion is commonly assumed to emerge when individuals in a group interact with neighbours via some combination of attraction, repulsion and alignment forces. Alignment has been the most elusive and controversial force to study in experimental setups, with previous works differing about its existence. Here we revisit the topic by introducing a force map technique depending on the relative velocities of neighbours. In contrast to commonly used force maps, our technique demonstrates evidence for experimental data of schooling fish of a selective alignment force when individuals move at slower speeds than their neighbours and an antialignment force when they move at higher speeds. We employ a simple model with alignment to demonstrate the validity and robustness of the proposed force map. Including a selective interaction where individuals only interact with faster neighbours allowed us to reproduce the alignment interactions in the experimental data. Finally, we link this idea to leader-follower interactions, justifying that faster individuals act as leaders with respect to their neighbours.

Invited Talk DY 35.5 Thu 10:30 TOE 317

Statistical Physics of Spatially Organized Catalytic Particles — •Ulrich Gerland — Technical University of Munich, Germany

Catalytic particles are spatially organized in a number of biological systems across different length scales, from enzyme complexes to metabolically coupled cells. Despite operating on different scales, these systems all feature localized reactions involving partially hindered diffusive transport, which is determined by the collective arrangement of the catalysts. We explore how different arrangements affect the interplay between the reaction and transport dynamics, which ultimately determines the flux through the reaction pathway. Two fundamental trade-offs arise, the first between efficient inter-catalyst transport and the depletion of substrate, and the second between steric confinement of intermediate products and the accessibility of catalysts to substrate. We find that the question of optimal catalyst arrangements generalizes the well-known Thomson problem of electrostatics [1]. Furthermore, we map the problem of optimally arranging enzymes to an economic investment problem, which helps to formulate and understand a possible design principle for synthetic biomolecular systems [2].

[1] F. Hinzpeter, F. Tostevin, A. Buchner, and U. Gerland (2022), Trade-offs and design principles in the spatial organization of catalytic particles, Nature Phys. 18, 203-211.

[2] G. Giunta, F. Tostevin, S. Tanase-Nicola, and U. Gerland (2022), Optimal spatial allocation of enzymes as an investment problem, Commun. Phys. 5, 319.

15 min. break

DY 35.6 Thu 11:15 TOE 317

Collective Dynamics of Multi-Scale Interacting Complex Systems — •Fabrizio Olmeda[1,2] and Steffen Rulands[1,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]IST Austria, Vienna, Austria — [3]Ludwigs-Maximilians-Universitat Munchen, Arnold Sommerfeld Center for Theoretical Physics, Munich, Germany

Understanding the conditions under which complex systems are stable is pivotal for understanding their response to perturbations. Theoretical work has shown that for global interactions between components a minimal complex system is stable if the standard deviation of linearised interaction rates is sufficiently small. In biological systems, which often contain a small number of important and interactions are mediated by diffusing agents, stochasticity and non-locality may influence stability. Here, we generalise these results to stochastic, spatial systems with interaction on multiple length scales. Starting from a microscopic description we derive a coarse-grained field theory and identify a transition between a regime defined by giant density fluctuations and one exhibiting a spatial instability with a finite wave length. The latter is suppressed by non-reciprocity in the interactions between components. Our work provides a rigorous framework to infer col-

lective dynamics and stability in complex systems, with applications ranging from ecosystems to morphogenesis.

DY 35.7 Thu 11:30 TOE 317

Physical mechanism of erythrocytes sedimentation rate — •Alexis Darras, Thomas John, Lars Kaestner, and Christian Wagner — Experimental Physics, Saarland University; D-66123 Saarbrücken, Germany

Red blood cells (or erythrocytes) sedimentation rate (ESR) is a physical parameter of blood which is often checked in medical diagnosis. It is indeed well known that in case of inflammation, the increase in fibrinogen and other proteins induces a higher ESR.

Until recently, researchers thought that the increase of fibrinogen accelerates the ESR by creating bigger aggregates of red blood cells (RBC). Fibrinogen is indeed an aggregation agent of RBCs, and bigger aggregates tend to sediment faster in Stokes regime. However, modeling the ESR measurements with this hypothesis is challenging and often requires physical assumptions specific to this system.

Besides, modern colloidal science has shown that attractive particles, in suspensions with a high volume fraction, form percolating aggregates, as wide as the container. The sedimentation of those colloids then follows a so-called "colloidal gel collapse" regime, governed by the geometry of the percolating aggregate acting as a porous material. In this talk, we show that RBCs actually follow the same behavior. We also demonstrate that a porous-material model naturally leads to an efficient description the RBC sedimentation, which also provides a long-sought dependency of the ESR as a function of the initial RBC volume fraction (i.e. the hematocrit).

DY 35.8 Thu 11:45 TOE 317

Stochastic wavelength selection and pattern fixation — •Tom Burkart[1,2], Anastasiia Petrova[2,3], Laeschkir Würthner[1,2], Claudia Veigel[2,3], and Erwin Frey[1,2,4] — [1]Arnold Sommerfeld Center for Theoretical Physics (ASC), Department of Physics, LMU München, Munich, Germany — [2]Center for NanoScience, LMU München, Munich, Germany — [3]Department of Cellular Physiology, Biomedical Center (BMC), LMU München, Planegg-Martinsried, Germany — [4]Max Planck School Matter to Life, Munich, Germany

Biological pattern-forming processes are typically driven by a chemical fuel (out-of-equilibrium systems) or by a relaxation towards a thermodynamic equilibrium (phase separation). In these cases, pattern wavelength selection results from translational shifts of high-density regions and mass redistribution in between such regions. Here, we study how a pattern with a characteristic wavelength can form when high-density regions can only grow, but neither mass redistribution nor translation are allowed. The corresponding wavelength selection mechanism relies on thermal fluctuations, irreversible fixation of randomly occurring high-density regions, and long-ranged interactions between these regions. To model the density dynamics and the long-ranged interaction, we derive a set of reaction-diffusion equations from a free energy functional. In addition, we derive the statistics of pattern wavelengths from order statistics, emphasising the stochastic nature of the underlying mechanism. Our results constitute an alternative path to pattern formation next to out-of-equilibrium dynamics and phase separation processes.

DY 35.9 Thu 12:00 TOE 317

Control of non-equilibrium chemical reactions via phase separation — •Sudarshana Laha[1,2], Jonathan Bauermann[1,2], Tyler S. Harmon[3], Frank Jülicher[1,2], Thomas C.T. Michaels[4], and Christoph A. Weber[5] — [1]Max Planck Institute for the Physics of Complex Systems Dresden , Germany — [2]Center for Systems Biology Dresden , Germany — [3]IFW Dresden, Germany — [4]ETH Zürich, Switzerland — [5]Institute of Physics, University of Augsburg, Germany

Fuel-driven out-of-equilibrium chemical reactions are spatially organized using compartments in living cells. To what extent the properties of chemical reactions are altered by the compartments relative to homogeneous systems and the underlying physical principles are less explored. Here, we derive a theoretical framework to study such chemical reactions in the presence of compartments. We highlight the different governing kinetic equations for the reactants in diffusion-limited and reaction-limited regimes. We show that for two-state transition processes, the turnover of the product can be significantly affected in the limit of infinitely fast diffusion of the components. We can further derive the optimal compartment volume analytically which shows how phase separation parameters can affect the turnover. We further observe that the initial rate can be strongly modified for enzymatic and nucleation processes. These aspects allow us to understand better the control of such processes and exemplify the role of enzymes in compartments to speed up the reaction. This understanding is crucial for synthetically designing of cells as compartments and establishing communication between them.

DY 35.10 Thu 12:15 TOE 317

Microphase separation of living cells — •François Detcheverry, Adrien Carrère, Joseph d'Alessandro, Olivier Cochet-Escartin, Julie Hesnard, Nasser Ghazi, Charlotte Rivière, Christophe Anjard, and Jean-Paul Rieu — University of Lyon, Université Claude Bernard Lyon 1, CNRS, Institut Lumière Matière, F-69622, VILLEURBANNE, France

Self-organization of cells is key to a variety of biological systems and physical concepts inspired from condensed matter have proven essential in understanding some of their properties. Here we demonstrate that microphase separation, long known in polymeric materials and other inert systems, has a natural counterpart in living cells. When placed below a millimetric film of liquid nutritive medium, a quasi two-dimensional population of *Dictyostelium discoideum* cells spontaneously self-assembles into compact domains. Their typical size of 100 μm is governed by a balance between competing interactions: an adhesion which acts as a short-range attraction and promotes aggregation, and an effective long-range repulsion stemming from aerotaxis in near anoxic condition. We present a combination of experimental data, analytical modelling and cell-based simulations that all support this scenario. Our findings establish a generic mechanism for self-organization of living cells and highlight oxygen regulation as an emergent organizing principle for biological matter.

[Preprint: bioRxiv https://doi.org/10.1101/2022.05.25.493184]

DY 35.11 Thu 12:30 TOE 317

Hydrationa and crowding effects on SOD1 sequestration into FUS biocondensates — Luis Enrique Coronas[1], Emeline Laborie[2], Stepan Timr[2], Fabio Sterpone[2], and •Giancarlo Franzese[1,3] — [1]Interdisciplinary and Statistical Physics Section–Department of Condensed Matter Physics, Physics & Institute of Nanoscience and Nanotechnology (IN2UB), Universitat de Barcelona, Barcelona, Spain — [2]CNRS Laboratoire de Biochimie Théorique, Institut de Biologie Physico-Chimique, Université Paris Denis Diderot, Paris, France — [3]Max Planck Institut für Physik Komplexer Systeme, Dresden, Germany

Superoxide Dismutase 1 (SOD1) is a protein related to amyotrophic lateral sclerosis that, under Heat Stress (HS), is sequestered into Stress Granules in vivo and Fused in Sarcoma (FUS) biomolecular condensates in vitro. Experiments show that an in vitro cytomimetic medium, using Bovine Serum Albumin (BSA) as crowder, decreases the SOD1 partition coefficient (PC) even after 60 min of HS. Implicit-water OPEP simulations show no preferential interactions of SOD1 with BSA. Here, by combining the OPEP with a coarse-grained water model, accounting for water contributions to the interactions in large biological systems, we show that SOD1 has one preferred associative state in FUS but three in BSA, whose transition rates and residency times are controlled by their hydration. We conclude that the SOD1 PC's decrease in FUS condensate, when BSA crowders are present, is due to the hydration entropy increase in BSA, a mechanism possibly relevant also in vivo.

DY 35.12 Thu 12:45 TOE 317

Stochastic heat production in phase-separated systems out of equilibrium — •Kathrin Laxhuber, Jonathan Bauermann, and Frank Jülicher — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Phase-separated multi-component systems in the presence of chemical reactions provide interesting examples of non-equilibrium systems. We complement the dynamics of phase separation by a heat transport equation which is coupled to diffusive matter transport. On a microscopic scale, fluctuations become relevant, which we include by developing a stochastic lattice model that we link to the macroscopic continuum dynamics. We then implement this model in a kinetic Monte Carlo simulation of spatial flows of energy and matter as well as local reactions. By coupling to reservoirs or by fueling reactions, a system can be driven out of equilibrium. Using a toy system of a single phase-separated droplet, we discuss how temperature fluctuations affect the droplets' dynamics and the noise in the system. We furthermore show how the fluxes due to the driving give rise to a stochastic production of

latent heat and reaction heat. The systems we discuss serve as models for biological condensates and the study of energetics in cells.

DY 36: Wetting, Fluidics and Liquids at Interfaces and Surfaces I (joint session CPP/DY)

Time: Thursday 9:30–13:00 Location: MER 02

DY 36.1 Thu 9:30 MER 02

Dynamic wetting of concentrated granular suspensions — •Reza Azizmalayeri, Peyman Rostami, and Günter K. Auernhammer — Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

Concentrated granular suspensions are employed in a variety of processes where the contact line dynamics and internal structure of the suspension interact. The process can be characterized using individual particle analysis and average suspension descriptions. Along the contact line, particles interact with each other and the substrate, and the shear rate influence the suspension's non-Newtonian rheological behavior. In this study, we use fluorescently-labeled tracer particles in a refractive index-matched silica suspension. We track the motion of the tracer particles in the concentrated suspension with astigmatism particle tracking velocimetry (APTV). Averaging over single tracks gives the flow profile in a droplet near the advancing contact line. In addition, side-view allows characterizing the drop shape. The behavior of high-concentration suspensions near contact lines differs significantly from that of simple liquids. Near the advancing contact line, we observe the fast-moving layering of suspensions close to the substrate, which is controlled by the suspension's rheology. Near the receding contact line, the suspension adheres to its previous layer and moves on top of it. Initially, there is an unsteady motion, which becomes stationary with time.

DY 36.2 Thu 9:45 MER 02

Sliding drops: towards a universal law of friction — Xiaomei Li[1], Francisco Bodziony[2], Mariana Yin[2], Holger Marshall[2], Rüdiger Berger[1], and •Hans-Jürgen Butt[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz — [2]Computational Multiphase Flows, Technische Universität Darmstadt, Alarich-Weiss-Straße 10, 64287 Darmstadt

Liquid drops moving on tilted surfaces are an everyday phenomenon and are important for many industrial applications. Still, it is not possible to predict their velocity. To make a step forward in quantitative understanding, we measured the velocity U, width w, length, advancing Θ_a, and receding contact angle Θ_r of liquid drops sliding down inclined flat surfaces. By solving the equation of motion, we determined the friction force versus slide velocity for different hydrophobic surfaces. The friction force acting on moving drops of polar and non-polar liquids with viscosities ranging from 10^{-3} to 1 Pa s can empirically be described by $F_f(U) = F_0 + \mu w Ca^{\alpha}$ for the whole relevant velocity range. Here, $Ca = U\eta/\gamma$ is the capillary number, in which η is the viscosity and γ the surface tension of the liquid. The friction coefficient μ is in the range of 1 - 3 N/m for all liquid/surface combinations. For viscosities above 0.006 Pa s, we find $\alpha = 1.0$. Bulk and wedge viscous dissipation can fully account for the velocity-dependent friction force. These results were confirmed by direct numerical diffuse-interface simulations of the flow pattern inside sliding drops. We demonstrate that the Furmidge-Kawasaki equation, is also valid in the dynamic case.

DY 36.3 Thu 10:00 MER 02

Spreading of soft elasto-viscoplastic droplets — •Maziyar Jalaal[1], Cassio Oishi[1], and Hugo França[1,2] — [1]Institute of Physics, University of Amsterdam, Amsterdam, The Netherlands — [2]Sao Paulo State University, Sao Paulo, Brazil

The spreading under surface tension of a droplet of complex fluid with elastic and plastic properties is studied. Unlike Newtonian fluids, the droplet converges to a final equilibrium shape once the driving stresses inside the droplet fall below the critical yield stress. Scaling laws are presented for the final radius and complemented with an asymptotic analysis for shallow droplets. Moreover, numerical simulations using the volume-of-fluid method and an elastoviscoplastic (EVP) constitutive law, and experiments with an aqueous solution of Carbopol, are presented.

DY 36.4 Thu 10:15 MER 02

Stick-slip Contact Line Dynamics in Forced Wetting of Polymer Brushes — •Daniel Greve[1], Simon Hartmann[1], and Uwe Thiele[1,2] — [1]Institut für Theoretische Physik, WWU Münster — [2]Center for Nonlinear Science (CeNoS), WWU Münster

We study the wetting of adaptive substrates using a mesoscopic hydrodynamic model for a liquid droplet on a polymer brush, refining the model in [1]. First, we show that Young's law still holds for the macroscopic equilibrium contact angle and that on the mesoscale a Neumann-type law governs the shape of the wetting ridge (comparable to the case of elastic substrates [2]). Further, we numerically examine the wetting ridge dynamics for a moving meniscus, i.e., we consider an "inverse Landau-Levich geometry" where a brush-covered plate is introduced into a bath. We find stick-slip motion in good qualitative agreement with experimental observations [3,4] and discuss criteria for the onset of the corresponding instability.

[1] U. Thiele and S. Hartmann, *Eur. Phys. J.-Spec. Top.*, 2020, 229, 1819-1832.
[2] B. Andreotti and J. H. Snoeijer, *Annu. Rev. Fluid Mech.*, 2020, 52, 285-308.
[3] S. Schubotz et al., *Adv. Colloid Interface Sci.*, 2021, 294, 102442.
[4] L. Wan, X. Meng, Y. Yang, J. Tian and Z. Xu,*Sci. China Chem.*, 2010, 53, 183-189.

DY 36.5 Thu 10:30 MER 02

Demixing of liquid PDMS during dewetting into the equilibrium state — •Khalil Remini[1], Leonie Schmeller[2], Dirk Peschka[2], Barbara Wagner[2], and Ralf Seemann[1] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Weierstrass-Institute, Berlin University, Berlin, Germany

The study of micrometer-sized equilibrium droplets on elastic substrates is of great interest because, due to negligible gravity, other interactions such as elastic or capillary forces and their mutual influence can easily be investigated, so deviations from the expected behaviour at larger scales becomes visible. This applies in particular to soft solids like PDMS that are typically considered as ideal rubbers on the macro scale. Our experimental system is composed of liquid polystyrene (PS) droplets on a viscoelastic substrate consisting of cross-linked polydimethylsiloxane (PDMS) of different elasticities. Using atomic force microscopy (AFM), we analyse the topography of the materials and thus their contact angles with high precision, we also use AFM to demonstrate the existence of non-cross-linked liquid PDMS that migrates from the elastic PDMS toward the three-phase contact line TPCL to form a demixed liquid ring around the dewetted PS droplet. In that situation, on the nanometer distance around the TPCL, liquid PS meets liquid PDMS instead of being in direct contact with the soft solid PDMS. Further analysis allows us to say that this phenomenon also exists during the dewetting of liquid polystyrene in the same type of elastic solids.

DY 36.6 Thu 10:45 MER 02

How droplets dry on stretched soft substrates — •Binyu Zhao, Yixuan Du, and Günter K. Auernhammer — Leibniz Institute of Polymer Research Dresden, Dresden 01069, Germany

Droplets evaporation on solid substrates is a ubiquitous phenomenon and relevant in many natural and industrial processes. Well known are the coffee-ring. Many studies have succeeded in promoting, suppressing or even reversing the formation of coffee-ring by using non-spherical particles, surfactants, patterned substrates, and so on.

Here, we show that a uniaxial stretching of soft substrates strongly controls the dynamics of droplet evaporation and particle deposition through controlling the contact line motion. Water droplet evaporates with an elongated non-circular contact line on the stretched substrates and switches the elongation direction during evaporation. The contact line evolution depends on the orientation of the contact line relative to the stretching direction. When nanoparticles are added into the liquid, the circular deposition pattern, i.e., the so-called coffee-ring, becomes elongated along the direction perpendicular to the stretching direction. Particularly, such non-circular deposition pattern ex-

hibits periodic height gradients along its rim. The finer structure of the pattern can be controlled by applying different stretching ratios to the soft substrate and thus are correlated to the anisotropic surface stresses near the contact line. The findings broaden our understanding of droplet wetting and evaporation on soft and anisotropic substrates, and open the way to reshaping the coffee-ring to allow anisotropic, non-circular patterning.

DY 36.7 Thu 11:00 MER 02

Gradient dynamics model for sessile drop evaporation in a gap: from simple to applied scenarios — •Simon Hartmann[1], Uwe Thiele[1], Christian Diddens[2], and Maziyar Jalaal[3] — [1]Institut für Theoretische Physik and Center for Nonlinear Science, Universität Münster — [2]Physics of Fluids group, Max Planck Center Twente for Complex Fluid Dynamics, and J. M. Burgers Center for Fluid Dynamics, University of Twente — [3]Van der Waals-Zeeman Institute, Institute of Physics, University of Amsterdam

We consider an evaporating drop of volatile partially wetting liquid on a rigid solid substrate. In addition, the setup is covered with a plate, forming a narrow gap with the substrate. First, we develop an efficient mesoscopic description of the liquid and vapor dynamics in a gradient dynamics form. It couples the diffusive dynamics of the vertically averaged vapour density in the narrow gap to an evolution equation for the drop profile. The dynamics is purely driven by a free energy functional that incorporates wetting, bulk and interface energies of the liquid as well as vapour entropy.

Subsequently, we employ numerical simulations to validate the model against both experiments and simulations based on Stokes equation. Finally, we show that the gradient dynamics approach allows for extensions of our model to cover more intricate scenarios, e.g., spreading drops of volatile liquid on polymer brushes or on porous media.

15 min. break

DY 36.8 Thu 11:30 MER 02

Modeling the temporal evolution and stability of thin evaporating films for wafer surface processing — •Max Huber[1,2,3], Xiao Hu[1,2,3], Andreas Zienert[1,2,3], and Jörg Schuster[1,2,3] — [1]Fraunhofer Institute for Electronic Nano Systems ENAS, Technologie-Campus 3, 09126 Chemnitz, Germany — [2]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Rosenbergstr. 6, 09126 Chemnitz, Germany — [3]Center for Microtechnologies, Chemnitz University of Technology, Reichenhainer Str. 70, 09126 Chemnitz, Germany

Thin liquid films play a crucial role for many applications, e.g., coating, particle deposition, wafer bonding, and the cooling of electronic devices. As an example, we investigate the evaporation of thin water films on $LiTaO_3$. *Ab initio* density functional theory is used to calculate the Gibbs free energy of adsorption. These results are fitted to an expression of the Gibbs free energy which is derived from the disjoining pressure, consisting of molecular and structural components. In this way, the parameters for the disjoining pressure can be determined. A combination of literature-known models for spin drying and evaporation is used to analyze the temporal evolution of the water layer. The vapor above the water layer is modeled by diffusion and a mass balance is applied at the water-air interface. The results can be used to optimize the process time needed to reach the equilibrium thickness of the water layer. In addition, computational fluid dynamics simulations are utilized to investigate the evaporation in a wafer bond chamber during pump-down.

DY 36.9 Thu 11:45 MER 02

Electrokinetic, electrochemical and electrostatic surface potentials of the pristine water liquid-vapor interface — •Maximilian R Becker and Roland R Netz — Freie Universität Berlin, Berlin, Germany

Although conceptually simple, the interface between liquid water and vapor displays rich behavior and is subject to intense experimental and theoretical investigations. Different definitions of the electrostatic surface potential as well as different calculation methods, each relevant for distinct experimental scenarios, lead to widely varying potential magnitudes. Here, based on density-functional-theory (DFT) molecular dynamics (MD) simulations, different surface potentials are evaluated and compared to force-field (FF) MD simulations. The laterally averaged electrostatic surface potential, accessible to electron holography, is dominated by the trace of the water molecular quadrupole moment and therefore differs strongly between DFT and FF MD. Thus, when predicting electrostatic potentials within water molecules DFT simulation methods need to be used. The electrochemical surface potential inside a neutral atom, relevant for ion transfer reactions and ion surface adsorption, is much smaller and depends specifically on the atom radius. Charge transfer between interfacial water molecules leads to a sizable surface potential as well. However, when probing electrokinetics by explicitly applying a lateral electric field in DFT-MD simulations, the electrokinetic zeta-potential turns out to be negligible. Thus, interfacial polarization charges from charge transfer between water molecules do not lead to a significant electrokinetic mobility.

DY 36.10 Thu 12:00 MER 02

How Charges Separate at Moving Contact Lines — •Aaron D. Ratschow[1], Lisa S. Bauer[1], Pravash Bista[2], Stefan A. L. Weber[2,3], Hans-Jürgen Butt[2], and Steffen Hardt[1] — [1]Technische Universität Darmstadt, Darmstadt, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany — [3]Johannes Gutenberg Universtität, Mainz, Germany

Spontaneous charge accumulation in sliding drops is ubiquitous in nature and has been the subject of research activities for over two decades. Despite the growing number of experimental investigations in recent years, the physical mechanism behind the charging remains poorly understood. We identify the origin of charge separation as the dewetting of the immobilized part of the electric double layer (EDL) by the moving contact line. This layer of physically or chemically bound surface charges depends strongly on the local EDL structure, which is disturbed by the vicinity of the gas-liquid interface and the flow in the liquid. We summarize the physics of charge separation in an analytical model that predicts parametric dependencies on surface chemistry, wetting, and liquid properties. The results agree well with our experiments and numerical simulations and uncover decreasing charge separation with decreasing dynamic contact angle and increasing contact line velocity. Our findings reveal the universal mechanism of charge separation at moving contact lines, not limited to drops, with broad implications for the field of wetting.

DY 36.11 Thu 12:15 MER 02

Beyond the plate capacitor: Calculating the full dielectric tensor for arbitrary system geometries — •David Egger, Christoph Scheurer, and Karsten Reuter — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Realistic models for catalytic reactions at aqueous interfaces require a profound understanding of the electrostatic properties in the vicinity of the solvated catalytic complex, in particular for (photo-)electrochemical reactions with charged intermediates. However, explicit quantum mechanical simulations of these systems on the required length- and time-scales remain oftentimes out of reach. Coarse-graining the electrostatic response of the molecular solvent into a continuum dielectric, described by the dielectric permittivity tensor $\boldsymbol{\varepsilon}$, can hence be a necessity. Existing coarse-graining protocols for $\boldsymbol{\varepsilon}$ typically assume a separation of the dielectric response parallel and perpendicular to the active interface. This approximation is equivalent to two decoupled sets of in-series plate capacitors and ignores potential non-zero off-diagonal elements in the $\boldsymbol{\varepsilon}$ tensor.

In this contribution, we present a comprehensive and general formalism to coarse-grain molecular solvents into a truly anisotropic $\boldsymbol{\varepsilon}$ beyond this approximation. We obtain the full, spatially resolved dielectric tensor for arbitrary system geometries with no prior assumptions on boundary conditions. Common bulk and slab formulas are obtained as special cases. The approach is applied exemplarily to bulk water, water-dichloroethane liquid-liquid interfaces, and solvated platinum nanoparticles following from Wulff constructions.

DY 36.12 Thu 12:30 MER 02

Asymmetric Sessile Compound Drops — •Jan Diekmann and Uwe Thiele — Westfälische Wilhelms-Universität, Münster, Germany

We consider compound drops of two immiscible liquids on a rigid solid substrate. Having established a mesoscopic model (amending [1]) consistent with the macroscopic description of [2,3], we show for one-dimensional (1D) substrates that asymmetric compound drops can be energetically favoured using continuation techniques. Furthermore, we investigate selected dewetting and coarsening processes and discuss emerging steady compound drops for two-dimensional (2D) substrates, thereby discussing the relation of 1D and 2D results.

[1] A. Pototsky et al., "Morphology changes in the evolution of liquid

two-layer films". J. Chem. Phys. 122, 224711, 2005.

[2] L. Mahadevan, M. Adda-Bedia, and Y. Pomeau., "Four-phase merging in sessile compound drops". J. Fluid Mech. 451, 411-420, 2002.

[3] M. J. Neeson et al., "Compound sessile drops". Soft Matter 8, 11042-11050, 2012.

DY 36.13 Thu 12:45 MER 02

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

Droplets are set in motion on substrates with a spatio-temporal wettability pattern as generated, for example, on light-switchable surfaces. To study such cases, we implement the boundary-element method to solve the governing Stokes equations for the fluid flow field inside and on the surface of a droplet and supplement it by Cox–Voinov friction for the dynamics of the contact line. One objective of our research is targeted microfluidic transport of such droplets. In earlier work we investigated how a droplet can be steered by imposing a wettability pattern on the substrate [Grawitter and Stark, Soft Matter **17**, 2454 (2021)]. As a next step, we have recently extended our method to include substrates the height profile of which varies temporally in a prescribed manner.

We compare two cases: First, we investigate a droplet on substrates with planar-wave wettability pattern by varying the speed and wave length of the pattern. Second, we investigate a droplet on substrates with a planar-wave height profile. In both scenarios, for small wave velocities the droplet moves steadily forward. In contrast, above a wave velocity the droplet performs steady oscillations. These speed oscillations correlate with oscillations in the shape of the droplet which decay linearly as a function of pattern speed.

DY 37: Data Analytics of Complex Dynamical Systems (joint session DY/SOE)

Time: Thursday 9:30–12:00 Location: MOL 213

DY 37.1 Thu 9:30 MOL 213

Reverse-engineering method for XPCS studies of non-equilibrium dynamics — •Anastasia Ragulskaya[1], Vladimir Starostin[1], Nafisa Begam[1], Anita Girelli[1], Hendrik Rahmann[2], Mario Reiser[2], Fabian Westermeier[3], Michael Sprung[3], Fajun Zhang[1], Christian Gutt[2], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]Universität Siegen, Germany — [3]DESY, Germany

X-ray photon correlation spectroscopy (XPCS) is a powerful tool for the investigation of dynamics covering broad time and length scales [1]. For non-equilibrium states, the resulting time-dependent dynamic behavior can be described using the two-time correlation function (TTC), which often contains more interesting features than only the component along the diagonal, and cannot be easily interpreted via classical simulation methods. Here, a reverse-engineering (RE) approach is proposed based on particle-based simulations [1]. This approach is applied to XPCS measurements on a protein solution undergoing liquid-liquid phase separation. We demonstrate that the rich features of experimental TTCs can be well connected with the key control parameters including size distribution, concentration, viscosity, and mobility of domains. The dynamic information obtained from this RE analysis goes beyond existing theory. The RE approach established in this work is applicable to other processes such as film growth, domain coarsening, or phase transformations.

[1] A. Ragulskaya et. al., IUCrJ 9 (2022), 439.

DY 37.2 Thu 9:45 MOL 213

Sensitivity of principal components to changes in the presence of non-stationarity — •Henrik Bette and Thomas Guhr — Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Deutschland

Non-stationarity affects the sensitivity of change detection in correlated systems described by sets of measurable variables. We study this by projecting onto different principal components. Non-stationarity is modeled as multiple normal states that exist in the system even before a change occurs. The studied changes occur in mean values, standard deviations or correlations of the variables. Monte Carlo simulations are performed to test the sensitivity for change detection with and without knowledge about the non-stationarity for different system dimensions and numbers of normal states. A comparison clearly shows that the knowledge about the non-stationarity of the system greatly improves change detection sensitivity for all principal components. This improvement is largest for those components that already provide the greatest possibility for change detection in the stationary case.

DY 37.3 Thu 10:00 MOL 213

Inferring partial differential equations from molecular dynamics simulations — •Oliver Mai, Tim Kroll, Uwe Thiele, and Oliver Kamps — Institute of Theoretical Physics and Center for Nonlinear Science, University of Münster

Although integral to scientific or engineering applications, deriving partial differential equations (PDEs) solely from experimental data proves quite challenging and in most cases relies on physical principles in addition to qualitative behaviour of the system. In the last decade various efforts based on empirical data have been put forth to supplement first-principle derivations in theoretical sciences. That is in place of or in addition to typical conservation laws or phenomenological observations, time series data has been used to yield analytic expressions to describe the spatio-temporal evolution of a given dynamical system. While there have been various improvements in the sparsity and interpretability of the results, we provide another approach to optimization using the predictive power of the estimation when integrating it. Additionally aggregated small scale behaviour in macro- or mesoscopic experiments may exhibit unknown governing laws and as such a way for comparing data more directly to models derived in statistical physics may prove critical in furthering our understanding. To this end we study the application of system identification methods on molecular dynamics (MD) simulations.

DY 37.4 Thu 10:15 MOL 213

Reproducibility of analysis workflows in biomedical physics — •Alexander Schlemmer[1,4], Inga Kottlarz[1,2], Baltasar Rüchardt[1,3,4], Ulrich Parlitz[1,2,4], and Stefan Luther[1,2,3,4] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, Georg-August-Universität Göttingen, Germany — [3]Institute of Pharmacology and Toxicology, University Medical Center Göttingen, Germany — [4]German Center for Cardiovascular Research (DZHK), Partner Site Göttingen, Germany

Sustainable and well-documented data analysis workflows are essential for effectiveness and reproducibility in data-intensive research. In our terminology, documentation includes method and algorithm descriptions as well as human- and machine-readable representations of parameters, initial conditions and data, versions and dependencies and a well-defined software execution environment.

In practice, many software frameworks for reproducibility fail to achieve a widespread adoption. Using examples from data analysis in cardiac research, we illustrate typical challenges and show, how simple guidelines - when implemented in a pragmatic way - can already lead to a high degree of documentation and reproducibility. Furthermore, we discuss the employment of containers and semantic data management which simplify reproducibility, findability and interoperability.

DY 37.5 Thu 10:30 MOL 213

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

Complex systems in nature, technology and society can undergo sudden transitions between system states with very different behaviour. In order to avoid undesired consequences of these tipping events, statistical measures have been proposed as leading indicators. They can give a hint of an ongoing bifurcation-induced (B-tipping) destabilization process. However, we present an alternative approach that is open-source available and more robust under numerous aspects. It assumes the dynamical system to be described by a Langevin equation.

Starting from this stochastic description, we combine MCMC sampling, rolling window methods and Bayesian reasoning to derive the drift slope as an alternative early warning sign including credibility bands which make it easier to distinguish significant leading indicator trends prior to B-tipping. Furthermore, our approach provides information about an increasing noise level in a multi-stable system. This is an important information related to the Kramers escape rate of a noise-induced tipping (N-tipping) event. We show some results and discuss the method's potential to be applied in N-tipping scenarios and under more complex conditions like correlated non-Markovian or multiplicative noise. Finally, possible limitations and tasks of future research are mentioned.

15 min. break

Invited Talk DY 37.6 Thu 11:00 MOL 213

Power law error growth rates – a dynamical mechanism for a strictly finite prediction horizon in weather forecasts — Hynek Bednar[1,2], Jonathan Brisch[1], Burak Budanur[1], and •Holger Kantz[1] — [1]Max Planck Insstiute for the Physics of Complex Systems, Dresden, Germany — [2]Dept. of Atmospheric Physics, Charles University, Prague, Czech Republic

While conventional chaotic systems have a finite positive Lyapunov exponent, physical arguments and observations suggest that the maximal Lyapunov exponent of the model equations of the atmosphere is the larger the smaller are the resolved spatial scales. Specifically, a power law divergence of the scale dependent error growth rate would translate into a strictly finite prediction horizon, since due to the divergence, additional accuracy of initial conditions is not translated into longer prediction times. We present conceptual toy models with such behavior, we show its presence in a more realistic spatially extended system with advective transport, and we present numerical results from turbulence simulations where the largest Lyapunov exponent scales as an inverse power of spatial resolution. The idea of a power law scale dependence of error growth rates and of a finite prediction horizon is also supported by re-analysis of numerical error growth experiments performed with an operational weather model. Altogether, this suggests that the prediction horizon of numerical weather prediction is strictly finite.

DY 37.7 Thu 11:30 MOL 213

Wave Digital Optimization of a Modified Compact Models of 1T-1R Random Resistive Access Memory Cells — •Bakr Al Beattie[1], Max Uhlmann[2], Gerhard Kahmen[2], and Karlheinz Ochs[1] — [1]Ruhr-Universität Bochum, Lehrstuhl für digitale Kommunikationssysteme, Bochum, Deutschland — [2]Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Deutschland

Random Resistive Access Memory (RRAM) cells are popular memristive devices that are commonly used in neuromorphic applications. In this context, RRAM cells are usually utilized to embed synaptic plasticity, a property that is exhibited by biological synapses, into analog-based artificial neural networks. However, since RRAM-based technology has yet to reach a state of maturity, circuit designers are usually forced to make use of compact models to avoid dealing with device-to-device variabilities. The Stanford PKU model is a well-established compact model that has been developed to capture the dynamics of 1T-1R RRAM cells. In this contribution, we present a modified compact model, based on the Stanford PKU model, that takes more properties of real RRAM cells into account, such as the RESET voltage shift in multilevel devices. To demonstrate the capabilities of our model, we exploit the wave digital concept to apply a live parameter optimization, which fits the model parameters to a technologically reproducible device from the Leibniz Institute for High Performance Microelectronics (IHP).

DY 37.8 Thu 11:45 MOL 213

Discovering Causality and Coupling in high dimensional nonlinear dynamical systems — •Tim Kroll[1,2] and Oliver Kamps[2] — [1]Westfälische Wilhelms-Universität Münster, 48149 Münster — [2]Center for Nonlinear Science, Westfälische Wilhelms-Universität Münster, 48149 Münster

In this talk we present a method to infer causal relationships between observables from data of systems where the underlying dynamics are not known a priori. The method is based on the hypothesis that the system of interest can in principle be described by a set of coupled nonlinear ordinary differential equations. Following the work of Prusseit and Lehnertz in 2008 we can then determine the couplings between observables by integrating out all other observables. Since the estimation of the underlying dynamical system invokes the efficient representation in terms of polynomials the method can be applied also to hight dimensional systems. We demonstrate the capabilities of the method by inferring the network structure of coupled Rössler-Attractors.

DY 38: Active Matter IV (joint session DY/BP/CPP)

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

Invited Talk DY 38.1 Thu 9:30 ZEU 160

Acoustically propelled nano- and microparticles: From fundamentals to applications — •Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Among the existing types of artificial active colloidal particles, acoustically propelled nano- and microparticles have a particularly high potential for future applications in fields like medicine and materials science. However, despite intensive research on this type of motile particles in recent years, the understanding of their properties is still very limited. A reason for the limited understanding is that the previous research has mostly been experimental and that it is difficult to study the dependence of certain system parameters on the propulsion of the particles in experiments since the parameters can often not be varied independently of the other parameters and in ranges of reasonable size. In this talk, I will give an overview about our theoretical investigation of the properties of acoustically propelled nano- and microparticles and the challenges that remain for future research.
Funded by the Deutsche Forschungsgemeinschaft (DFG) – 283183152 (WI 4170/3).

DY 38.2 Thu 10:00 ZEU 160

Force on probe in a confined active fluid — Shuvojit Paul[1], •Ashreya Jayaram[2], N Narinder[1], Thomas Speck[2], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, 78464 Konstanz, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55128 Mainz, Germany

When immersed in a dispersion of smaller "depletants", a colloidal particle experiences depletion forces in the presence of another colloidal particle or under confinement. While the nature of these forces is well-established for passive systems, much less is known about the consequence of making the depletants self-propelled or "active". In this work, we consider a large, optically trapped probe under circular confinement surrounded by smaller active Janus particles. We find that the force experienced by the probe varies non-monotonically as the distance between the colloid and the confinement is increased. To rationalize this observation, we relate the measured force to the active stress and, subsequently, to the microstructure of the surrounding active fluid. Going beyond synthetic active matter, our work could shed light on the organization of intracellular entities in biological systems.

DY 38.3 Thu 10:15 ZEU 160

Symmetry-breaking refractive index profiles as a propulsion mechanism for active Brownian particles — •Julian Jeggle[1], Matthias Rüschenbaum[2], Cornelia Denz[2], and Raphael Wittkowski[1] — [1]Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Institut für Angewandte Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Active Brownian particles (ABPs) have been realized with various propulsion mechanisms such as self-diffusiophoresis, self-electrophoresis or acoustic scattering. Typically, these mechanisms induce flow fields around the particles that represent a deviation from the "pure" ABP model. Here, we present a novel implementation of ABPs in the form of transparent microswimmers with a symmetry-breaking refractive index gradient. Utilizing the momentum transfer

associated with light refraction as the driving force induces no flow fields beyond Stokes flow. Unlike optothermally driven particles, this archetype of ABPs also allows for sensitivity to the phase and polarization of the driving light field thus improving the spatio-temporal control of light-based propulsion mechanisms. Using non-light-absorbing particles enables bulk volume systems and allows the introduction of feedback loops, therefore making this approach a promising foundation for adaptive matter systems.

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

DY 38.4 Thu 10:30 ZEU 160

The interaction-expansion method: a systematic derivation strategy for active field theories* — •Michael te Vrugt[1,2], Jens Bickmann[1,2], Stephan Bröker[1,2], Tobias Frohoff-Hülsmann[1], Eyal Heifetz[3], Michael E. Cates[4], Uwe Thiele[1,5,6], and Raphael Wittkowski[1,2,5] — [1]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]SoN, Westfälische Wilhelms-Universität Münster — [3]Porter School of the Environment and Earth Sciences, Tel Aviv University, 69978 Tel Aviv, Israel — [4]DAMTP, Centre for Mathematical Sciences, University of Cambridge, Cambridge CB3 0WA, United Kingdom — [5]CeNoS, Westfälische Wilhelms-Universität Münster — [6]CMTC, Westfälische Wilhelms-Universität Münster

Field-theoretical models have made enormous contributions to our understanding of the collective dynamics of active matter. In this contribution, we introduce the interaction-expansion method (IEM) [1], which allows for a systematic derivation of active field theories from the microscopic dynamics of individual particles. We then discuss some recent applications of the IEM to particles with orientation-dependent propulsion speed [2] and particles with inertia [3].

[1] M. te Vrugt et al., in preparation (2022)
[2] S. Bröker et al., arXiv:2210.13357 (2022)
[3] M. te Vrugt et al., Nature Communications (provisionally accepted), arXiv:2204.03018 (2022)

Funded by the Deutsche Forschungsgemeinschaft (DFG)– 283183152

DY 38.5 Thu 10:45 ZEU 160

Entropy production in active turbulence — •Byjesh Nalini Radhakrishnan, Thomas Schmidt, and Etienne Fodor — Department of physics and material science, University of Luxembourg

Active particles like bacteria and sperm cells sustain a continuous intake and dissipation of energy. Consequently, they are intrinsically out of equilibrium which leads to a non-vanishing entropy production rate (EPR) even in steady states. Quantifying how the EPR varies in different collective phases is crucial in developing a thermodynamic framework for active matter. In this work, we look at the EPR in active turbulence. We use Active Model H, a continuum model for active particles in a momentum-conserving fluid, to study turbulence in contractile scalar active systems. We measure the local EPR in numerical simulations, which unveils the role of the noise and activity parameters on the EPR in active turbulent systems.

15 min. break

DY 38.6 Thu 11:15 ZEU 160

Phase transitions in multicomponent active matter: a quantitative kinetic theory — •Jakob Mihatsch[1], Thomas Ihle[1], Rüdiger Kürsten[2], and Horst-Holger Boltz[1] — [1]Institute for Physics, University of Greifswald, Greifswald, Germany — [2]Departament de Física de la Matèria Condensada, University of Barcelona, Barcelona, Spain

We consider a multicomponent model of self-propelled particles with Kuramoto-type alignment interactions. Starting from the N-particle Fokker-Planck equation we observe that the usual factorization Ansatz of the probability density, often called Molecular Chaos approximation, predicts a relaxation behavior which qualitatively disagrees with agent-based simulations. Therefore, we develop a kinetic theory which takes the time-evolution of the two-particle correlation function explicitly into account, i.e. goes beyond the mean-field approximation. We show that this theory predicts the relaxation behavior of the system as well as the order-disorder transition with high precision in certain parameter ranges. In particular, the dependence of the transition threshold on the particle speed is predicted correctly.

DY 38.7 Thu 11:30 ZEU 160

Emergent collective behaviour due to virtual interactions between robotic swimmers — •Samudrajit Thapa[1,2], Bat-El Pinchasik[1,3], and Yair Shokef[1,2,3] — [1]School of Mechanical Engineering, Tel Aviv University, Tel Aviv 69978, Israel — [2]Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv 69978, Israel — [3]Center for the Physics and Chemistry of Living Systems, Tel Aviv University, 69978, Tel Aviv, Israel

Many organisms in nature use local interactions to realize global collective behaviour. Here we study how simple two body distance-based interactions between active Brownian particles results in collective motion. The interactions are not physical but virtual, wherein each particle senses the presence of other particles nearby and changes its behaviour accordingly. We study the radial distribution function to quantify the emergent interactions for both social and anti-social behaviour. Using Langevin dynamics simulations, we discover that under certain conditions positive correlations of the motion can emerge even in the case of anti-social behaviour. Our results might be potentially useful for designing robotic swimmers that can swim collectively just based on sensing the distance to their neighbours.

DY 38.8 Thu 11:45 ZEU 160

Kinetic Event-Chain Algorithm for Active Matter — •Nico Schaffrath, Thevashangar Sathiyanesan, Tobias Kampmann, and Jan Kierfeld — Physics Department, TU Dortmund University, 44221 Dortmund, Germany

We present a cluster kinetic Monte-Carlo algorithm for active matter systems of self-propelled hard particles. The kinetic event-chain algorithm is based on the event-chain Monte-Carlo method and is applied to active hard disks in two dimensions. The algorithm assigns Monte-Carlo moves of active disks a mean time based on the mean and variance of the move length in force direction. This time is used to perform diffusional rotation of their propulsion force. We show that the algorithm reproduces the motility induced phase separated region in the phase diagram of hard disks correctly and efficiently.

DY 38.9 Thu 12:00 ZEU 160

Emergent pattern formation in communicating active matter — •Robert Grossmann[1], Zahra Mokhtari[2], Robert I.A. Patterson[3], and Felix Höfling[2,4] — [1]Institut für Physik und Astronomie, Universität Potsdam — [2]Institut für Mathematik, Freie Universität Berlin — [3]WIAS Berlin — [4]Zuse Institut Berlin

Inspired by trail formation as observed in colonies of driver ants, for example, we study ensembles of agent particles that communicate via deposition and sensing of pheromones. These chemical traces are produced by the agents themselves and encode their current position and walking direction. Other agents passing by will then tend to align with the orientation inscribed in the pheromone traces. In the limit of short pheromone lifetime, the dynamics of this system reduces to the seminal Vicsek model and, thus, yields the formation of transversally moving bands. In the opposite limit, the effective agent-agent interaction represents a form of delayed feedback and yields the spontaneous formation of macroscopic, persistent trails, which are followed and reinforced by the agents [New J. Phys. **24** 013012 (2022)]. In this talk, we present large-scale simulations of the agent model and establish the phase diagram as function of the lifetime of pheromones. We rationalize our findings by analyzing mean-field equations that are systematically derived from the stochastic particle model. Combining numerical solutions of these order parameter equations and a linear stability analysis, we show how transversal bands, common in the Vicsek model, are destabilized, giving rise to the formation of "longitudinal" trails, pointing in the mean direction of motion.

DY 38.10 Thu 12:15 ZEU 160

Binary Mixture of Deforming Particles — •Yiwei Zhang, Alessandro Manacorda, and Etienne Fodor — DPhyMS, University of Luxembourg, Luxembourg, Luxembourg

Phase separation occurs in miscible liquids where components have distinct properties. In reactors, components undergo stochastic change in their properties which affect the liquid composition. While phase separation and reaction-diffusion have already been studied extensively as separate ingredients, how they combine in non-ideal reactors remains poorly understood. To bridge this gap, we consider repulsive particles with fluctuating size subject to one-body landscape and nonequilibrium synchronisation. The landscape features minima which, regarding size as reaction coordinate, distinguish three states: Particles with

finite size, either A- or B-type, and point particles. In this context, synchronisation penalizes A particles in B-rich phases, and vice versa, so that the system eventually accommodates a uniform state. We report the phase diagram depending on the stability of each state and the corresponding particle sizes. Combining hydrodynamic and phenomenological arguments, we recapitulate how metastability regulates the interplay between synchronisation and repulsion. Our results reveal the role of nonequilibrium kinetic factors at play in non-ideal reaction-diffusion systems.

DY 38.11 Thu 12:30 ZEU 160

Self-organization of model catalytic cycles — •Vincent Ouazan-Reboul[1], Jaime Agudo-Canalejo[1], and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, D-37077, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, OX1 3PU, Oxford, UK

We study analytically and numerically a model metabolic cycle composed of an arbitrary number of species of catalytically active particles. Each species converts a substrate into a product, the latter being used as the substrate by the next species in the cycle. Through a combination of catalytic activity and chemotactic mobility, the catalytic particles develop effective interactions with particles belonging to neighbouring species in the cycle. These interactions, being fully out-of-equilibrium, show some unusual features, in particular being non-reciprocal. We find that such model metabolic cycles are able to self-organize through a macroscopic instability, with a strong dependence on the characteristics of the cycle. For instance, cycles containing an even number of species are able to minimize repulsion between their component particles by aggregating all even-numbered species in one cluster, and all odd-numbered species in another. Such a grouping is not possible if the cycle contains an odd number of species, which can lead to oscillatory steady states in the case of chasing interactions.

DY 38.12 Thu 12:45 ZEU 160

Reentrant condensation transition in a model of driven scalar active matter with diffusivity edge — Berx Jonas[2], •Bose Aritra[1], Mahault Benoit[1], and Golestanian Ramin[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany — [2]Institute for Theoretical Physics, KU Leuven, B-3001 Leuven, Belgium — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

A class of scalar active matter for which the effective diffusivity vanishes beyond a certain density threshold, hereby referred to as diffusivity edge, triggers the formation of a condensate when confined in a harmonic potential. The condensation transition exhibits remarkable similarities with a Bose-Einstein Condensation (BEC). Here we study the effect of a diffusivity edge in a system of scalar active matter confined by a periodic potential and driven by an external force.

We find that this system shows qualitatively distinct stationary regimes depending on the amplitude of the driving force with respect to the potential barrier. For small driving, the diffusivity edge induces a condensation analogous to the BEC-like transition reported for the nondriven case, which is characterised by a density-independent steady state current. Conversely, large external forces lead to a qualitatively different phase diagram where condensation is not possible below a density threshold and the associated transition at moderate densities above the threshold the transition is reentrant due to the existence of a subsequent evaporation transition at low effective temperatures.

DY 39: Networks: From Topology to Dynamics II (joint session SOE/DY)

Time: Thursday 9:30–10:00 Location: ZEU 260

Invited Talk DY 39.1 Thu 9:30 ZEU 260

Networks in space and time – Exploring the physics in graph learning — •Ingo Scholtes — Julius-Maximilians-Universität Würzburg, Chair of Machine Learning for Complex Networks, Center for Artificial Intelligence and Data Science, D-97074 Würzburg, Germany

Network Analysis and Graph Neural Networks have become cornerstones for the application of data science and machine learning to complex systems. Addressing geometric machine learning in non-Euclidean data, I will introduce key concepts that help to apply deep learning to graphs. We cover message passing algorithms, convolutional filters, discrete Laplacians and neural representation learning and highlight relationships between graph learning and physics.

We finally explore how time-resolved data on dynamic networks helps us to better understand complex systems and how we can incorporate the time dimension into deep graph learning. We introduce De Bruijn Graph Neural Networks (DBGNNs), a novel time-aware graph neural network architecture. Our approach accounts for temporal-topological patterns that unfold via causal walks, i.e. temporally ordered sequences of links by which nodes can influence each other over time. We develop a graph neural network architecture that utilizes De Bruijn graphs of multiple higher orders to implement a message passing scheme that follows a non-Markovian dynamics, which enables us to learn patterns in the causal topology of complex networks.

DY 40: Stochastic Thermodynamics

Time: Thursday 10:00–12:30 Location: ZEU 250

DY 40.1 Thu 10:00 ZEU 250

Optimized Work Protocols for the Higgs RNA-Model — •Peter Werner and Alexander K. Hartmann — Institute of Physics, University of Oldenburg, Germany

When a system is driven from one state to another in a *finite* amount of time $t \in [0, \ldots, \tau]$ by changing an external control parameter according to a protocol $\lambda(t)$, some work W is performed. Here $\langle W \rangle \geq \Delta F$ holds, where ΔF is the equilibrium free energy difference between initial and final states. The protocol $\lambda^*(t)$ minimizing the average amount of work is of interest, since it tightens the upper bound to ΔF. The optimum protocols of simple Brownian-particle systems exhibit distinct jumps especially at the beginning and end of the process [1,2] and it was speculated that these are a generic feature for arbitrary systems.

Here the *many-particle* Higgs RNA model [3] is considered, where work is performed by stretching the RNA through changing an external force. For this model, an exact calculation of the free-energy differences ΔF and the sampling of the equilibrium initial state can be performed in polynomial time. The work processes are realized by means of nonequilibrium Monte-Carlo simulations [4]. The optimum protocols are obtained numerically with the parallel-tempering approach. Also for this complex system, the optimum protocols exhibit distinct jumps at the beginning and end.

[1] T. Schmiedl and U. Seifert, Phys. Rev. Lett., **98**, 108301 (2007)
[2] H. Then and A. Engel, Phys. Rev. E **77**, 041105 (2008)
[3] P. G. Higgs, Phys. Rev. Lett., **76**, 704 (1996)
[4] P. Werner and A. K. Hartmann, Phys. Rev. E **104**, 034407 (2021)

DY 40.2 Thu 10:15 ZEU 250

Coherence of oscillations in the weak-noise limit — •Benedikt Remlein, Volker Weissmann, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

In a noisy environment, oscillations lose their coherence, which can be characterized by a quality factor. We determine this quality factor for oscillations arising from a driven Fokker-Planck dynamics along a periodic one-dimensional potential analytically in the weak-noise limit. With this expression, we can prove for this continuum model the analog of an upper bound that has been conjectured for the coherence of oscillations in discrete Markov network models. We show that our approach can also be adapted to motion along a noisy two-dimensional limit cycle. Specifically, we apply our scheme to the noisy Stuart-

Landau oscillator and the thermodynamically consistent Brusselator as a simple model for a chemical clock. Our approach thus complements the fairly sophisticated extant general framework based on techniques from Hamilton-Jacobi theory with which we compare our results numerically [1].

[1] B. Remlein, V. Weissmann, and U. Seifert, Phys. Rev. E 105, 064101 (2022)

DY 40.3 Thu 10:30 ZEU 250

Work extraction potential for a single spin in equilibrium with a non-isotropic environment — •Felix Hartmann[1] and Janet Anders[1,2] — [1]Institut für Physik und Astronomie, University of Potsdam, 14476 Potsdam, Germany — [2]Department of Physics and Astronomy, University of Exeter, Stocker Road, Exeter EX4 4QL, UK

Thermal equilibrium properties of nanoscale systems deviate from standard macroscopic predictions due to a non-negligible coupling to the environment. For non-isotropic three-dimensional materials, we derive the mean force corrections to the equilibrium state of a single classical spin vector. The result is valid at arbitrary coupling strength.

Specifically, we consider cubic, orthorhombic, and monoclinic symmetries, and compare differences in their spin expectation values as a function of temperature. We underpin the correctness of the mean force state by evidencing its match to the steady state of the simulated non-Markovian spin dynamics. Our results show an explicit dependence on the symmetry of the material in which the spin is confined.

Further, we quantify how the mean force-generated inhomogeneities in the energy shells lead to a work extraction potential. Such inhomogeneities constitute a classical equivalent to quantum coherences.

DY 40.4 Thu 10:45 ZEU 250

Time-resolved statistics of snippets as general framework for model-free entropy estimators — •Jann van der Meer, Julius Degünther, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart

Irreversibility is commonly quantified by entropy production. An external observer can estimate it through measuring an observable that is antisymmetric under time-reversal like a current. We introduce a general framework that, inter alia, allows us to infer a lower bound on entropy production through measuring the time-resolved statistics of events with any symmetry under time-reversal, in particular, time-symmetric instantaneous events. We emphasize Markovianity as a property of certain events rather than of the full system and introduce an operationally accessible criterion for this weakened Markov property. Conceptually, the approach is based on snippets as particular sections of trajectories, for which a generalized detailed balance relation is discussed.

DY 40.5 Thu 11:00 ZEU 250

Anomalous relaxation from a non-equilibrium steady state: An isothermal analog of the Mpemba effect — •Julius Degünther and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

The Mpemba effect denotes an anomalous relaxation phenomenon where a system initially at a hot temperature cools faster than a system that starts at a less elevated temperature. We introduce an isothermal analog of this effect for a system prepared in a non-equilibrium steady state that then relaxes towards equilibrium. Here, the driving strength, which determines the initial non-equilibrium steady state, takes the role of the temperature in the original version. As a paradigm, we consider a particle initially driven by a non-conservative force along a one-dimensional periodic potential. We show that for an asymmetric potential relaxation from a strongly driven initial state is faster than from a more weakly driven one at least for one of the two possible directions of driving. These results are first obtained through perturbation theory in the strength of the potential and then extended to potentials of arbitrary strength through topological arguments.

[1] Julius Degünther and Udo Seifert, EPL, 139 4 (2022) 41002

15 min. break

DY 40.6 Thu 11:30 ZEU 250

Measurement phase transitions in the no-click limit as quantum phase transitions of a non-hermitean vacuum. — •Caterina Zerba[1,2,3] and Alessandro Silva[2] — [1]Technical University of Munich, 85748 Garching, Germany — [2]International School for Advanced Studies (SISSA), via Bonomea 265, 34136 Trieste, Italy — [3]Università degli Studi di Trieste, via Alfonso Valerio 2, 34127 Trieste, Italy

We study dynamical phase transitions occurring in the stationary state of the dynamics of integrable many-body non-hermitian Hamiltonians, which can be either realized as a no-click limit of a stochastic Schrödinger equation or using spacetime duality of quantum circuits. In two specific models, the Transverse Field Ising Chain and the Long Range Kitaev Chain, we observe that the entanglement phase transitions occurring in the stationary state have the same nature as that occurring in the vacuum of the non-hermitian Hamiltonian: an area law phase when the imaginary part of the quasi-particle spectrum is gapped and a logarithmic growth for gapless imaginary spectrum. This observation suggests the possibility to generalize the area-law theorem to non-Hermitian Hamiltonians

DY 40.7 Thu 11:45 ZEU 250

Thermodynamics of growth in chemical reaction networks — •Shesha Gopal Marehalli Srinivas, Francesco Avanzini, and Massimiliano Esposito — Complex Systems and Statistical Mechanics, Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg

Open chemical reaction networks show a variety of complex dynamical behaviour such as chemical waves, oscillations, chaotic dynamics, multistability, and so on. Progress in stochastic thermodynamics has enabled us to identify the energetic costs of these phenomena. However, very little attention has been paid to chemical growth. We will identify the necessary conditions under which open homogeneous CRNs evolving with mass action kinetics show asymptotic growth. Our main results show that growth with nonequilibrium abundances requires nonlinear CRNs with the influx of at least one species from the surrounding. Linear CRNs, on the other hand, can only grow with equilibrium abundances. Our results illustrate the important interplay between topology and the chemostatting procedure in determining the asymptotic dynamics of CRNs.

DY 40.8 Thu 12:00 ZEU 250

Irreversible fluctuations herald dynamical phases in non-Hermitian phase-field models — •Thomas Suchanek[1], Klaus Kroy[1], and Sarah Loos[2] — [1]Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany — [2]DAMTP, University of Cambridge, Cambridge, United Kingdom

We study the time-reversal symmetry (TRS) breaking of fluctuations in phase-field models that exhibit dynamical phases. We focus on two typical scenarios in which dynamical phases can be born, namely, oscillatory instabilities and the recently uncovered $\mathcal{PT}$-symmetry breaking transitions in non-Hermitian systems [1] that are accompanied by Exceptional Points. Quantifying the TRS breaking by the informatic entropy production rate [2] and analytically investigating the zero noise limit, we find divergent behavior at both transitions. We discuss an example model of two nonreciprocally coupled Chan-Hilliard fields, and offer interpretations of the TRS breaking in terms of interface dynamics, the $\mathcal{PT}$-symmetry breaking and the amplification of dissipative noise near Exceptional Point transitions.

[1] M. Fruchart, R. Hanai, P. B. Littlewood, and V. Vitelli, Nonreciprocal phase transitions, Nature 592, 363-369 (2021).
[2] C.Nardini, E. Fodor, E. Tjhung, F. van Wijland, J. Tailleur, and M. E. Cates, Entropy production in field theories without time-reversal symmetry: Quantifying the non-equilibrium character of active matter, Phys. Rev. X 7, 021007 (2017).

DY 40.9 Thu 12:15 ZEU 250

Large deviations theory for noisy non-linear electronics — •Ashwin Gopal, Massimiliano Esposito, and Nahuel Freitas — University of Luxembourg, L-1511 Luxembourg, Luxembourg

The latest generations of transistors are nanoscale devices whose performance and reliability are limited by thermal noise in low-power applications. Therefore, developing efficient methods to compute the voltage and current fluctuations in such non-linear electronic circuits is essential. In this presentation, I will describe the large deviations approach to compute these fluctuations using the stochastic thermodynamic description of CMOS-based electronics (Phys. Rev. B 106, 155303). Starting from the thermodynamically consistent description of the charge transfer at a single electron level, I will then consider the macroscopic limit. This corresponds to scaling up the transistor's physical dimensions, resulting in an increase in the number of elec-

trons on the conductors. In this limit, the thermal fluctuations satisfy a Large Deviations Principle which I will show is also remarkably precise in settings involving only a few tens of electrons, by comparing our results with Gillespie simulations and spectral methods. Traditional approaches, using the stationary Gaussian white noise, are recovered by resorting to an ad hoc diffusive approximation revealing their inconsistencies. To illustrate these findings, I will use the case study of the low-power CMOS inverter, or NOT gate, which is a basic primitive in electronic design. Finally, I will briefly comment on thermodynamic uncertainty (TUR) relations and information processing, in the context of such electronic circuits.

DY 41: Networks: From Topology to Dynamics III (joint session SOE/DY)

Time: Thursday 10:00–10:45 Location: ZEU 260

DY 41.1 Thu 10:00 ZEU 260

Understanding Braess' Paradox in power grids — •Benjamin Schäfer[1], Thiemo Pesch[2], Debsankha Manik[3], Julian Gollenstede[4], Guosong Lin[4], Hans-Peter Beck[4], Dirk Witthaut[2], and Marc Timme[5,3] — [1]Karlsruhe Institute of Technology — [2]Forschungszentrum Jülich — [3]Max Planck Institute for Dynamics and Self-Organization — [4]Clausthal University of Technology — [5]Technical University of Dresden

The ongoing energy transition requires power grid extensions to connect renewable generators to consumers and to transfer power among distant areas. The process of grid extension requires a large investment of resources and is supposed to make grid operation more robust. Yet, counter-intuitively, increasing the capacity of existing lines or adding new lines may also reduce the overall system performance and even promote blackouts due to Braess' paradox. Braess' paradox was theoretically modeled but not yet proven in realistically scaled power grids. Here, we present an experimental setup demonstrating Braess' paradox in an AC power grid and show how it constrains ongoing large-scale grid extension projects. We present a topological theory that reveals the key mechanism and predicts Braessian grid extensions from the network structure. These results offer a theoretical method to understand and practical guidelines in support of preventing unsuitable infrastructures and the systemic planning of grid extensions.

DY 41.2 Thu 10:15 ZEU 260

Evolutionary Optimization of networks towards complexity: role of link distribution and cross-consistency of network complexity measures — Archan Mukhopadhyay and •Jens Christian Claussen — University of Birmingham, UK

In a framework utilizing complexity measures for optimizing graphs and networks towards complexity, we use one complexity measure as fitness function of an evolutionary algorithm, and evaluate the resulting graphs through other complexity measures and network properties. We consider both evolution of graphs where the total number of links can evolve, as well as the case of constrained number of links. We find that in a certain range MAg optimizes towards degree-regular graphs, which is not observed for other complexity measures. We also investigate the consistency among the complexity measures on artificial and real-world datasets.

DY 41.3 Thu 10:30 ZEU 260

On the role of deleterious mutant regime in steering long-term evolution — Nikhil Sharma[1], •Joachim Krug[2], and Arne Traulsen[1] — [1]Department of Evolutionary Theory, Max Planck Institute for Evolutionary Biology, 24306 Plön, Germany — [2]Institute for Biological Physics, University of Cologne, Köln, Germany

Evolutionary Graph Theory aims to understand the interplay of natural selection and genetic drift on spatial structures. A spatial structure is modeled as a graph with nodes representing asexually reproducing individuals, and edges dictate the interaction among these individuals. Based on the fixation probabilities of mutants on graphs, graphs are mainly categorised as amplifiers of selection and suppressors of selection. We study Moran Birth-death origin fixation dynamics on graphs, see https://doi.org/10.1073/pnas.2205424119. As expected, amplifiers of selection attain higher steady-state average fitness than the complete graph. However, we found that a suppressor of fixation, having a lower probability of fixing mutants regardless of their fitness values compared to the complete graph, beats the complete graph in the long term by attaining higher average fitness. It happens because of the suppressor's ability to reject deleterious mutants more efficiently. Similarly, an amplifier of fixation, a structure with a higher probability of fixing mutants regardless of their fitness values, attains lower steady-state average fitness. It happens because of the amplifier's poor ability to reject deleterious mutants. These two examples illustrate the importance of the deleterious mutant regime in steering long-term evolution, which, to our knowledge, has been overlooked in the literature.

DY 42: Poster: Active Matter, Soft Matter, Fluids

Time: Thursday 13:00–16:00 Location: P1

DY 42.1 Thu 13:00 P1

Transition to mesoscale turbulence in an active fluid — •Henning Reinken[1], Sebastian Heidenreich[2], Markus Bär[2], and Sabine H.L. Klapp[1] — [1]Technische Universität Berlin — [2]Physikalisch-Technische Bundesanstalt

Microwsimmer suspensions, a paradigmatic example of an active fluid, self-organize into complex spatio-temporal flow patterns, including regular vortex lattices and mesoscale turbulence, a highly dynamical state that exhibits a characteristic length scale. This work investigates the transition to this turbulent state using a continuum-theoretical approach for the effective microswimmer velocity field [1], where the dynamics is governed by the competition between relaxation to a regular vortex lattice and destabilization by nonlinear advection. For the unconstrained bulk flow, we show how to identify the onset of mesoscale turbulence analytically. To this end, we determine the linear stability of the vortex lattice state by explicitly taking into account the coupling between multiple modes via the nonlinear terms. Recent experiments [2] have also demonstrated how vortex lattices can be stabilized by small obstacles [3]. Using the continuum-theoretical approach, we further show numerically that the formation of these patterns exhibits features of a continuous second-order equilibrium phase transition in the 2D Ising universality class [4].

[1] Reinken et al., Phys. Rev. E **97**, 022613 (2018)
[2] Nishiguchi et al., Nat. Commun. **9**, 4486 (2018)
[3] Reinken et al., Commun. Phys. **3**, 76 (2020)
[4] Reinken et al., Phys. Rev. Lett. **128**, 048004 (2022)

DY 42.2 Thu 13:00 P1

Dynamics and clustering of active run-and-tumble particles on two-dimensional lattices — •Lars Torbjørn Stutzer and Peter Sollich — Institut für Theoretische Physik, Georg-August Universität Göttingen

We study the dynamics of run-and-tumble particles on two-dimensional lattices, focusing on the effects of lattice geometry (square, triangular and hexagonal) and maximum occupation number $n_{\max}$ per lattice site. We identify three phases in the stationary state: a cluster (C) phase with extensive clusters formed by motility-induced phase separation, which appears only for $n_{\max} \geq 2$; a gas (G) phase consisting of finite-sized clusters; and a new sponge (S) phase where small fluctuating clusters percolate. The nature of the transitions between these phases depend on lattice type and density. C-G transitions are mostly, but not always, first order, while C-S transitions are continuous. Single particle displacement distributions become non-Gaussian at higher densities, with intermediate exponential tails. Considering finally the transient dynamics from a random initial condition, the time it takes for clustering to appear in the system is independent of the tumble rate

α but grows with the lattice coordination number and (exponentially or stronger) with $n_{\max}$.

DY 42.3 Thu 13:00 P1

Pressure in inertial active particle systems with frictional contacts — •Kay-Robert Dormann, Lukas Hecht, and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt, Germany

In systems of isotropic overdamped active Brownian particles (ABPs), the pressure is a state function [1]. It can be shown, that an equation of state (EOS) also exists, if the ABPs are inertial [2]. Here, we explore inertial active Brownian particles [3,4] with additional frictional contacts and find that no EOS exists. We attribute this to the fact that the rotational diffusion depends on density in the presence of frictional contacts.

The breakdown of the EOS due to frictional contacts has interesting implications: for example, when embedding a passive Janus-sphere, whose two hemispheres show a different stiffness, into an active bath, the sphere shows active Brownian motion. In addition, we find that frictional contacts and the associated breakdown of the EOS also have interesting implications for motility-induced phase separation as we will specify on the poster.

[1] A. P. Solon et al., Phys. Rev. Lett. 114, 198301 (2015).
[2] Y. Fily et al., J. Phys. A Math. Theor. 51, 044003 (2018).
[3] S. Mandal et al., Phys. Rev. Lett. 123, 228001 (2019).
[4] L. Hecht et al., Phys. Rev. Lett. 129, 178001 (2022).

DY 42.4 Thu 13:00 P1

Advanced Sampling Methods for Non-Equilibrium Particles — •Thomas Kiechl, Michele Caraglio, and Thomas Franosch — Institute for Theoretical Physics, Universität Innsbruck, Innsbruck, Austria.

Active particles or microswimmers are capable of converting energy into directed motion - which is why they are classified as out-of-equilibrium systems. Microswimmers, such as bacteria or spermatozoa often find themselves in a *target search* situation, where the microswimmers have to make a transition from an initial area to a target area crossing complex environments. Transition Path Theory, a rigorous statistical mechanics description of transition processes, can be generalized to characterize the target search problem. A simple way of modeling a complex environment for the microswimmer is via an external potential, in which the metastable initial position is separated from the target by an energy barrier. This makes the target search a *rare event*, in which the timescales of the fluctuations in the metastable states and the transition process are separated. Brute force simulations solving the equations of motion are inefficient due to this gap in timescales. The main result is that a more efficient sampling method, Transition Path Sampling (TPS), originally developed for rare transitions of passive systems, can be generalized to Run-and-Tumble systems. TPS is a Monte Carlo simulation of successful trajectories where the new trajectory is accepted according to a metropolis rule based on a path integral formulation.

DY 42.5 Thu 13:00 P1

Markov state modelling of self-assembling active triblock Janus particles — •Salman Fariz Navas, Juri Schubert, and Sabine H.L. Klapp — ITP, Technische Universität Berlin, Germany

Active triblock Janus particles have been shown to form open-cell colloidal lattices in both experiments as well as simulations. Such structures are of particular interest owing to their novel optical and mechanical properties. However, the self-assembly of open-cell lattices is a multistep process involving the formation of many intermediate competing structures resulting in long time-scales.

Here, we develop a Markov State Model for a self-assembling active triblock Janus particle system [1] from particle resolved Brownian Dynamics simulations by reducing the continuous many particle dynamics into a discrete set of states [2],[3]. We use the local order parameters introduced in [4] to develop the discrete states. The transition probability matrix between these states can then be constructed using which, information regarding the metastable states, the relaxation times and the pathways relevant to the aggregation process can be extracted.

[1] S. A. Mallory and A. Cacciuto, J. Am. Chem. Soc. 141, 2500 (2019).
[2] J.-H. Prinz, H. Wu, M. Sarich, B. Keller, M. Senne, M. Held, J. D. Chodera, C. Schütte, and F. Noé, J. Chem. Phys. 134, 174105 (2011).
[3] S.F. Navas and S.H.L. Klapp, in preparation.
[4] H. Eslami, P. Sedaghat, and F. Müller-Plathe, Phys. Chem. Chem. Phys. 20, 27059 (2018).

DY 42.6 Thu 13:00 P1

Dynamics of an active agent subject to orientational resetting — •Yanis Baouche and Christina Kurzthaler — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We study the dynamics of an active particle whose swimming direction is subject to rotational diffusion and a stochastic resetting mechanism. The latter allows for taking into account the particle's response to external stimuli.

We use renewal processes to model the reorientation mechanism of the active agent and provide analytical expressions for the characteristic function of the stochastic process and its low-order moments.

Finally, the interplay between rotational diffusion and resetting of the particle's orientation is quantified for different resetting distributions.

DY 42.7 Thu 13:00 P1

Adaptive microvascular remodeling under flow — Fatemeh Mirzapour-Shafiyi, •Leonie Karr, and Karen Alim — School of Natural Sciences, Technische Universität München

Vessel morphology is adapted to minimise energetic costs of dissipation and homogenize flow transport in the network. Resource-deprived tissues produce chemotactic agents to induce vessel formation during development and in tissue homeostasis. The primitive, mesh-like vascular network formed initially through neovascularisation is highly ramified. Later, vascular network is normalised into a hemodynamically preferred tree-like structure. The normalisation process, termed vessel remodeling, leads to an organ-specific network architecture which better meets the metabolic needs of its surrounding tissue. As vessel growth and remodeling is found impaired in various disease states, several factors regulating vessel formation and branching morphology were identified over the past decades. However, while some of these factors have been undergoing clinical trials, their effects on transport properties of the altered vessel morphology are not fully elucidated yet. Establishing a perfusable human vasculature-on-a-chip (hVoC) model system, here we aim to investigate how vascular morphology correlates with flow field. Our hVoC model allows extensive quantitative analyses of network morphology and adaptive remodeling under fluid flow applied by a low-pressure syringe pump. Results of our analyses will contribute to the next generation therapeutics targeting vessel development.

DY 42.8 Thu 13:00 P1

Thermodynamics of active matter systems under coarse graining — •Robin Bebon and Thomas Speck — Institute for Theoretical Physics 4, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany

Over the last decade, dynamic field theories have proven useful in the description of collective behavior and large-scale dynamics of active matter systems. However, despite their popularity, surprisingly little is known about how to capture thermodynamics on the level of such hydrodynamic descriptions. This is partially due to the fact that common approaches, based on symmetry arguments and conservation laws, typically neglect degrees of freedom that play a crucial role in quantifying the system's energetics, e.g., the self-propulsion mechanism. To advance, we propose a bottom-up approach that starts with a thermodynamically consistent microscopic model of catalytic particles driven by a constant affinity and derive effective hydrodynamic equations via explicit coarse graining. To ensure that information of the self-propulsion mechanism and its energy consumption is preserved on the macro-scale, we introduce an additional field, which for the considered model tracks the local rate of successful chemical events. We find that, near equilibrium, particle current and chemical field couple linearly through their respective thermodynamic forces, closely resembling linear irreversible thermodynamics. This provides an access point to investigate the thermodynamic properties of our field theory and compare the results with their microscopic counterparts.

DY 42.9 Thu 13:00 P1

The Liquid-Glass-Jamming Rheology of Soft Active Particles — •Roland Wiese[1], Klaus Kroy[1], and Demian Levis[2,3] — [1]Institute for Theoretical Physics, Leipzig University, 04103 Leipzig, Germany — [2]Departement de Fisica de la Materia Condensada, Facultat de Fisica, Universitat de Barcelona, Marti i Franquès 1, 08028 Barcelona, Spain — [3]University of Barcelona Institute of Complex Systems (UBICS), Facultat de Fisica, Universitat de Barcelona, Marti

i Franquès 1, 08028 Barcelona, Spain

We study the linear and nonlinear rheology of an active Brownian particle suspension at different densities. In the low density and low shear limits the flow is Newtonian. In this regime its linear response viscosity can be calculated via the Green-Kubo autocorrelation method and is found to scale with an effective temperature. In the nonlinear regime of high shearing rates shear thinning is observed universally for all parameters considered in our study. Above the critical density of the glass transition the dynamics becomes arrested, marked by the appearance of a finite yield stress. Increasing the self-propulsion of the active particles shifts the glass transition to higher densities by melting the amorphous solid. The yield stress enables us to construct a phase diagram in the spirit of jamming phase diagrams, but exchanging temperature with activity. For suffienctly high activities glassy physics becomes suppressed and the yield stress scales with a power law in the density, known from jammed granular materials.

DY 42.10 Thu 13:00 P1

Wetting of reflecting plates by an Active Brownian fluid — •Matthieu Mangeat, Shauri Chakraborty, Adam Wysocki, and Heiko Rieger — Universität des Saarlandes, Saarbrücken, Germany

We study, using interacting active Brownian particles (ABP), the wall-wetting mechanism of active sedimenting fluid. We consider a minimal model of active particles under gravitational field, inside a two-dimensional rectangular box. An accumulation of particles near the bottom wall is observed, as well as the wetting of vertical plates by the rise of active particles against the gravity, even without any attractive force within the system. We characterize this wall-wetting by the meniscus height, calculated from stationary density profile and depending on the inter-particle repulsion. The maximum wetting height depends super-linearly on active sedimentation length for interacting ABP, and linearly for non-interacting ABP. We also observe two large vortices concentrated close to the meniscus, due to the persistence motion of ABP against the gravity. Moreover, with non-interacting ABP, a current flow is present near the boundaries for which we propose a coarse-grained description.

DY 42.11 Thu 13:00 P1

Force-free Ratcheting in Static Activity Landscapes — •Constantin Rein[1], Martin Kolár[2], Klaus Kroy[1], and Viktor Holubec[2] — [1]Leipzig University, Faculty of Physics and Earth Sciences, Institute for Theoretical Physics, Brüderstraße 16, 04081 Leipzig — [2]Charles University, Faculty of Mathematics and Physics, Department of Macromolecular Physics, V Holešovičkách 2, CZ-180 00 Praha

We study the possibility of rectifying active Brownian motion solely using time-independent activity landscapes. We argue that, in one dimension, spatially asymmetric activity does not suffice to induce directed transport, unless the activity is modulated in time or an additional potential is used, whereas, in higher dimensions, static activity landscapes alone can induce ratcheting. The underlying principle is similar to the ratcheting induced by asymmetric obstacles in microswimmer baths: swimmers with suitable orientations get channeled, while the others get trapped in low-activity regions until they lost their orientation. For landscapes with wedge-shaped low-activity regions, we numerically found an average transport velocity of the order of 1% of the particle's swim speed.

DY 42.12 Thu 13:00 P1

The nature of non-phononic excitations in disordered systems — •Walter Schirmacher[1,2], Matteo Paoluzzi[3], and Giancarlo Ruocco[2,4] — [1]Universität Mainz, Mainz, Germany — [2]Istituto Italiano di Tecnologia, Roma, Italy — [3]Universitat de Barcelona, Barcelona, Spain — [4]Universita di Roma "La Sapienza", Roma, Italy

We theoretically and numerically investigate the nature of the non-phononic excitations appearing in the vibrational spectrum of disordered materials of small systems, which do not allow for low-frequency waves (phonons). Using heterogeneous-elasticity theory and a new generalization, we are able to distinguish between two types of non-phononic vibrational excitations of disordered materials (glasses). A first type (Type-I) arises beyond the boson peak due to strong scattering from the structural disorder. These excitations are similar to the eigenvectors of random matrices. In very small systems, in the absence of low-frequency waves, the spectrum exhibits a gap, which, in a marginal-stable situation, may extend to zero frequency and features a DOS proportional to the square of the frequency. In such small systems, in a more stable situation, a second type of non-phononic excitations (Type-II) appears, which involve rotational oscillations around local frozen-in stresses. The frequency spectrum of these Type-II excitations is related to the interaction potential in the regime, where the potential contributions are small, rendering the frequency dependence non-universal. The frequently observed frequency scaling with the fourth power is shown to be an artifact due to the smooth tapering of the potential cutoff in the simulations.

DY 42.13 Thu 13:00 P1

Glass Transition in Modulated Liquids — •Abolfazl Ahmadirahmat[1], Michele Caraglio[1], Vincent Krakoviack[2], and Thomas Franosch[1] — [1]Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 21A, A-6020 Innsbruck, Austria — [2]Laboratoire de chimie, École normale supérieure de Lyon, 46 Allée d'Italie 69364 Lyon, Cedex 07, France

We have developed a theoretical description for the structural and dynamical properties of quasi-two-dimensional colloidal suspensions subject to periodic potentials using mode-coupling theory (MCT). We solve the MCT equations numerically for monodisperse hard disks modulated by a periodic external potential and, we show that the theory reduces to the conventional MCT equations of the glass transition for bulk systems if the external modulation vanishes. To do so, we elaborate numerical results for the long-time limits of suitably generalized intermediate scattering functions. We compare the nonergodicity parameter of a two-dimensional modulated liquid in zero modulation with the corresponding nonergodicity parameter for the bulk system in two dimensions.

DY 42.14 Thu 13:00 P1

Assembly of iron oxide nanocuboids directed by surface, ligand, and magnetic interactions — •Sindy J. Rodríguez Sotelo[1,2], Mario C.G. Paseggi Jr.[1,2], Carlos García[3], and Igor Stanković[4] — [1]Instituto de Física del Litoral IFIS-CONICET, Santa Fe, Argentina — [2]Facultad de Ingeniería Química, Universidad Nacional del Litoral UNL, Santa Fe, Argentina — [3]Departamento de Física and Centro Científico Tecnológico de Valparaíso-CCTVal, Universidad Técnica Federico Santa María, Valparaíso, Chile — [4]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Serbia

The direction of the dipole moment in the magnetite spherical nanoparticles is unrelated to the morphology particle. For non-spherical particles, a coupling between particle form and magnetic moment direction might result in unexpected behaviours, especially when the moment is not aligned along a particle symmetry axis [1,2]. We introduce energy models accounting for the directionality and magnitude of the van der Waals and dipolar interactions as a function of the shape of the nanocubes, illustrating the importance of the directional dipolar forces for the formation of the nanocube clusters, the dominance of the van der Waals multi-body interactions and exclusion forces of ligands. We illustrate how minimal energy structures depend on the assembly size, shape of the particles, and the balance of surface and magnetic dipolar coupling.

References [1] I. Stanković, *et al.* Nanoscale **12**, 19390, 2020. [2] L. Balcells *et al.* Nanoscale **11**, 14194, 2019.

DY 42.15 Thu 13:00 P1

Phase Behaviour of a Minimal Lattice Model with Chiral Interactions — •Boyi Wang[1,2], Patrick Pietzonka[1], and Frank Jülicher[1,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Institute of Physics, Chinese Academy of Sciences, Beijing, China — [3]Cluster of Excellence, Physics of Life, TU Dresden, Dresden, Germany

We introduce chiral interactions to a minimal lattice model based on the Ising model, adding second neighbour interactions that favour an L-shaped structure. We run Monte-Carlo simulations in equilibrium at low temperatures, and find two new ground states which exhibit chiral periodic tiling. We also study the phase behaviour analytically as a function of the strength of the chiral interaction and the external magnetic field. With number conservation, we observe the coexistence of chiral and achiral phases and the formation of droplets. Furthermore, we consider the role of chirality in this minimal lattice model with active driving forces.

DY 42.16 Thu 13:00 P1

Static and dynamical magnetic properties ferrofluid with ellipsoid-like nanoparticles — •Vladimir Zverev, Alla Dobroserdova, Ekaterina Ekaterina, Elena Pyanzina, and Alexey

Ivanov — Ekaterinburg, Russia

A system of magnetic ellipsoids with a point dipole at the particle center is considered. We take into account different shape's anisotropy and different positions of the magnetic moment inside the particle (parallel and perpendicular to the main axis of the ellipsoid). In order to study this system, molecular dynamics simulations are used. The ratio of the main semi-axis to the additional one was used as a measure of the particle anisotropy. In particular, we have studied the system in which the particles have magnetic moments, but there is no dipole-dipole interaction between them. As a result, the initial magnetic susceptibility (magnetic characteristic) and the radial distribution function (structural characteristic) were calculated. For the initial susceptibility, the data obtained in computer simulations differ from the Langevin magnetization (theoretical ideal case) within the statistical error. The data for the Radial Distribution Function (RDF) also match within the calculation error. The next stage of research was to take into account dipole-dipole interparticle interactions and also will be presented.

DY 42.17 Thu 13:00 P1

Hopping conduction in networks with site energy disorder — •Quinn Emilia Fischer, Marco Bosi, and Philipp Maass — Fachbereich Physik, Universität Osnabrück, Barabarastraße 7, D-49076 Osnabrück, Germany

Understanding conductivities due to hopping motion in disordered systems is an important problem with various applications ranging from electron transport in amorphous semiconductors to ion transport in glasses [1,2]. A prominent model is that of particle hopping on a lattice with random site energies, where each lattice site can be occupied by at most one particle. For this model, a theory has been proposed, where transport properties are determined by a mapping onto a random resistor network [3]. By comparison with extensive kinetic Monte Carlo simulations for different types of site energy distributions, we show that this theory gives good predictions for small and high particle concentrations but is less accurate for intermediate concentrations. We present a refined theory which takes into account nearest neighbour correlations between occupation numbers in current carrying nonequilibrium steady states. This theory yields an improved prediction of conductivities and their activation energies in very good agreement with the Monte Carlo results.

[1] M. Bosi, P. Maass, J. Phys. Chem. C 125 6260 (2021).
[2] M. Bosi, P. Maass, Z. Phys. Chem. 236, 1055 2022).
[3] V. Ambegaokar, B. I. Halperin, J. S. Langer, Phys. Rev. B 4, 2612 (1971).

DY 43: Poster: Quantum Dynamics and Many-Body Systems

Time: Thursday 13:00–16:00 Location: P1

DY 43.1 Thu 13:00 P1

applications of generalized coherent states in bosonic systems — •yulong qiao[1], Frank Grossman[2], and Joonsuk Huh[3] — [1]Institute for theoretical physics, TU Dresden, 01062 Dresden, Germany — [2]Institute for theoretical physics, TU Dresden, 01062 Dresden, Germany — [3]Department of Chemistry, Sungkyunkwan University, Suwon 16419, Republic of Korea

Generalized coherent states (GCS) are found to be very useful for studying bosonic systems with a fixed number of particles, such as the Bose-Hubbard model and boson sampling. Firstly, we present the non-equilibrium dynamics of the Bose-Hubbard model based on the time-dependent variational principle [1]. Increasing the multiplicity of GCS leads to converged results quickly for weak interaction strength, which indicates that GCS are a well-suited basis in the superfuild phase. Secondly, we investigate the boson sampling problem whose input state is a Fock state. Using an exact expansion of the Fock state in terms of GCS, we obtain the output state by means of a unitary rotation. By this process the total information is contained in a finite number of GCS. The specific structure of the GCS allows us to split the whole system into two parts easily and to study the entanglement entropy of the output state in detail [2].

[1] Y. Qiao and F. Grossmann, Exact variational dynamics of the multimode Bose-Hubbard model based on SU(M) coherent states, Phys. Rev. A 103, 042209 (2021).

[2] Y. Qiao, J. Huh, F. Grossmann, Entanglement in the full state vector of boson sampling, arXiv:2210.09915 [quant- ph] (2022).

DY 43.2 Thu 13:00 P1

Coupling in Optical Microcavity-Arrays — •Tom Rodemund and Martina Hentschel — Department of Physics, University of Applied Sciences Chemnitz, Chemnitz, Germany

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

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

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

DY 43.3 Thu 13:00 P1

From Dual Unitarity to Generic Quantum Operator Spreading — •Michael A. Rampp, Roderich Moessner, and Pieter W. Claeys — Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Dual-unitary circuits are paradigmatic examples of exactly solvable yet chaotic quantum many-body systems, but solvability naturally goes along with a degree of non-generic behaviour. By investigating the effect of weakly broken dual-unitarity on the spreading of local operators we study whether, and how, small deviations from dual-unitarity recover fully generic many-body dynamics. We present a discrete path-integral formula for the out-of-time-order correlator and use it to recover a butterfly velocity smaller than the light-cone velocity, $v_B < v_{LC}$, and a diffusively broadening operator front, two generic features of ergodic quantum spin chains absent in dual-unitary circuit dynamics. We find that the butterfly velocity and diffusion constant are determined by a small set of microscopic quantities and that the operator entanglement of the gates plays a crucial role.

DY 43.4 Thu 13:00 P1

Transmission of a single electron through a Berry ring — •Kenmoe Maseim Bassis — Universitätsstraße 31, 93053, Regensburg — Prüfeningerstraße 121, 93049, Regensburg

A theoretical model of transmission and reflection of an electron with spin is proposed for a mesoscopic ring with rotating localized magnetic moment. This model may be realized in a pair of domain walls connecting two ferromagnetic domains with opposite magnetization. If the localized magnetic moment and the traveling spin is ferromagnetically coupled and if the localized moment rotates with opposite chirality in the double path, our system is formulated in the model of an emergent spin-orbit interaction in a ring. The scattering problem for the transmission spectrum of the traveling spin is solved both in a single-path and a double-path model. In the double path, the quantum-path interference changes dramatically the transmission spectrum due to the effect of the Berry phase. Specifically, the spin-flip transmission and reflection are both strictly forbidden.

DY 43.5 Thu 13:00 P1

Optimal route to quantum chaos in the Bose-Hubbard model — Lukas Pausch[1,2], Edoardo Carnio[2,3], Andreas Buchleitner[2,3], and •Alberto Rodríguez[4] — [1]Département de Physique, Université de Liège, Belgium — [2]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3, D-79104, Freiburg, Germany — [3]EUCOR Centre for Quantum Science and Quantum Computing, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany — [4]Departamento de Física Fundamental, Universidad de Salamanca, E-37008 Salamanca, Spain

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

[1] L. Pausch *et al.*, Phys. Rev. Lett. 126, 150601 (2021)
[2] L. Pausch *et al.*, New J. Phys. 23, 123036 (2021)
[3] L. Pausch *et al.*, J. Phys. A 55, 324002 (2022)

DY 43.6 Thu 13:00 P1

Chaotic resonance modes in optical microcavities — •Florian Lorenz and Roland Ketzmerick — TU Dresden, Institut für Theoretische Physik, Dresden, Germany

Following a recently proposed conjecture, we show that resonance modes in dielectric cavities are a product of a conditionally invariant measure from classical dynamics and universal fluctuations [1]. The first factor describes the average of modes with similar lifetime and has a multifractal structure which we resolve on very fine scales. It is approximately described by conditionally invariant measures from classical dynamics [1]. However, increasing the openness of a dielectric cavity (i.e. by investigating TE modes or a small refractive index) is a challenge to the construction of appropriate classical measures.

[1] R. Ketzmerick, K. Clauß, F. Fritzsch, and A. Bäcker, Chaotic resonance modes in dielectric cavities: Product of conditionally invariant measure and universal fluctuations, Phys. Rev. Lett. **129**, 193901 (2022).

DY 43.7 Thu 13:00 P1

Classical and quantum escape dynamics in the vicinity of hyperbolic fixed points — •Alexander Hempel, Jonas Stöber, and Arnd Bäcker — TU Dresden, Institut für Theoretische Physik, Dresden, Germany

For an ensemble of orbits started in the vicinity of an inverse hyperbolic fixed point in the area-preserving standard map we find a slow, non-exponential decay of the survival probability. It turns out that this is governed by the geometry of the stable and unstable manifolds which form a partial barrier enclosing a resonance zone. An analysis of transit times through the resonance zone using the lobe dynamics of the partial barrier, including re-entrance of orbits, explains the non-exponential decay. Quantum mechanically, coherent states follow the classical behavior for remarkably long times.

DY 43.8 Thu 13:00 P1

Many-body localization in disordered Heisenberg-type spin chain models — •Yilun Gao and Rudolf A. Römer — Department of Physics, University of Warwick, Coventry, CV4 7AL, UK

Disordered quantum systems have become an important research topic in modern condensed matter physics ever since the discovery of Anderson localization. The investigation of many-body localization in quantum interacting systems has received much recent attention following the increase of computational power and improvement in numerical methods. One of the standard models that has been studied is the disordered spin-1/2 Heisenberg chain. It was shown that there exists a phase transition from ergodic states to many-body localized states as the disorder is increased. Here, we focus on a variant of the model where the exchange couplings between neighboring spins are taken to be disordered. We calculate the consecutive-spectral-gap ratio and its probability distribution for different system sizes and disorders. The result is compared with the case when the disorder is onsite. We average over many disorder realizations. We also plot the sample-to-sample variance against disorder and system size as a further characteristic of the phases across the MBL transition.

DY 43.9 Thu 13:00 P1

Nonlinear magnetoelectric effects in class AIII 3D topological insulators — •Nithin Thomas, Jan Wilhlem, and Ferdinand Evers — Institute of Theoretical Physics, Regensburg University, D-93053 Regensburg, Germany

We investigate nonlinear magnetoelectric effects in class AIII 3D topological insulators[1]. Within the framework of a tight-binding model, we numerically observe a quadratic scaling of wrapping currents with the electric field strength. Starting with the theory of nonlinear Hall effect induced by Berry curvature dipole[2], we develop an analytic description of our numerical findings.

Shinsei Ryu et al 2010 New J. Phys. 12 065010 (2010) Inti Sodemann and Liang Fu, Phys. Rev. Lett. 115, 216806 (2015)

DY 43.10 Thu 13:00 P1

Flat band physics for dispersive bands — •Jie Liu[1], Carlo Danieli[2], and Rudolf A. Römer[3] — [1]School of Physics and Optoelectronics, Xiangtan University, Xiangtan 411105, China — [2]Department of Physics, University of Sapienza, Piazzale Aldo Moro 5, 00185 Rome, Italy — [3]Department of Physics, University of Warwick, Coventry, CV4 7AL, United Kingdom

Lieb models provide a convenient test bed for the characterization of compactly localized states (CLS) in "flat" energy bands. The CLS have been discussed as potential candidates for information storage applications. However, they are typically sensitive to perturbations. Uncorrelated onsite disorder in most cases lifts the existence of CLS irrespective of the disorder strength and induces wave localization in flat band lattices. In certain cases, however, local symmetries within flat band lattices suggest local correlations in the onsite disorder which result in anomalous localization features. Here we make use of these ideas to proposed an engineered "disorder" that allows to keep the compactness of the CLS while it at the same time changes half of the dispersive states to become more CLS-like. The work has potential applications for the many situations where flat-band physics has been shown to be relevant, effectively stabilizing the CLS.

DY 43.11 Thu 13:00 P1

Electron cavity optics in bilayer graphene billiards — •Lukas Seemann[1], Angelika Knothe[2], Klaus Richter[2], and Martina Hentschel[1] — [1]Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [2]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Rapid developments in the field of 2D materials and their nanostructures make it possible to trap charge carriers with different dispersions in various confinement geometries with a high degree of control. This progress now allows studying 2D electron optics phenomena enriched by the charge carriers' different electronic and topological properties compared to the photonic. Here, we demonstrate the differences induced by deviating from an isotropic dispersion relation by theoretically investigating cavities in gapped bilayer graphene characterized by the presence of a trigonally warped band structure [1]. We employ an approach based on ray-wave correspondence [2] and find dramatic deviations from the optical-case behavior with clear signatures in phase space. We show that the fermion optics characteristics can be conveniently tuned by gate voltages and illustrate the experimentally relevant consequences.

[1] C. Gold, A. Knothe, A. Kurzmann, A. Garcia-Ruiz, K. Watanabe, T. Taniguchi, V. Fal'ko, K. Ensslin, T. Ihn, Phys. Rev. Lett. 127, 046801 (2021).
[2] J.-K. Schrepfer, S. Chen, M.-H. Liu, K. Richter, and M. Hentschel, Phys. Rev. B 104, 155436 (2021).

DY 43.12 Thu 13:00 P1

Quantum many-body dynamics in two dimensions using tree tensor networks — •Wladislaw Krinitsin[1], Niklas Tausendpfund[1,2], Matteo Rizzi[1,2], and Markus Schmitt[1] — [1]Forschungszentrum, Jülich, Deutschland — [2]Institut der Theoretischen Physik, Köln, Deutschland

Many body systems out of equilibrium are notoriously difficult to solve due to the rapid growth of entanglement with time. In particular the rapidly expanding possibilities to address 2-dimensional systems in quantum simulation turn a spotlight on the lack of reliable numerical methods in this regime. We explore an approach to solve the time dependence of 2-dimensional systems by applying the time-dependent variational principle (TDVP) to Tree Tensor Networks (TTNs). More specifically, this method is used to study non-ergodic dynamics in the quantum Ising model.

DY 43.13 Thu 13:00 P1

Numeric investigation of the Kibble-Zurek mechanism in 2D — •Seyedeh Parya Katoorani[1], Ralf Schützhold[2], Naser Ahmadiniaz[3], Gernot Schaller[4], and Friedemann

Queisser[5] — [1]Theoretical Physics(FWZ),HZDR,Dresden,Germany, — [2]Theoretical Physics(FWZ),HZDR,Dresden,Germany — [3]Theoretical Physics(FWZ),HZDR,Dresden,Germany — [4]Theoretical Physics(FWZ),HZDR,Dresden,Germany — [5]Theoretical Physics(FWZ),HZDR,Dresden,Germany

The two-dimensional classical Ising model can be approximately implemented on a Si(100) surface, where the dimers are anisotropically coupled. In particular, the setup allows for time-dependent temperatures, where the Kibble-Zurek mechanism predicts topological defect formation while traversing the critical point at a finite rate. We numerically investigate the corresponding relaxation dynamics of a two-dimensional extended Ising model with diagonal couplings and time-dependent temperature.

DY 43.14 Thu 13:00 P1

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

The Gorini-Kossakowski-Sudarshan-Lindblad Equation is a quantum master equation describing the time evolution of quantum mechanical states. It is used to model open quantum systems. We give explicit expressions of stationary solutions of the Lindblad equation in the case of a finite state space, using the concept of state transition networks of Markov chains. Our treatment is based on the so-called quantum-jump unravelling, which is an ensembles of stochastic quantum trajectories, compatible with the Lindblad equation. A single such trajectory is a piecewise deterministic process, which is interrupted by stochastic jumps. We discuss differences to the classical case and conditions, under which the Lindblad equation is asymptotically stable.

DY 43.15 Thu 13:00 P1

Generic partial barriers to chaotic transport in 4D symplectic maps — •Benjamin Hertzsch, Arnd Bäcker, and Roland Ketzmerick — TU Dresden, Institut für Theoretische Physik, Dresden, Germany

Chaotic transport in Hamiltonian systems is often restricted due to the presence of partial barriers, leading to a limited flux between different regions in phase phase. Typically, the most restrictive partial barrier in a 2D symplectic map is based on a cantorus, the Cantor set remnants of a broken 1D torus. Recently, for a weakly coupled 4D symplectic map, a partial barrier based on a normally hyperbolic invariant manifold with the structure of a cantorus has been established. We investigate how this can be extended to a generic 4D map, where the most restrictive partial barriers are expected to lie on the most irrational slopes between resonance channels in frequency space.

DY 43.16 Thu 13:00 P1

Stability analysis of a periodically driven ultra-cold Bose gas — •Larissa Schwarz, Simon B. Jäger, Dimo Claude, Imke Schneider, and Sebastian Eggert — Physics Department and Research Center OPTIMAS, Technische Universität Kaiserslautern, D-67663, Kaiserslautern, Germany

We theoretically study the dynamics of a Bose-Einstein condensate under periodic driving of the s-wave scattering length. In this setup, we first determine the stability of the condensate using Bogoliubov theory with time-periodic modulation. We find an exponential gain in the resonant k-modes due to a parameteric amplification which leads to a rapid condensate depletion. These findings are compared with the simulation of the Gross-Pitaevskii equation which shows the formation of a density-wave pattern with the predicted k-wavevector. We extend the Bogoliubov theory by including non-linearities which result in an effective damping of the k-modes. This enables the creation of stable density-wave pattern below a critical driving strength. Moreover, above this critical driving strength we analyze simple non-quadratic models and find macroscopic and stable occupation of the resonant k-mode.

DY 43.17 Thu 13:00 P1

Energy-conserving adaptive partitioning QM/MM simulations — •Marvin Nyenhuis[1,2] and Nikos Doltsinis[1,2] — [1]Institute for Solid State Theory, University of Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany — [2]Center for Multiscale Theory and Computation,, University of Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

Bachmann and Doltsinis have recently proposed an energy-conserving adaptive partitioning method between two different atomistic representations based on an extended Hamiltonian, which switches the system from a potential energy surface V_1 to another potential V_2. In this work, we develop this method further and implement it into the QM/MM molecular dynamics framework of the CP2K software package, enabling atoms travelling out of (or into) the QM region to adopt an MM (or QM) representation. For a test system consisting of a solvated sodium ion, we analyse the degree to which energy is conserved over a large number of switching events depending on the value chosen for the mass of the fictitious lambda particle. In addition, we investigate how this choice affects the switching speed and we seek the optimum mass that simultaneously ensures rapid switching and good energy conservation.

DY 43.18 Thu 13:00 P1

Classification of noisy spectra using machine learning — Aritra Mishra and •Alexander Eisfeld — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

A general problem in quantum mechanics is to obtain information of the eigenstates from the experimentally measured data which consists inherent noises. For an example, in the case of molecular aggregates, the information about excitonic eigenstates is vitally important to understand their optical and transport properties [1,2].

We show that it is possible to reconstruct the underlying delocalised aggregate eigenfunctions from near-field spectra using convolution neural networks [3]. We also investigate convolution neural networks for an eigenstate based classification of the spectra, in the presence of noise. Each aggregate eigenstate, corresponds to a distinctly looking spectrum. Therefore, we can assign a class to each of the eigenstate. We find that the network is also able to classify the spectra of different noise strengths along with the one it has been trained for.

[1] X. Gao and A. Eisfeld, J. Phys. Chem. Lett. 9, 6003 (2018)
[2] S. Nayak, F. Zheng and A. Eisfeld, J. Chem. Phys. 155, 134701 (2021)
[3] F. Zheng, X. Gao and A. Eisfeld, Phys. Rev. Lett. 123, 163202 (2019)

DY 43.19 Thu 13:00 P1

Exact time local equations of quantum dissipation with minimal state space — •Meng Xu[1], Vasilii Vadimov[2], Malte Krug[1], Jürgen T. Stockburger[1], and Joachim Ankerhold[1] — [1]Institute for Complex Quantum Systems and IQST, Ulm University — [2]QCD Labs, QTF Centre of Excellence, Aalto University, Finland

We present a minimal state space approach to unravel the Feynman path integral influence functional for open quantum system dynamics. The resulting time local evolution equation for the density in minimally extended state space is exact and in combination with tensor network methods, can be very efficiently propagated with very high precision also for long times [1]. It is capable to treat the full non-Markovian dynamics, regardless of low temperature, structured reservoir, and strong system-bath coupling. On a formal level, its intriguing structure allows to demonstrate that the new equation is closely related to an entire family of representations (Lindblad-type, Fokker-Planck-type). Alternative perturbative and non-perturbative formulations of quantum dissipation can be derived from it, with our new approach being favorable through a comparably low dimension of auxiliary dimensions. With the new platform at hand, lab-based high-precision simulations in parallel to actual experiments with, for example, superconducting qubits are within reach.

[1] M. Xu *et al.*, Phys. Rev. Lett. **129**, 230601 (2022).

DY 43.20 Thu 13:00 P1

Training Restricted Boltzmann Machines for Spin-1 Quantum Magnets — •Abhiroop Lahiri and Michele Casula — IMPMC, Sorbonne Université, Paris, France

Neural Network Quantum states (NQS) have gained popularity in recent times for their ability to study quantum many-body systems. Restricted Boltzmann Machines (RBMs) have been quite successful in providing an accurate representation of the ground states of spin-1/2 quantum systems both in one and two dimensions. Based on recent studies of the spin-1 representation of RBMs using one-hot encoding and a quadratic energy function, we aim to test these ansatze for spin-1 models in various configurations. We train the network parameters and investigate their behaviour to resolve the ground state of these systems.

DY 43.21 Thu 13:00 P1

Enhancement and suppression of charge transport in or-

ganic semiconductors under strong light-matter coupling — •Sebastian Stumper and Junichi Okamoto — University of Freiburg, Institute of Physics

We study a model of an organic semiconductor coupled to a cavity with variable disorder and electronic filling factors as well as dissipative effects. It represents a fermionic generalization of the Dicke model such that charges can move between lattice sites.

Different mechanisms are explored to explain experimentally observed conductivity enhancements in the strong coupling regime. These are either based on an increase of the charge mobility or of the charge density. Mobilities and the generalized inverse participation ratio, which characterizes localization, are accessible from various two- and four-point correlators that we obtain by a Lanczos technique. In agreement with several previous studies, we find that excitons are indeed delocalized under strong light-matter coupling and show an enormously increased mobility. The same is not true for electrons and holes.

Charge densities are increased by excitation of electrons to the upper band through counter-rotating light-matter interaction terms. However, this is counteracted by the cavity-mediated formation of bound electron-hole states. We analyze the relative strengths of these processes under finite size scaling, and how the formation of bound states is affected by disorder and dephasing. In certain limits for an undoped system, the Dicke model is recovered.

DY 43.22 Thu 13:00 P1

Investigation of two-dimensional quantum billiards with mixed dynamics in microwave resonators — •Lennart Anderson and Andreas Wieck — Angewandte Festkörperphysik, Ruhr-Universität Bochum

Based on the analogy of the stationary Schrödinger equation and the Helmholtz equation for a flat electromagnetic resonator, two-dimensional quantum mushroom billiards are studied in the microwave regime. We give a practical approach, ranging from the construction process of the resonator to the eigenvalue statistics. I.e. the frequency spectrum is measured for different stem widths. The obtained nearest neighbour spacings are fitted with respect to three different distribution functions for systems with mixed dynamics respectively. The degrees of chaoticity are determined analytically, dependent on the stem width, and compared with the fitted data. The presented approach is of both conceptual and educational interest.

DY 44: Poster: Statistical Physics

Time: Thursday 13:00–16:00 Location: P1

DY 44.1 Thu 13:00 P1

Understanding probability and irreversibility in the Mori-Zwanzig projection operator formalism — •Michael te Vrugt — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Center for Soft Nanoscience, Philosophisches Seminar, 48149 Münster, Germany

Explaining the emergence of stochastic irreversible macroscopic dynamics from time-reversible deterministic microscopic dynamics is one of the key problems in philosophy of physics. The Mori-Zwanzig (MZ) projection operator formalism, which is one of the most important methods of modern nonequilibrium statistical mechanics, allows for a systematic derivation of irreversible transport equations from reversible microdynamics and thus provides a useful framework for understanding this issue. However, discussions of the MZ formalism in philosophy of physics tend to focus on simple variants rather than on the more sophisticated ones used in modern physical research. In this work [1], I will close this gap by studying the problems of probability and irreversibility using the example of Grabert's time-dependent projection operator formalism. This allows to better understand how general proposals for understanding probability in statistical mechanics, namely (a) quantum approaches and (b) almost-objective probabilities, can be accomodated in the MZ formalism.

[1] European Journal for Philosophy of Science 12, 41 (2022)

DY 44.2 Thu 13:00 P1

Finite-temperature absorption spectrum of Al_2O_3 from first principles — •Angela F. Harper[1], Bartomeu Monserrat[2], and Andrew J. Morris[3] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]University of Cambridge, UK — [3]University of Birmingham, UK

Advancing the next generation of materials for solid-state devices requires an understanding of their underlying electronic structure. One such material is alumina (Al_2O_3), which is used to enhance performance in electronic devices from Li-ion batteries to perovskite solar cells and field effect transistors. By including phonon-assisted transitions within plane-wave DFT methods for calculating the X-ray absorption spectrum (XAS) we obtain the Al K-edge XAS at 300 K for two crystalline Al_2O_3 phases. The 300 K XAS reproduces the pre-edge peak for α-Al_2O_3, which is not visible at the static-lattice level of approximation. The 300 K XAS for γ-Al_2O_3 correctly describes two out of the three experimental peaks. We show that the second peak arises from 1s to mixed *s-p* transitions and is absent in the 0 K XAS. The method presented here is generalizable to any element and absorption edge, and is a feasible way to calculate finite temperature spectroscopy for any crystalline material.

DY 44.3 Thu 13:00 P1

Potts model with invisible states on a scale-free network — •Mariana Krasnytska[1,2,3] and Petro Sarkanych[1,2] — [1]ICMP, NAS of Ukraine, Lviv, Ukraine — [2]L4 Collaboration Leipzig-Lorraine-Lviv-Coventry — [3]Université de Lorraine, Nancy, France

Different models are proposed to understand magnetic phase transitions through the prism of competition between the energy and the entropy. One of such models is a (q+r)-state Potts model with invisible states. This model introduces r invisible states such that if spin lies in one of them, it does not interact with the rest. We consider such a model using the mean-field approximation on an annealed scale-free network where the probability of a randomly chosen vertex having a given degree is governed by the power law with decay exponent λ. Our results confirm that q, r and λ play a role of global parameters that influence the critical behaviour of the system. Depending on their values the phase diagram is divided into three regions with different critical behaviour. However, the topological influence, presented by the marginal value of $\lambda c(q)$, has proven to be dominant over the entropic one, governed by the number of invisible states r [arXiv:2211.14048].

DY 44.4 Thu 13:00 P1

Thermodynamics of $su(n)$-symmetric integrable models and their continuum limit — •Ingryd Passos and Andreas Klümper — Bergische Universität Wuppertal, Wuppertal, Germany

Traditionally the computation of the partition function of integrable quantum chains is achieved by means of the thermodynamic Bethe ansatz (TBA). On the other hand, an alternative formulation which relies on finite sets of nonlinear integral equations has been developed and successfully applied to seminal cases like for example the spin-1/2 Heisenberg chain, the supersymmetric t-J model and quantum chains with $su(3)$ and $su(4)$ invariance. This approach, known as the Quantum Transfer Matrix (QTM) method, allows for faster numerical computations and calculation of finite temperature correlation lengths. However, the derivation of these alternative equations was done in case by case studies in which by trial and error suitable auxiliary functions were identified. Another shortcoming of the QTM method is its applicability in the case of continuum integrable models. A way to circumvent this issue is to identify the proper lattice model from which the continuum model follows after a suitable scaling limit. This way, it is possible, for example, to determine the thermodynamics of multicomponent Bose gases from anisotropic spin chains. In this work we present a way to derive systematically finite sets of nonlinear integral equations for $su(n)$-symmetric integrable lattice models and discuss a scaling limit of these equations in the case of the $su(3)$-invariant anisotropic spin chain.

DY 44.5 Thu 13:00 P1

Simple-to-complex phase transition for longest increasing subsequences (Ulam's problem) — •Tammo Lentsch and Alexander K. Hartmann — Institute of Physics, University of Old-

enburg, Germany

It is possible to calculate the LIS length L by efficient algorithms in polynomial time. Finding and analyzing LIS was first considered numerically in the 1950s by Stanislav Ulam. The LIS problem has applications in bioinformatics and data analysis but is also studied in mathematics and statistical physics [1].

Recently, an algorithm to count the number of LIS [2] was extended to directly sample LIS [3]. The phase space where σ are random permutations was studied by calculating the distribution $P(q)$ of overlaps, revealing a complex structure similar to Replica Symmetry Breaking.

Here we consider the effect of randomly partially presorting σ with $O(n^\alpha)$ sorting steps. For sequences up to length $n = 8192$, we analyzed the LIS length L and $P(q)$. The results indicate a phase transition at a critical value α_c from $O(n)$ to $O(\sqrt{n})$ LIS length scaling and from simple to complex phase-space structure.

[1] J. Börjes, H. Schawe, A.K. Hartmann, Phys. Rev. E **99**, 042104 (2019).
[2] P. Krabbe, H. Schawe, A.K. Hartmann, Phys. Rev. E **101**, 062109 (2020).
[3] P. Krabbe, H. Schawe, A.K. Hartmann, arXiv:2208.14955 (2022).

DY 44.6 Thu 13:00 P1

Nonergodicity of scaled fractional Brownian motion with nonliner time and space clocks — •Yingjie Liang[1,2], Wei Wang[2], Andrey G. Cherstvy[2], and Ralf Metzler[2,3] — [1]Hohai University — [2]University of Potsdam — [3]Asia Pacific Center for Theoretical Physics

Experimental evidences show that diffusion processes are not always Brownian motion. It is anomalous diffusion with the mean squared displacement (MSD) being a power law in time, ultraslow diffusion with a logarithmic law, and superfast diffusion with an exponential law. To describe different types of non-Brownion motion in heterogeneous media, this study provides scaled fractional Brownian motion (SFBM) with nonliner time and space clocks. In the Langevin system for the FBM runnning with a nonliner time clock, i.e., the time scaled FBM, the real time is a temporal function of the original times in FBM. For the FBM runnning with a nonliner space clock, i.e., the space scaled FBM, the real position is a nonlinear spatial function of the orginial positions in FBM. The nonergodicity properties of SFBM are quantified based on single particle trajectories of the fractional Brownian motion running with time and space clocks. The simulations are consistent with the general analytical results in specific values of the dominated parameters for the behaviors of the MSD, time averaged mean squared displacement (TAMSD) and aging. Potential applications of these results are encountered in diverse scientific fields, such as biophysical, soft matter and hydrology systems.

DY 44.7 Thu 13:00 P1

The Griffiths Phase: A Large Deviations Study — •Lambert Münster[1], Martin Weigel[1], and Alexander K. Hartmann[2] — [1]Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany — [2]Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg, Germany

For spin systems with quenched disorder, the Griffiths phase is the thermal region between the phase transition in the pure system and the corresponding transition in the disordered system. The standard example is a dilute ferromagnet, where a certain fraction of bonds is missing [1]. The physical behavior of this phase is characterized by large fluctuations in the order parameter which are visible in the tails of the distribution of the magnetic susceptibility. To directly investigate this property, we combine a large-deviation Monte Carlo sampling algorithm [2,3] with a Gaussian modified ensemble [4], thus allowing us to study the distribution of physical quantities on a much larger range of the support as compared to previous studies [5], i.e., in the region of exponential small probabilities. In addition to considering the susceptibility distribution we also study other observables such as the specific heat, thus shedding new light on this intriguing physical phenomenon.

[1] A. J. Bray, Phys. Rev. Lett. **59**, 586 (1987).
[2] A. K. Hartmann, Phys. Rev. E **65**, 056102 (2002).
[3] A. K. Hartmann, Eur. Phys. J. B **84**, 627 (2011).
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[5] K. Hukushima, Y. Iba, J. Phys. **95**, 012005 (2008).

DY 44.8 Thu 13:00 P1

Transport Properties of Brownian Particles: Analytical Results and Computer Simulations — •Regina Rusch[1], Gerhard Jung[2], and Thomas Franosch[1] — [1]Institute for Theoretical Physics, Universität Innsbruck, Innsbruck, Austria. — [2]Laboratoire Charles Coulomb (L2C), Université de Montpellier, CNRS, 34095 Montpellier, France.

The results of computer simulations for Brownian particles can be improved by using a novel noise cancellation algorithm, with which the velocity autocorrelation function (VACF) can be measured more precisely. The algorithm is based on the fact that the Brownian noise can be stored in computer simulations and thus the noise can be subtracted from a simulated trajectory. Doing this, a reduced motion of the particle due to interactions or an external force is obtained. It could be shown that the VACF of the reduced motion is connected with the original VACF up to a cross-correlation term, which is shown to be sufficiently small. For the system of a Brownian particle in a periodic step potential the noise cancellation algorithm decreases the error of the VACF by about one order of magnitude. A power-law decay in the VACF is found by employing Monte-Carlo simulations. We also present analytical results for the probability distribution of the particle position using the Bloch theorem. This enables us to compute further correlation functions such as the intermediate scattering function which is in quantitative agreement with simulations.

DY 44.9 Thu 13:00 P1

First passage time as thermodynamical parameter — •Vasiliy Ryazanov — Institute for nuclear research NANU, Kiev, Ukraine

The first-passage time is proposed as an independent thermodynamic parameter of the statistical distribution that generalizes the Gibbs distribution. The thermodynamic parameter conjugated to the first-passage time is the same as the Laplace transform parameter of the first-passage time distribution in the partition function. The thermodynamic parameter conjugated to the first-passage time can be expressed in terms of the deviation of the entropy from the equilibrium value. Thus, all the moments of the distribution of the first passage time expressed in terms of the deviation of the entropy from its equilibrium value and the external forces acting on the system. By changing the thermodynamic forces, you can change of the first passage time.

An analogy is drawn between version of non-equilibrium thermodynamics a distribution-based containing an additional thermodynamic first-passage time parameter, nonequilibrium statistical operator method and extended irreversible thermodynamics with flows as an additional thermodynamic parameter. Various conditions for the dependence of the distribution parameters of the first-passage time on the random value of energy, the first thermodynamic parameter, are considered. Expressions are obtained for the thermodynamic parameter, the conjugate of the first passage time through the entropy change, and for the average first passage time through the flows.

DY 44.10 Thu 13:00 P1

Stochastic dynamics with multiplicative noise under resetting — •Trifce Sandev[1,2,3], Ljupco Kocarev[1,3], Ralf Metzler[2,4], and Aleksei Chechkin[2,5,6] — [1]Macedonian Academy of Sciences and Arts, Skopje, Macedonia — [2]University of Potsdam, Germany — [3]Ss. Cyril and Methodius University in Skopje, Macedonia — [4]Asia Pacific Center for Theoretical Physics, Pohang, Republic of Korea — [5]Wroclaw University of Science and Technology, Poland — [6]Akhiezer Institute for Theoretical Physic, Kharkiv, Ukraine

We analyze different stochastic processes with multiplicative noise under resetting in non-homogeneous media. We use the subordination approach, which is a powerful technique for solving various diffusion and Fokker-Planck equations, to analyze the probability density functions and the mean squared displacements. Additionally, we show that such systems under stochastic resetting reach non-equilibrium stationary states. The transition to the non-equilibrium stationary states is analyzed in terms of the large deviation function, by employing the Laplace approximation of the integral in the renewal equation for the probability density of the process with resetting events.

[1] T. Sandev, V. Domazetoski, L. Kocarev, R. Metzler, A. Chechkin, J. Phys. A: Math. Theor. 55, 074003 (2022).
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DY 44.11 Thu 13:00 P1

Quench-Probe Setup as an Analyzer of Fractionalized Entanglement Spreading — •Nicolas P. Bauer[1], Jan Carl Budich[2], Björn Trauzettel[1], and Alessio Calzona[3] — [1]Julius Maximilians Universität Würzburg, Würzburg, Germany — [2]TU Dresden, Dresden, Germany — [3]IQM Quantum Computers, München, Germany

We propose a novel spatially inhomogeneous setup for revealing quench-induced fractionalized excitations in entanglement dynamics. In this quench-probe setting, the region undergoing a quantum quench is tunnel-coupled to a static region, the probe. Subsequently, the time-dependent entanglement signatures of a tunable subset of excitations propagating to the probe are monitored. We exemplify the power of this generic approach by identifying a unique dynamical signature associated with the presence of an isolated Majorana zero mode in the post-quench Hamiltonian. In this case excitations emitted from the topological part of the system give rise to a fractionalized jump of $\log(2)/2$ in the entanglement entropy of the probe. This dynamical effect is highly sensitive to the localized nature of the Majorana zero mode, but does not require the preparation of a topological initial state.

DY 44.12 Thu 13:00 P1

Exploiting Skyrmion motion for computing — •Alessandro Pignedoli, Björn Dörschel, and Karin Everschor-Sitte — University of Duisburg-Essen, Duisburg, Germany

Brownian motion is a natural phenomenon that can be exploited for energy efficient computing. Here, an assemblage of simple parts evolves in an energetic labyrinth to a low energy state which is isomorphic to the desired solution of a computation [1]. Magnetic Skyrmions [2] are topologically stable magnetic whirls that have been shown to behave like interacting Brownian particles [3,4]. We use a Langevin model to describe and investigate the motion of Skyrmions by means of correlations and statistical observables to carry out Brownian computation. We show that besides the Brownian motion of individual Skyrmions, their interactions and external driving forces break ergodicity. This allows for a rapid convergence to the low-energy state of the system and thus solves the calculation faster.

[1] C. H. Bennett, Int. J. Theor. Phys. 21, 905 (1982) [2] K. Everschor-Sitte, J. Masell, R. M. Reeve and M. Kläui, J. Appl. Phys.124, 240901 (2018) [3]J. Zázvorka, et al. Nat. Nanotechnol. 14, 658 (2019) [4] T.Nozaki, et al Appl. Phys. Lett. 114, 012402 (2019)

DY 44.13 Thu 13:00 P1

A generalised rotational diffusion approach to modeling of the dielectric relaxation processes with resetting — •Irina Petreska[1], Ljupco Pejov[1,2], Trifce Sandev[1,3,4], Ljupco Kocarev[1,3], and Ralf Metzler[4] — [1]Ss. Cyril and Methodius University in Skopje, Macedonia — [2]University of Stavanger, Norway — [3]Macedonian Academy of Sciences and Arts, Skopje, Macedonia — [4]University of Potsdam, Germany

We consider the rotational diffusion equation with a generalised memory kernel in the context of dielectric relaxation processes in a medium composed of polar molecules. We give an overview of existing models on non-exponential relaxation and introduce an exponential resetting dynamic in the corresponding process, providing a detailed analysis of the autocorrelation function and complex susceptibility. It is shown that stochastic resetting leads to a saturation of the autocorrelation function to a constant value, in contrast to the case without resetting, for which it decays to zero. The behaviour of the autocorrelation function, as well as the complex susceptibility in the presence of resetting, confirms that the dielectric relaxation dynamics can be tuned by an appropriate choice of the resetting rate.

[1] I. Petreska, Lj. Pejov, T. Sandev, Lj. Kocarev and R. Metzler, *Fractal Fract.* **6**, 88 (2022).

DY 44.14 Thu 13:00 P1

Dividing Active Brownian Particles — •Till Welker and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Germany.

We aim to combine active motion with cell division to answer questions like: Does nutrient input induce clustering? How does a non-uniform nutrient distribution effects population dynamics?

To include cell division and death in the model of active Brownian particles, we propose a simple rule: *in a time interval dt, each particle has a probability* $dt \cdot g(s)$ *to divide and* $dt \cdot d$ *to die.* The growth rate g depends on the nutrient concentration s at the position of the bacterium and is described by the Monod function. The nutrient diffuses with the diffusion coefficient D_N. We add a source with steady input rate S_0, in addition, each particle takes up nutrient with a rate $\gamma g(s)$.

The population dynamics strongly depends on nutrient diffusion: For large D_N, the population oscillates before reaching a steady population number N^*. For small D_N, the population is stronger damped and equilibrates quickly. N^* is independent of D_N, but the population fluctuation decreases for lower D_N due to the damping. The collective behavior is also influenced by the nutrient: First, for large D_N the swarm has a strongly asymmetric shape during the transient phase which then becomes symmetric in the steady state. Second, the swarm is less dense for larger D_N, but the relationship between spread of nutrient and bacteria is not linear.

We show that combining two key aspects of microbial life, mobility and growth, gives rise to interesting population and spatial dynamics.

DY 44.15 Thu 13:00 P1

Ornstein-Uhlenbeck process and generalizations: influence of comb geometry and stochastic resetting on the particle dynamics — •Petar Jolakoski[1], Pece Trajanovski[1], Kiril Zelenkovski[1], Alexander Iomin[2], Ljupco Kocarev[1,4], and Trifce Sandev[1,3,4] — [1]Macedonian Academy of Sciences and Arts, Skopje, Macedonia — [2]Department of Physics, Technion, Haifa, Israel — [3]University of Potsdam, Germany — [4]Ss. Cyril and Methodius University in Skopje, Macedonia

The Ornstein-Uhlenbeck (O-U) process can be interpreted as a Brownian motion in a harmonic potential. The process is an established Gauss-Markov process that has a bounded variance and admits a stationary probability distribution, in contrast to the standard Brownian motion. Over time, the process tends to drift towards its mean function: such a process is called mean-reverting. Here, we study the effects of stochastic resetting on the O-U process and its generalizations which were hitherto unexplored. In particular, we investigate the dynamics with and without resetting on comb-like structures. For the studied specific 2D comb geometry, we compute the first moment, the non-equilibrium stationary state and the mean squared displacement, and find that the global resetting hinders the particle's transport in the two dimensions. Moreover, the two divergent forces, namely the resetting and the drift towards the mean, lead to compelling results both in the case of O-U process with resetting and its generalization on a 2D comb structure.

DY 44.16 Thu 13:00 P1

Theoretical design of Geometric Brownian Information Engine: Analysis of output work — •Syed Yunus Ali, Rafna Rafeek, and Debasish Mondal — IIT Tirupati, Yerpedu, Andhrapradesh, India

We design a geometric Brownian information engine by considering overdamped Brownian particles inside a 2-D monolobal confinement with irregular width along the transport direction. Under such conditions, particles experience an effective entropic potential. We employ a feedback control protocol as an outcome of error-free position measurement.The protocol comprises three stages: measurement, feedback, and relaxation. We show that the upper bound of the achievable work shows a cross-over from $(5/3-2\ln 2)k_BT$ to $k_BT/2$ when the system changes from an entropy-dominated regime to energy dominated one. Next, we determine the benchmarks for utilizing the available information in an output work and the optimum operating requisites for best work extraction in asymmetric feedback protocol. Transverse bias force (G) tunes the entropic contribution in the effective potential and hence the equilibrium marginal probability distribution standard deviation(σ).We recognize that the amount of extracted work reaches a global maximum when $x_f = 2x_m$ with $x_m = 0.6\sigma$, irrespective of the extent of the entropic limitation.

References:

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DY 44.17 Thu 13:00 P1

Diffusion and order in mixed lattice gas of hard squares — Niklas Raake[1], •Piotr Nowakowski[2], and Ana-Sunčana Smith[1,2] — [1]Friedrich–Alexander–Universität Erlangen–Nürnberg, Erlangen, Germany — [2]Institut Ruđer Bošković, Zagreb, Croatia

We study a lattice gas composed of hard square particles of 1×1 and 2×2 size (measured in lattice constant) undergoing Brownian motion on a two–dimensional square lattice. For different concentrations of both types of particles we determine numerically the diffusion coefficients and compare them with predictions of a model based on a persistent random walk with one or two step memory. Good agreement is observed only for very low and very high concentration of particles. The deviations present in between these regimes suggest that the correlations play an important role in the dynamics of the system.

Additionally, we introduce a configurational order parameter that

characterizes clustering of bigger squares. This allows us to study the continuous transition between unordered liquid and ordered crystal phases.

DY 44.18 Thu 13:00 P1

Non-Markovian modeling of non-equilibrium fluctuations and dissipation in active viscoelastic biomatter — •Amir Abbasi[1], Roland R. Netz[1], and Ali Naji[2] — [1]Freie University of Berlin, Berlin, Germany — [2]Institute for Research in Fundamental Sciences (IPM), Tehran, Iran

Viscoelastic gels such as permanently or transiently cross-linked networks of semiflexible polymers are important soft biological materials. The polymeric nature of such gels is responsible for their salient rheological properties, including their frequency-dependent response to external forces.

Here, based on a Hamiltonian that incorporates the elastic coupling between a tracer and active particles, we derive a generalized Langevin model for the non-equilibrium mechanical response of active viscoelastic biomatter. Our model accounts for the power-law viscoelastic response of the embedding polymeric network as well as for the non-equilibrium energy transfer between active and tracer particles. Our analytical expressions for the frequency-dependent response function and the positional autocorrelation function agree nicely with experimental data for red blood cells and actomyosin networks with and without ATP. The fitted effective active-particle temperature, elastic constants and effective friction coefficients of our model allow straightforward physical interpretation.

DY 44.19 Thu 13:00 P1

Ornstein-Uhlenbeck process on three dimensional comb structure under stochastic resetting — •Pece Trajanovski[1], Petar Jolakoski[1], Kiril Zelenkovski[1], Alexander Iomin[2], Ljupco Kocarev[1,4], and Trifce Sandev[1,3,4] — [1]Macedonian Academy of Sciences and Arts, Skopje, Macedonia — [2]Department of Physics, Technion, Haifa, Israel — [3]University of Potsdam, Germany — [4]Ss. Cyril and Methodius University in Skopje, Macedonia

The Ornstein-Uhlenbeck (O-U) process is a generalised diffusion process, introduced as a model for the velocity of a particle undergoing a Brownian motion confined in harmonic potential. The process is a stationary, meaning that over time, it tends to drift towards its long-time mean function: such a process is called mean-reverting. Here, we investigate the influence of the three dimensional comb structure and the stochastic resetting on the particle dynamics governed by O-U processes along the backbone (x-direction) and the main fingers (y-direction) and standard Wiener process along the secondary fingers of the comb (z-direction). The explicit analytical expressions for the first moment and mean squared displacement along all three directions are calculated and confirmed numerically. The marginal probability density functions along all directions are simulated by using coupled Langevin equations for comb geometry.

DY 44.20 Thu 13:00 P1

Generalized molecular Stokes-Einstein and Stokes-Einstein-Debye relations including temperature-dependent slip and effective radius — •Sina Zendehroud, Jan O. Daldrop, Yann von Hansen, and Roland R. Netz — Freie Universität Berlin, Department of Physics, Arnimallee 14, 14195 Berlin, Germany

We perform molecular dynamics simulations of water at different temperatures and calculate the viscosities as well as the rotational and translational self-diffusion constants of water molecules in the lab frame and in the comoving coordinate frame of the molecules. Instead of interpreting the results as deviations from the Stokes-Einstein and Stokes-Einstein-Debye relations, we simultaneously determine the slip length and the effective hydrodynamic radius from the simulation data. We show that the viscosity dependence of the diffusion constants of water can be understood in terms of an almost constant effective radius and a pronounced temperature dependence of the slip length.

DY 44.21 Thu 13:00 P1

Energy transfer between the librational and the inter- and intramolecular vibrational modes of liquid water — •Louis Lehmann and Roland Netz — Fachbereich Physik, Freie Universität Berlin

The molecular dynamics of liquid water can be split into librational and inter- and intramolecular vibrational modes. By applying the Eckart decomposition scheme, the infrared absorption spectrum can be exactly decomposed into contributions from these different modes. The complete energy transfer network of the librational and inter- and intramolecular vibrational modes in liquid water is established based on the energy transfer rates determined from equilibrium molecular dynamics simulations with conventional and many-body force fields. The results are validated by comparison with non-equilibrium molecular dynamics simulations that mimic pump-probe experiments.

DY 44.22 Thu 13:00 P1

Domain Drift and Diffusion in Cell-Polarization Processes — •Johannes Ewald and Jürgen Vollmer — Institute of Theoretical Physics, Universität Leipzig, Brüderstr. 16, D-04103 Leipzig, Germany

Cell polarization can be driven by the formation of signaling patterns on cell membranes. They can be modeled by two species of membrane proteins that can bind to cytosolic enzymes. The enzymes drive the conversion between cell membranes. These chemical reactions drive the coarsening of domains on the cell surface. Polarization amounts to the situation where the cell surface is covered by only two domains on opposing sides of the cell. Certain aspects of the domain coarsening are reminiscent to ripening of spin-up and spin-down domains in ferromagnets. In this analogy the conversion of membrane proteins takes the role of spin flips of the magnetic system. However, there are also distinct differences in the dynamics because the conversion is driven by a dissipative chemical reaction, while spin-flips arise due to thermal fluctuations. Based on the analytical solutions for domain drift and diffusion in the two models we will discuss differences and communalities of the processes.

DY 45: Poster: Nonlinear Dynamics, Pattern Formation and Networks

Time: Thursday 13:00–16:00 Location: P1

DY 45.1 Thu 13:00 P1

A systematic approximation scheme mapping systems with time delays to sets of ordinary differential equations — •Daniel Henrik Nevermann and Claudius Gros — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Deutschland

Mathematically, delayed differential equations evolve in infinite dimensional state spaces. It is hence conceivable that time-delayed systems can be approximated by a set of $N+1$ ordinary differential equations, with the trajectory of the primary variable converging to the solution of the original time-delayed system when $N \to \infty$. We show that this program can be carried out using sequences of time-delay kernels related to discrete gamma distributions.

We present several analytical and numerical results for the proposed approximation scheme, finding that the instability of fixed points due to increasing time delays is captured accurately already for $N \sim 10$. For the Mackey-Glass system we find that the locus of a limit-cycle doubling are recovered in good approximation only for substantially larger $N \sim 10^2 - 10^3$, with the transition to chaos requiring an even larger state space. In general, we find that relative approximation errors scale as $1/N$. In addition, we discuss how the approximation proposed can be applied to the case of distributed time delays.

It is in general an approximation to model a given experimental protocol by a dynamical system characterized by a single time delay T. Using a distribution of time delays peaked at T, with width $\sim 1/N$, can hence be argued to provide a more accurate description of real-world non-Markovian processes.

DY 45.2 Thu 13:00 P1

Preprocessing algorithms for the estimation of ordinary differential equation models with polynomial nonlinearities — •Oliver Strebel — Angelstr. 17, 75392 Deckenpfronn

The data analysis task of determining a model for an ordinary differential equation (ODE) system from given noisy solution data is addressed. Based on a previously published parameter estimation method for ODE models [1] four related model estimation algorithms were developed. The algorithms are tested for over 20 different polynomial ordinary equation systems comprising 60 equations at various noise levels. Two algorithms frequently compute the correct model [2]. They are compared to the prominent SINDy-family for those SINDy-algorithms that have simple default hyperparameters [3]. A novel and successful method for determining the parameter of Tikhonov regularization when calculating numerical differentials is also presented.

[1] O. Strebel: http://dx.doi.org/10.1016/j.chaos.2013.08.015
[2] O. Strebel: https://osf.io/89djt/
[3] S. Brunton et al: http://dx.doi.org/10.1073/pnas.1517384113

DY 45.3 Thu 13:00 P1

Testing Jump-Diffusion in Epileptic Brain Dynamics: Impact of Daily Rhythms — •Jutta G. Kurth[1,2], Klaus Lehnertz[2], and Thorsten Rings[2] — [1]Georg-August-Universität Göttingen — [2]Rheinische Friedrich-Wilhelms-Universität Bonn

Stochastic approaches to complex dynamical systems have recently provided broader insights into spatial-temporal aspects of epileptic brain dynamics. Stochastic qualifiers based on higher-order Kramers-Moyal coefficients derived directly from time series data indicate improved differentiability between physiological and pathophysiological brain dynamics. It remains unclear, however, to what extent stochastic qualifiers of brain dynamics are affected by other endogenous and/or exogenous influencing factors. Addressing this issue, we investigate multi-day, multi-channel electroencephalographic recordings from a subject with epilepsy. We apply a recently proposed criterion to differentiate between Langevin-type and jump-diffusion processes and observe the type of process most qualified to describe brain dynamics to change with time. Stochastic qualifiers of brain dynamics are strongly affected by endogenous and exogenous rhythms acting on various time scales*ranging from hours to days. Such influences would need to be taken into account when constructing evolution equations for the epileptic brain or other complex dynamical systems subject to external forcings.

Keywords: diffusion process; jump-diffusion process; time series analysis; brain; epilepsy; biological rhythms

DY 45.4 Thu 13:00 P1

Temporal localized states and square waves in semiconductor micro-resonators with strong time delayed feedback — •Elias R. Koch[1,2], Thomas Seidel[1], Julien Javaloyes[2], and Svetlana V. Gurevich[1] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany — [2]Departament de Física & IAC-3, Universitat de les Illes Balears, C/ Valldemossa km 7.5, 07122 Mallorca, Spain

Recent works demonstrated the promising potential of injected micro-resonators enclosed into external cavities as high-power, tunable sources of Frequency Combs in the near infra-red. It was shown that the natural modeling approach consists in using singularly perturbed time delayed systems. Departing from former studies that considered a single intensity dependent refractive index (i.e. Kerr nonlinearity) we explore in this contribution the impact of a semiconductor Quantum-Well as the nonlinear element. A first principle model for the optical response is employed which allows to explore the influence of the detuning with respect to the band-gap. We show that this extended model predicts the existence of a bistable set of bright and dark temporally localized states as well as square-waves, with a periodic of twice the delay in the case of antiresonant optical feedback.

Finally, in order to clarify the influence of the second and third order chromatic dispersion and of the frequency dependence of the quantum-well response, we perform a multiple time-scale analysis in the so-called good cavity limit. The resulting normal form PDE shows a good agreement with the original, first principle, time delayed model.

DY 45.5 Thu 13:00 P1

Antipersistent random walks in time-delayed systems — •Tony Albers[1], David Müller-Bender[1], and Günter Radons[1,2] — [1]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Institute for Mechanical and Industrial Engineering, Chemnitz, Germany

In this contribution, we show that the occurrence of chaotic diffusion in a typical class of time-delayed systems with linear instantaneous and nonlinear delayed term can be well described by an antipersistent random walk. We numerically investigate the dependence of all relevant quantities characterizing the random walk on the strength of the nonlinearity and on the delay. With the help of analytical considerations [1], we show that for a decreasing nonlinearity parameter the resulting dependence of the diffusion coefficient is well described by Markov processes of increasing order.

[1] Tony Albers, David Müller-Bender, and Günter Radons, Phys. Rev. E **105**, 064212 (2022)

DY 45.6 Thu 13:00 P1

Advection dependent pulse dynamics — •Adrian Misselwitz[1], Susanne Lafon[2], Jean-Daniel Julien[2], and Karen Alim[1,2] — [1]School of Natural Sciences, Technische Universität München — [2]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen

Models of pulse formation in nerve conduction have provided manifold insight not only into neuronal dynamics but also the non-linear dynamics of pulse formation in general. Recent observation of neuronal electro-chemical pulses also driving mechanical deformation of the tubular neuronal wall and thereby generating ensuing cytoplasmic flow now question the impact of flow on the electro-chemical dynamics of pulse formation. We, here, theoretically investigate the classical Fitzhugh-Nagumo model now accounting for advective coupling between the pulse propagator typically describing membrane potential and here triggering mechanical deformations and, thus, governing flow magnitude, and the pulse controller, a chemical species advected with the ensuing fluid flow. Employing analytical calculations and numerical simulations we find, that advective coupling allows for a linear control of pulse width while leaving pulse velocity unchanged. We therefore uncover an independent control of pulse width by fluid flow coupling.

DY 45.7 Thu 13:00 P1

(Broken) gradient-dynamics description of reactive thin liquid films — •Florian Voss, Fenna Stegemerten, and Uwe Thiele — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Ger-

many

After reviewing the gradient dynamics formulation of chemical reactions, applied e.g. in [1] to reacting phase-separating systems, we apply the concept to thin liquid films and shallow drops that are either covered by reactive surfactants [2] or react with the solid substrate [3]. Next we discuss how the breaking of the variational form by imposed fluxes results in intricate spatio-temporal dynamics of the film/drop and reactant density profiles. As an example we consider a simple model for oscillatory behaviour in droplets of slime mould.

[1] D. Zwicker, Current Opinion in Colloid & Interface Science, 61, 101606 (2022),

[2] A. Pereira, P. M. J. Trevelyan, U. Thiele, and S. Kalliadasis, Phys. Fluids 19, 112102 (2007),

[3] K. John, M. Bär, and U. Thiele, Eur. Phys. J. E 18, 183 (2005).

DY 45.8 Thu 13:00 P1

Coupling short-range signaling and tissue mechanics for biological pattern formation — •Valèria Ribelles Pérez, Stephan Kremser, Mareike Bojer, Sabina Orazov, and Ulrich Gerland — Physics Department, Technical University of Munich

Pattern formation phenomena are ubiquitous in natural and synthetic multicellular systems. Both mechanical forces and biochemical interactions between cells play key roles in tissue dynamics. While much is known about these physical and biochemical processes separately, their interplay is still poorly understood. Here, we focus on short-range signaling between cells, modelled by cellular automata, coupled to a vertex model incorporating mechanical interactions, to investigate patterning principles during tissue homeostasis and growth. We test the modelling framework in the context of salt-and-pepper-like patterns that arise for instance in epithelial tissues.

DY 45.9 Thu 13:00 P1

Robust, precise, and modular solutions to the French flag problem in two dimensions without global signaling — •Lukas Zett, Stephan Kremser, Gabriel Vercelli, and Ulrich Gerland — Technical University of Munich

The formation of axial patterns with broad regions in multicellular systems has been conceptualized by Wolpert in his famous French flag problem. Both of Wolpert's proposed solutions, the balancing and gradient model, utilize long-range signaling between cells. Models relying on short-range signaling, based on cellular automata (CA) rules as modeling tool, have also computationally been shown to successfully solve the French flag problem in one dimension (1D). Here, we extend these models to two spatial dimensions (2D) to investigate whether the 1D solutions can be generalized to the 2D case and to search for novel solutions existing only in 2D. We dissect the 2D problem into two coupled, 1D pattern formation processes along and perpendicular to the axis of the French flag. Using evolutionary algorithms and consensus procedures as well as engineering approaches, CA dynamics which solve the French flag problem are found. We show that these solutions form more precise patterns and are in general more robust than their 1D counterparts, while still being able to scale with system size. Depending on the desired robustness and precision of the solution, different patterning modules along the two axes can be combined. Using the regulatory logics of these underlying modules could therefore serve as a basis for the design of synthetic patterning systems with a range of different specifications.

DY 45.10 Thu 13:00 P1

Kinetic Monte Carlo Model for Computing Functionalities in Nanoparticle Networks — •Jonas Mensing[1] and Andreas Heuer[2] — [1]Institut für Physikalische Chemie, WWU Münster — [2]Institut für Physikalische Chemie, WWU Münster

We want to achieve reconfigurable computational unctionality in a nanoparticle network for energy efficient machine learning applications. Previous research has shown that disordered networks of functionalized gold nanoparticles can be configured to behave like Boolean logic gates and binary classifiers. In this regard, gold nanoparticles serve as switchable single-electron transistors, while organic molecules connecting the nanoparticles act as tunable tunnel barriers. The resulting network is then placed within an array of electrodes that manipulate the charge and potential landscape of the network to evolve the system into its desired emergent functionality. In total, the network is able to mimic the mechanism of a brain-like neural network. The theoretical underpinning of these networks is investigated with a highly optimized physical model and subsequent simulations. The model is able to simulate the charge transport within the network stochastically, i.e. with a kinetic Monte Carlo approach. Requirements for various computing functionalities such as Boolean logic are examined. Besides graph theory and data-driven tools allow mapping network and electrode properties to the appearance of computational functionalities. The simulations are carried out in close comparison with corresponding experiments.

DY 45.11 Thu 13:00 P1

Randomised mixed labyrinth fractals — •Janett Prehl[1], Ligia Loretta Cristea[2], and Daniel Dick[1] — [1]Technische Universität Chemnitz, Chemitz, Germany — [2]Technische Universität Graz, Graz, Austria

Fractals, introduced by Benoit Mandelbrot in the early 1980s, allow the analysis of physical properties of natural geometries and structures in non-integer dimensions. It has been shown recently, that utilizing fractals structures, for instance for gas sensors made of carbon nanotubes increase their efficiency or give new insights to complex quantum phenomena. Here, we are interested how the effect of randomness, as observed in real materials, alter the topology and thus dynamics of the resulting fractal structures in comparison to the pure cases. We focus on a special class of Sierpinski carpets, i.e., the labyrinth fractals [1], that can be used for dendritic networks or porous materials. Therefore, we mix to fractal patterns, with different properties, i.e., shortest path and random walk dimension, randomly together at different mixing ratios. Surprisingly we found that even in cases where the initial patterns exhibit the same non-integer dimensions the resulting randomised fractals give a different property [2].

[1] L.L. Cristea and B. Steinsky, *Proc. Edinburgh Math. Soc.* **54.4** (2011) 329.
[2] J. Prehl, D. Dick, and L.L. Cristea, to be submitted to *Fractals* (2023).

DY 45.12 Thu 13:00 P1

How Can Cell-Like Inflated Shells Control Their Shape? —A Stability Analysis — •Paul Nemec and Ulrich Gerland — Physics Department, Technical University of Munich

This work follows a long history of studying how biological organisms arrive at and maintain their shape [1]. Inspired by the question of how E. coli maintain their cylindrical shape during growth [2], we study the growth of pressurised cell-like structures. The model is this: a cell is an inflated elastic shell, where internal and fine grained details are neglected. Growth is the time evolution of the reference or undeformed configuration of the cell, which may depend on geometric and mechanical properties like curvature and stress. Growth must be local and invariant under translations and rotations of the entire cell. Under these constraints, how can cells robustly achieve simple target geometries like a sphere given arbitrarily perturbed initial conditions? This poster presents some initial insights.

[1] Goriely, A. The Mathematics and Mechanics of Biological Growth, Springer (2017).

[2] Amir, A., van Teeffelen, S. Getting into shape: How do rod-like bacteria control their geometry?. *Syst Synth Biol* **8**, 227–235 (2014).

DY 45.13 Thu 13:00 P1

Stimulating self-optimisation of flow networks for transport — •Swarnavo Basu and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

Flow transport in networks is ubiquitous in biology (e.g. blood vasculature) and engineering (e.g. porous media). Many biological networks are adaptive and can self-organise in response to external stimuli. They homogenise flow to achieve optimal perfusion and a uniform flow of chemicals across the network. In contrast, engineered networks of random media have heterogeneous flow velocity distributions across the network. Self-organising engineered networks that can homogenise flow will have many applications, ranging from microfluidic networks for cooling batteries and chemical reactors to *in vitro* vasculature for perfusing tissues and implants. We propose a model of a network whose tube radii can be controlled using periodic inflows of pulses of an eroding agent that erodes the network's walls. We observe that such networks self-organise in response to the eroding agent, leading to a homogenised flow. This provides a framework for engineering networks that can self-organise to achieve optimal perfusion.

DY 45.14 Thu 13:00 P1

Fixation probabilities in network structured meta-

populations — •Sedigheh Yagoobi[1] and Arne Traulsen[2] — [1]Max-Planck institute for evolutionary biology — [2]Max-Planck Institute for Evolutionary Biology

The effect of population structure on evolutionary dynamics is a long-lasting research topic in evolutionary ecology and population genetics. Evolutionary graph theory is a popular approach to this problem, where individuals are located on the nodes of a network and can replace each other via the links. We study the effect of complex network structure on the fixation probability, but instead of networks of individuals, we model a network of sub-populations with a probability of migration between them. We ask how the structure of such a meta-population and the rate of migration affect the fixation probability. Many of the known results for networks of individuals carry over to meta-populations, in particular for regular networks or low symmetric migration probabilities. However, when patch sizes differ we find interesting deviations between structured meta-populations and networks of individuals. For example, a two patch structure with unequal population size suppresses selection for low migration probabilities.

DY 45.15 Thu 13:00 P1

Ising model with variable spin/agent strengths on graphs — Mariana Krasnytska[1,2,3], Yurij Holovatch[1,2,4], •Bertrand Berche[2,3], and Ralph Kenna[2,4] — [1]ICMP, NAS of Ukraine, Lviv, Ukraine — [2]L4 Collaboration Leipzig-Lorraine-Lviv-Coventry — [3]Université de Lorraine, Nancy, France — [4]Coventry University, UK

We consider a generalization of the Ising model in which individual spin strengths can vary [1]. The model describes the ordering in systems comprised of agents which, although matching in their binarity (i.e., maintaining the iconic Ising features of spin 'up'/'down', 'yes'/'no'), differ in their strengths. With inhomogeneous physical systems in mind, but also anticipating interdisciplinary applications, we present the model on graph structures of varying degrees of complexity: complete graph, Erdös-Rényi graph, and on a scale-free network. This allows us to explore the interplay of two types of randomness: individual strengths of spins or agents and collective connectivity between them. We find the delicate interplay between variable properties of nodes and interactions between them leads to new universality classes.

[1] M. Krasnytska, B. Berche, Yu. Holovatch, R. Kenna, J. Phys. Complex., 1 (2020) 035008; Entropy, 23(9) (2021) 1175.

DY 45.16 Thu 13:00 P1

Homeostatic plasticity in a minimal model for brain criticality — •Marco Schmidt and Stefan Bornholdt — Institut für Theoretische Physik, Universität Bremen

The 'criticality hypothesis' asserts that real-world neural networks operate near a critical phase transition. Experimental evidence exists and numerous models studying the possible underlying mechanisms accumulated during the last 20 years.

Early models based on simple threshold networks tune to a critical connectivity $K = 2$, which is not a realistic value when compared to real-world neural networks.

However, a phase transition in high degree threshold networks using the inhibition to excitation ratio as a control parameter does exist [1], as well as a corresponding self-organized critical toy model [2]. It features an adaptive threshold network, self-tuning to the critical inhibition to excitation ratio by using an activity based rewiring process that results in a highly clustered network and reaches criticality independent of K.

Here we present a new version of the model, incorporating a simple homoestatic plasticity mechanism as it appears in biological systems.

[1] L. Baumgarten, S. Bornholdt, Critical excitation-inhibition balance in dense neural networks, Phys. Rev. E 100, 010301 (2019).
[2] L. Baumgarten, S. Bornholdt, A toy model for brain criticality: self-organized excitation/inhibition ratio and the role of network clustering, arXiv:2202.03330.

DY 46: Poster: Machine Learning and Data Analytics

Time: Thursday 13:00–16:00 Location: P1

DY 46.1 Thu 13:00 P1

Time series analysis of loudness fluctuations in musical performances and psychophysical experiments — •Benjamin Schulz[1,2], Corentin Nelias[1,2], and Theo Geisel[1,2,3] — [1]MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Physics Dept., Georg-August University, Göttingen, Germany — [3]Bernstein Center for Computational Neuroscience, Göttingen, Germany

Over the last decades, the study of fluctuations in musical time series showed power spectral densities that exhibit a $1/f^{\beta}$-shape across certain frequency regions, indicating long range correlations. So far time series of pitch, rhythm, or timing were investigated across different musical epochs, composers and styles, showing a variety of β-values between 0 and 2. Whether the fluctuations of musical dynamics, or in other words loudness fluctuations, have similar spectral properties, is an open question, however. We have carried out in-depth studies of manually recorded data sets in different musical settings. A first set results from psychophysical tapping experiments. A second one consists of drum performances recorded in a musical environment. All participating musicians were professionals. The tapping and drumming data consistently show the clear occurrence of a $1/f^{\beta}$-shape in the power spectral density. Furthermore, the presence of a metronome click in the tapping experiment leads to the strengthening of specific periodic structures in the loudness fluctuations and also seems to have an impact on the coefficient β.

DY 46.2 Thu 13:00 P1

Battery modeling: Fusing equivalent circuit models with data-driven surrogate modelling — •Limei Jin[1,2], Franz P. Bereck[2], Josef Granwehr[2], Rüdiger-A. Eichel[2], Karsten Reuter[1], and Christoph Scheurer[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]IEK-9, Forschungszentrum Jülich, Jülich, Germany

Electrochemical impedance spectroscopy (EIS) is widely used to characterize electrochemical energy conversion systems. The traditional analysis with equivalent circuit models (ECM) has recently been augmented by a transform based distribution of relaxation times (DRT) analysis which allows one to reduce the ambiguity in the construction of ECMs and thus overfitting. Experimentally determined ECM parameters vary depending on operating conditions and the lifetime history of battery usage. Here we focus on State of Health (SOH) and State of Charge (SOC) as a basis for operando diagnosis and functionality optimization in the setting of fast-charging. Within pure ECM approaches, aging effects can only be represented to a limited extent, as aging is related to a variety of different factors whose impact on cell impedance are not sufficiently understood, yet. The highly complex interplay of factors motivates the development of data-driven Machine Learning (ML) models as a basis for future battery management systems. We present ML enabled ECMs based on experimental impedance analyses and a data-driven ML approach that computationally samples an abstract target space for classification and recognition of cells at vastly different SOC/SOH combinations.

DY 46.3 Thu 13:00 P1

Machine learning categorization of the Anderson model — •Quangminh Bui-Le and Rudolf Römer — Department of Physics, University of Warwick, Coventry, CV4 7AL

Machine learning (ML) methods have been used to identify phase transitions of physical systems by categorizing systems based on the Ψ^2 values of their wave-functions into extended and localized states, which a model is then trained on in order to identify between the extended and localized states. Here we want to see if ML is powerful enough to categorize systems into even more specific groups by attempting to categorize Anderson model data into categories based on the disorder of the wave-function. We are using a PyTorch model to create a convolutional neural network using a ResNet18 model. This model will be trained on 3D Anderson model Ψ^2 values from 17 disorder values spanning a range of 15 to 18.

DY 46.4 Thu 13:00 P1

Neural-network based Monte Carlo Markov chain simulation of spin glasses — •Michael Engbers and Alexander K. Hart-

MANN — Carl von Ossietzky University, Oldenburg, Germany

Spin glasses exhibit a complex equilibrium and non-equilibrium behavior at low temperatures. The reason is the existence of an energy landscape with many local minima and high barrieres. In computer simulations, this leads to long correlation times when investigating large systems. Due to this numerical hardness, the model has motivated the development of many new algorithmic approaches like generalized Wolff cluster algorithms, parallel tempering or genetic algorithms.

Recently, it has been shown that the application of generative neural networks can accelerate Monte Carlo simulations, also for simple spin models with apparently promising results.

Here, we use an autoregressive distribution estimator (NADE) to perform a Monte Carlo simulation of spin glasses [1]. We embedded the NADE into a Metropolis-Hastings Markov-chain approach, therefore ensuring detailed balance. We confirm previous results that the acceptance rates of the NADE approach surprisingly increase with decreasing temperature. Nevertheless, we show that crucial observables, such as the distribution of spin overlaps, indicate that this neural-network approach suffers from the lack of effective ergodicity.

[1] B. McNaughton, M.V. Milosević, A. Perali, and S. Pilati, Phys. Rev. E **101**, 053312 (2020).

DY 46.5 Thu 13:00 P1

Influence of mode-coupling on the information processing rate of Spin-VCSEL reservoir computer — •LUKAS MÜHLNICKEL, LINA JAURIGUE, and KATHY LÜDGE — Institut f. Physik, Technische Universität Ilmenau, Weimarer Str. 25, 98684 Ilmenau, Germany

The relative simplicity of reservoir computing, when comparing it to other machine learning methods, makes it suitable for efficient hardware implementation. The needed high dimensional reservoir dynamics can be provided by adding feedback to only one single nonlinear node, while driving the system with time multiplexed inputs. One promising realization utilizes the fast polarization dynamics of power efficient Spin-VCSELs. These fast field interactions are related to birefringence, dichroism and electron transition rates in the cavity material and occur on shorter time scales than the relaxation oscillations. Thus, compared to typical semiconductor lasers, much higher cutoff frequencies in the system response are observed for the Spin-VCSELs. We investigate the influence of these fast polarization oscillation dynamics on the reservoir performance when increasing data processing rates.

DY 46.6 Thu 13:00 P1

Deep learning-based clogging prediction in outflow of hard and soft grains — •SEDDIGHEH NIKIPAR, DMITRY PUZYREV, JING WANG, and RALF STANNARIUS — Institute of Physics and MARS, Otto von Guericke University Magdeburg, Universitätsplatz 2, D- 39106 Magdeburg, Germany

Studying the outflow of granular materials has been recognized as a challenging topic in physics due to their unexpected behavior, such as segregation, blockage, and other dynamical events [1]. In particular, the early detection of clogging during discharge of granular materials through narrow orifice in silo has significant challenges. In this work, the possibility of early prediction of clogging was investigated through implementation of image-based deep learning approach, which turns out to be a promising strategy to predict the time until the next clog [2]. For this purpose, experiments on discharge of mixtures of hard and soft spheres from a quasi-two dimensional (2D) silo have been conducted [3]. The image dataset of flowing particles was used to train the Convolutional Neural Networks of various architectures and to CNN-LSMT architecture specifically designed for time series analysis. The trained networks demonstrate considerable accuracy in clogging prediction.

This study is supported by DLR projects VICKI and EVA (50WM2252 and 50WM2048)

[1] Perge C, et al. Phys. Rev. E 85 021303 (2012) [2] Hanlan J, APS March Meeting, abstract id.M09.010 (2022) [3] J Wang, et al. Soft Matter, 17, 4282 (2021)

DY 46.7 Thu 13:00 P1

Optical reservoir computing with incoherent optical memory — •MINGWEI YANG[1,2], ELIZABETH ROBERTSON[1,2], LEON MESSNER[1,3], NORMAN VINCENZ EWALD[1], LUISA ESGUERRA[1,2], and JANIK WOLTERS[1,2] — [1]Deutsches Zentrum für Luft- und Raumfahrt, Institute of Optical Sensor Systems, Berlin, Germany. — [2]Technische Universität Berlin, Berlin, Germany. — [3]Humboldt-Universität zu Berlin, Berlin, Germany.

Reservoir computing is a machine learning method that is particularly suited for dynamic data processing. A fixed reservoir projects the input information to a high-dimensional feature space, and only the readout weights need to be trained, allowing fast data processing with low energy consumption [1,2]. In this work, we demonstrate an optical reservoir computing using incoherent memory in a cesium vapor cell to predict time-series data. The information is stored in the reservoir by controlling the pump and probe process on the Cs D2 transitions. The coupling between the reservoir and both the input and output data is realized by acousto-optic modulators. [1] G. Tanaka, T. Yamane, J. B. Héroux, R. Nakane, N. Kanazawa, S. Takeda, H. Numata, D. Nakano, and A. Hirose, *Recent advances in physical reservoir computing: A review,* Neural Networks 115, 100*123 (2019). [2] L. Jaurigue, E. Robertson, J. Wolters, and K. Lüdge, *Photonic reservoir computing with non-linear memory cells: interplay between topology, delay and delayed input,* in Emerging Topics in Artificial Intelligence (ETAI) 2022, vol. 12204 (SPIE, 2022), pp. 61*67.

DY 46.8 Thu 13:00 P1

Metadynamics Simulations of Chemical Reactions in Solution — •AZAD KIRSAN, SAGARMOY MANDAL, and BERND MEYER — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

For four important chemical reactions we have benchmarked two different method for reconstructing the free energy surface (FES) and for estimating the free energy barrier from *ab initio* molecular dynamics (AIMD) simulations: standard metadynamics (MTD) and the recently introduced well-sliced metadynamics (WS-MTD) approach [1], which is a combination of umbrella sampling and MTD. The chosen reactions are a Diels-Alder reaction, an aromatic decarboxylation, an aromatic Claisen rearrangement, and the base-catalyzed hydrolysis of formamide. This selection includes a cycloaddition, an elimination, an intermolecular rearrangement, and an OH^- addition, thus covering a wide range of different reaction types and mechanisms. By utilizing our recently improved version of the CPMD code [2] it was possible to obtain many ns long trajectories of the reactions in the gas phase as well as in an explicitly included solvent.

[1] S. Awasthi, V. Kapil, N. Nair, J. Comput. Chem. **37** (2016) 1413
[2] T. Klöffel, G. Mathias, B. Meyer, Comput. Phys. Commun. **260** (2021) 107745

DY 46.9 Thu 13:00 P1

Analyzing Extreme Fluctuations of the Randomly Forced Nonlinear Schrödinger Equation via Large Deviation Theory — •SUMEJA BUREKOVIĆ[1], TOBIAS SCHÄFER[2], and RAINER GRAUER[1] — [1]Institute for Theoretical Physics I, Ruhr-University Bochum, Germany — [2]Department of Mathematics, College of Staten Island, Staten Island, United States of America

Recently, the focusing nonlinear Schrödinger equation with additive noise has been proposed as a model for finite-time singularity mediated turbulence [1]. Among other findings, the authors of [1] show through direct numerical simulations that the statistics of quantities such as the energy dissipation rate and structure functions are intermittent. Here, in order to explain these observations and to quantify the effect of extreme fluctuations on the turbulence statistics, we employ methods from large deviation theory or instanton calculus [2]. In the first step, the probability density function or expectation for the quantities of interest is approximated by the Freidlin-Wentzell action of the large deviation minimizer or instanton. Additionally, our aim is to improve this approximation by taking into account Gaussian fluctuations around the instanton, harnessing the techniques of [3].

[1] Josserand, C., Pomeau, Y., & Rica, S. (2020). Phys. Rev. Fluid, 5(5), 054607. [2] Grafke, T., Grauer, R., & Schäfer, T. (2015). J. Phys. A Math. Theor., 48(33), 333001. [3] Schorlepp, T., Grafke, T., & Grauer, R. (2021). J. Phys. A Math. Theor., 54(23), 235003.

DY 46.10 Thu 13:00 P1

Light propagation in media with electric and magnetic disorder: 3D Anderson localization — •WALTER SCHIRMACHER[1,2], THOMAS FRANOSCH[3], MARCO LEONETTI[1,4], and GIANCARLO RUOCCO[1,5] — [1]Istituto Italiano di Tecnologia, Roma, Italy — [2]Universität Mainz, Mainz, Germany — [3]Universität Innsbruck, Innsbruck, Austria — [4]SLML, Consiglio Nationale delle Richerche, Roma, Italy — [5]Universita "La Sapienza", Roma Italy

We consider Maxwell's equations in a 3-dimensional material, in which both, the electric permittivity, as well as the magnetic permeability,

fluctuate in space. Differently from all previous treatments, we transform the fields in such a way that the linear operator in the equations is manifestly Hermitian, in order to deal with a proper eigenvalue problem. We use an appropriate version of the Coherent-Potential approximation (CPA) to calculate the density of states and scattering-mean-free path. We find that in the presence of both electric and magnetic disorder the spectral range of Anderson localization appears to be much larger than in the case of electric (or magnetic) disorder only.

DY 47: Wetting, Fluidics and Liquids at Interfaces and Surfaces II (joint session CPP/DY)

Time: Thursday 15:00–16:15 Location: MER 02

DY 47.1 Thu 15:00 MER 02

Hierarchical superhydrophobic composite membrane for enhanced distillation with excellent fouling resistance — •Prexa Shah[1], Youmin Hou[2], Michael Kappl[1], and Hans Jürgen Butt[1] — [1]Max-Planck-Institute for Polymer Research, Physics at Interfaces group, Ackermannweg 10, 55128 Mainz, Germany. — [2]School of Power and Mechanical Engineering, Wuhan University, 430072, Wuhan, China.

In arid areas near the coast, seawater desalination has become an essential supply of clean water. As a result, energy-efficient desalination systems must be developed to avoid overburdening the restricted energy supply. Membrane distillation (MD) is gaining popularity as a hybrid thermal/membrane-based desalination approach that may use waste heat for small-scale desalination as well as treating high-salinity brines. The objective is now to maximize the distillation rate while avoiding membrane wetting and fouling. In this work, composite membranes with multiscale pore sizes are formed by depositing a thin layer of nano-porous nanofilaments over microporous membranes. Distillation performance and fouling resistance are explored utilizing low surface tension impurities, which might enhance the chance of membrane wetting. The resistance of protein adsorption to organic fouling is also examined. Our unique multiscale porous membranes outperform traditional hydrophobic membranes in terms of fouling resistance while achieving better distillation flow. This research shows how to optimize MD procedures for wastewater and saltwater treatment.

DY 47.2 Thu 15:15 MER 02

Surface tension of cavitation bubbles — •Marine Bossert[1], Panayotis Spathis[2], Pierre-Étienne Wolf[2], Laurent Cagnon[2], Isabelle Trimaille[3], and Étienne Rolley[4] — [1]Institut of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Institut Néel, Grenoble, France — [3]Institut des NanoSciences de Paris, Paris, France — [4]Laboratoire de Physique de l'École Normale Supérieure, Paris, France

The evaporation of a fluid contained in a porous material occurs by cavitation when the pores are connected to the outer gas reservoir through small constrictions. Using monolithic transparent porous samples, we have measured the cavitation rate J as a function of the departure from equilibrium for hexane at room temperature [1] and nitrogen over a wide temperature range.

When the radius of the critical nucleus R* is large, our measurements are in agreement with the prediction of the Classical Nucleation Theory. However, when the thickness of the interface is not negligible compared to R*, we find that J is much larger than predicted. We show that this shift can be accounted for if the liquid-vapor surface tension is allowed to depend on the interface curvature. This dependence is in reasonable agreement with Density Functional calculations for Lennard-Jones fluid, including the correction to second order in curvature.

[1] V. Doebele, et al, Phys. Rev. Lett. 125 (2020) 255701.

DY 47.3 Thu 15:30 MER 02

Simulations for Wetting of Biomembranes — •Marcel Mokbel and Sebastian Aland — TU Bergakademie Freiberg, Freiberg, Germany

The dynamics of membranes, shells, and capsules in fluid flow has become an active research area in computational physics and computational biology. The small thickness of these elastic materials enables their efficient approximation as a hypersurface, which exhibits an elastic response to in-plane bending and out-of-plane stretching deformations. If such a closed thin shell is filled with (and/or surrounded by) multiple fluids, capillary forces on the contact line between the fluids and the shell may arise and force the shell to deform.

In this work, we present a novel Arbitrary Lagrangian-Eulerian (ALE) method to simulate such elastic surfaces immersed in Navier-Stokes fluids, which is combined with a phase field approach to model droplets inside and/or outside the surface. This method combines high accuracy with computational efficiency, since the grid is matched to the elastic surface and can therefore be resolved with relatively few grid points near the surface. We formulate elastic surface forces and propose an evolving finite-element discretization. Several wetting test cases demonstrate the versatility of the proposed method. Examples are simulations of single or multiple droplets deforming a vesicle-like shell.

DY 47.4 Thu 15:45 MER 02

Dilute suspensions of chemically active particles in thin liquid films — •Tilman Richter, Paolo Malgeretti, and Jens Harting — HELMHOLTZ-INSTITUT ERLANGEN-NÜRNBERG FÜR ERNEUERBARE ENERGIEN, Erlangen, Germany

Thin liquid films are important for many microfluidic applications such as printing or coating of e.g. printable electronics or photovoltaic cells as well as so called lab-on-a-chip devices. Also in catalysis at liquid interfaces thin film dynamics are important. It is well known that a thin film on a solid substrate can be unstable and droplet formation may arise.

The dynamics of thin liquid films and their instability has been the subject of intensive experimental, analytical, and numerical studies, the latter often based on the thin film equation. We propose a set of newly developed equations for the influence of chemical active colloids suspended in a thin liquid film based on the lubrication and Fick-Jackobs approximation. For this novel set of equations we perform a linear stability analysis (LSA) that reveals surprisingly interesting dynamics. We identify the subset of parameters for which the thin film becomes stable i.e. is not rupturing, as well as a variety of different dominating wave-modes. This allows us to control not only the stability but also the droplet size distribution after film rupture, as well as the time it takes for an initially flat film to rupture.

In order to assess the asymptotic state of the thin film, the LSA results are compared against numerical simulations using the Lattice Boltzmann method.

DY 47.5 Thu 16:00 MER 02

Light properties and water resistant of combined sobrerol methacrylate cellulose thin films. — •Constantin Harder[1,2], Alexandros E. Alexakis[3], Marie Betker[1,3], Yusuf Bulut[1,2], Benedikt Sochor[1], Huaying Zhong[2], Guangjiu Pan[2], Manuel Reus[2], Korneliya Goordeyeva[3], Apostolos Vagias[2,4], Daniel Söderberg[3], Eva Malmström[3], Peter Müller-Buschbaum[2,4], and Stephan V. Roth[1,3] — [1]DESY, 22607 Hamburg, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [3]KTH Royal Institute of Technology, 10044 Stockholm, Sweden — [4]MLZ, TUM, 85748 Garching, Germany

Functionalization of porous materials in terms of optical, chemical and mechanical properties is achieved by applying fully wood-based layers materials. In this project, the refraction index, extinction coefficient and water adhesion properties of cellulose thin films combined with sobrerol methacrylate colloids are investigated together with their topography and morphology. Cellulose nanofibrils (CNF) are a hydrophilic material, and form networks during the drying with specific refraction index, extinction coefficient. Applying additional colloids, their optical properties and water-contact angle can be tuned. Hence, in order to produce water-resistant thin film, a combination of CNF and colloids is a perfect candidate.

DY 48: Dynamics and Chaos in Many-Body Systems I (joint session DY/TT)

Time: Thursday 15:00–17:30 Location: MOL 213

DY 48.1 Thu 15:00 MOL 213

Imperfect Many-Body Localization in Exchange-Disordered Isotropic Spin Chains — •Julian Siegl and John Schliemann — University of Regensburg

We study many-body localization in isotropic Heisenberg spin chains with the local exchange parameters being subject to quenched disorder. The Hamiltonian is invariant under global SU(2)- rotations and incorporates therefore a nonabelian symmetry. Systems of common spin length 1/2 and 1 are studied numerically using random matrix techniques. In both cases we find a transition from an ergodic phase at small disorder strength to an incompletely localized phase at stronger disorder. The transition is signaled by a maximum of the sample-to-sample variance of the averaged consecutive-gap ratio. The incompletely localized phase found here is distinguished from a fully localized system by the scaling behavior of the sample-to-sample variance.

DY 48.2 Thu 15:15 MOL 213

Magnetic Dipole Clusters - Resurrection of Catastrophe Machines — •Ingo Rehberg and Simeon Völkel — Experimental Physics, University of Bayreuth

Hysteretic transitions between stable configurations of a hexagonal magnetic dipole cluster [1] are set in a broader context by revealing the nature of the corresponding instabilities [2]. Following the animation of this bifurcation scenario [3], we present an experimental setup where the height of the centre dipole serves as the bifurcation parameter. This catastrophe machine demonstrates the two instabilities forming the hysteresis loop, and it might provide a hint to the unresolved puzzle of the slowing down of one of the eigenmodes [4].

[1] Andrew D.P. Smith et al., JMMM 549, 168991 (2022).
[2] Simeon Völkel et al., JMMM 559, 169520 (2022).
[3] https://doi.org/10.5281/zenodo.6380539 (18.5.2022).
[4] Peter T. Haugen et al., Chaos 32, 063108 (2022).

DY 48.3 Thu 15:30 MOL 213

Signatures of the interplay between chaos and local criticality on the dynamics of scrambling in many-body systems — Felix Meier[1], •Mathias Steinhuber[2], Juan Diego Urbina[2], Daniel Waltner[1], and Thomas Guhr[1] — [1]University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany — [2]University of Regensburg, Universitätsstr. 31, 93040 Regensburg, Germany

Fast scrambling, quantified by the exponential initial growth of Out-of-Time-Ordered-Correlators (OTOCs), is the ability to efficiently spread quantum correlations among the degrees of freedom of interacting systems, and constitutes a characteristic signature of local unstable dynamics. As such, it may equally manifest both in systems displaying chaos or even in integrable systems around criticality. We discuss the results from our recent publication [1], where we go beyond these two well-studied regimes with an exhaustive study of the interplay between local criticality and chaos. We address many-body systems with a well-defined classical (mean-field) limit, as coupled large spins and Bose-Hubbard chains, thus allowing for semiclassical analysis. Our aim is to investigate the dependence of the exponential growth of the OTOCs, defining the quantum Lyapunov exponent λ_q on quantities derived from the classical system with mixed phase space, specifically the local stability exponent of a fixed point λ_{loc} as well as the maximal Lyapunov exponent λ_L of the chaotic region around it.
[1] Meier, F., Steinhuber, M., Urbina, J. D., Waltner, D. & Guhr, T. arxiv:2211.12147

DY 48.4 Thu 15:45 MOL 213

Characterizing quantum chaoticity of kicked spin chains — •Tabea Herrmann, Maximilian F. I. Kieler, and Arnd Bäcker — TU Dresden, Institut für Theoretische Physik, Dresden, Germany

Quantum many body systems are commonly considered as quantum chaotic if their spectral statistics, such as the level spacing distribution, agree with those of random matrix theory. Using the example of the kicked Ising chain we demonstrate that even if both level spacing distribution and eigenvector statistics agree well with random matrix predictions, the entanglement entropy deviates from the expected Page curve. We propose a new measure of the effective spin interactions and obtain the corresponding random matrix result. By this the deviations of the entanglement entropy can be understood.

DY 48.5 Thu 16:00 MOL 213

Entanglement Characterization of Measurement-Induced Phase Transition in Fermionic Chains — •Jiangtian Yao[1,2], Sebastian Diehl[1], and Michael Buchhold[1] — [1]Institute for Theoretical Physics, University of Cologne, D-50937 Cologne, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

We report characterization of measurement-induced phase transition in Gaussian fermionic chains. We use various entanglement measures to characterize the two phases as well as the nature of the transition. Through a numerical study on the entanglement spectra, we observe closure of the entanglement gap in the critical phase and relate the scaling of the closure to the effective central charge of the system. In addition, we numerically extract the effective Luttinger liquid parameter of the system and use it to characterize the critical phase. Lastly, we use the scaling behavior of the effective Luttinger liquid parameter as well as the Schmidt gap to estimate the critical point for the phase transition.

15 min. break

DY 48.6 Thu 16:30 MOL 213

Dynamical characterization of the chaotic phase in the Bose-Hubbard model — David Peña Murillo and •Alberto Rodríguez — Departamento de Física Fundamental, Universidad de Salamanca, E-37008 Salamanca, Spain

We study the dynamical manifestation of the Bose-Hubbard model's chaotic phase [1] by analysing the temporal behaviour of connected two-point density correlations on experimentally accessible time scales up to a few hundred tunneling times. The time evolution of initial Mott states with unit density in systems including up to 17 bosons (Hilbert space dimension $\approx 10^9$) reveals that the chaotic phase can be unambiguously identified from the early time fluctuations of the considered observable around its equilibrium value [2]. The emergence of the chaotic phase is also seen to leave an imprint in the initial growth of the time signals. The possibility to discern specific features of this many-body chaotic phase, on top of the universal prediction of random-matrix theory, from these experimentally accessible measures is explored.

[1] L. Pausch *et al.*, Phys. Rev. Lett. 126, 150601 (2021)
[2] D. Peña Murillo, MSc Thesis, Universidad de Salamanca (2022)

DY 48.7 Thu 16:45 MOL 213

Universal Eigenvalue Distribution for Locally Interacting Quantum Systems — •Tobias Helbig, Tobias Hofmann, Ronny Thomale, and Martin Greiter — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg, Germany

Wigner has shown [1] that the eigenvalue distribution of a Gaussian orthogonal or unitary ensemble of random matrices approaches a semicircle in the thermodynamic limit. Here, we show that the joint eigenvalue distribution of locally interacting quantum systems, that is, ensembles of finite dimensional subsystems with local interactions between them, approaches a Gaussian distribution as the number of subsystems is taken to infinity [2]. In the talk, we present our analytical results supported by numerical data and discuss possible implications of a Gaussian density of states for physical problems.

[1] E. P. Wigner. On the statistical distribution of the widths and spacings of nuclear resonance levels. Mathematical Proceedings of the Cambridge Philosophical Society, 47(4): 790-798 (1951).

[2] T. Hofmann, T. Helbig, R. Thomale, and M. Greiter. In preparation.

DY 48.8 Thu 17:00 MOL 213

Power-law decay of correlations after a global quench in the massive XXZ chain — •Flávia Braga Ramos[1], Andrew Urichuk[2,3], Imke Schneider[1], and Jesko Sirker[3] — [1]Fachbereich Physik und Research Center OPTIMAS, Technische Universität Kaiserslautern, Kaiserslautern, Germany — [2]University of Manitoba, Winnipeg, Canada — [3]Bergische Universität Wuppertal, Wuppertal, Germany

While there have been great advances in understanding the final equilibration of integrable systems after a quantum quench, relatively little is known about their precise relaxation towards the steady state. In this context, the XXZ chain provides a playground for the investigation of interaction effects in out-of-equilibrium properties of quantum many-body systems. We investigate the relaxation dynamics of equal-time correlations in the antiferromagnetic phase of the XXZ spin-1/2 chain following a global quantum quench of the anisotropy parameter. In particular, we focus on the relaxation dynamics starting from an initial Néel state. Using the exact solution of an effective free-fermion model, state-of-art density matrix renormalization group simulations, and the quench-action approach, we show that the late-time relaxation is characterized by a power-law decay $\sim t^{-3/2}$ independent of anisotropy. Overall, we find remarkable agreement in the results obtained from the distinct approaches.

DY 48.9 Thu 17:15 MOL 213

Universal correlations in chaotic many-body quantum states: lifting Berry's Random Wave Model into Fock space — Rémy Dubertrand[1], Juan-Diego Urbina[2], Klaus Richter[2], and •Florian Schöppl[2] — [1]Department of Mathematics, Physics and Electrical Engineering, Northumbria University, NE1 8ST Newcastle upon Tyne, United Kingdom — [2]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Using a semiclassical analysis based on Berry's ansatz [1] we investigate the universal statistical features of eigenstate correlations in chaotic mesoscopic many-body quantum systems, focusing on Bose-Hubbard lattices, where the existence of a classical (mean-field) limit allows for the use of many-body semiclassical methods [2]

For this, we first have to lift Berry's ansatz into the many-body space by expanding the microscopic correlations and the conjectured multivariant Gaussian distribution of expansion coefficients into the Fock space of quantum fields. Together with numerical evidence, which supports the extension to multi-point correlations of the known Gaussian distribution for a single expansion coefficient, the universality of eigenstate correlations can be extended well beyond random matrix theory, where these correlations are absent. Our results bring the correlation backbone of eigenfunctions into a precise signature of quantum chaos in many-body mesoscopic systems.

[1] M. V. Berry, Journal of Physics A: Mathematical and General **10**, 2083 (1977) [2] K.Richter, J.D. Urbina, and S. Tomsovic. "Semiclassical roots of universality in many-body quantum chaos," (2022)

DY 49: Critical Phenomena and Phase Transitions

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

DY 49.1 Thu 15:00 ZEU 160

Metastate analysis for two-dimensional Ising spin glasses — •Alexander K. Hartmann[1] and A. Peter Young[2] — [1]University of Oldenburg, Germany — [2]University of California, Santa Cruz, USA

Spin glasses (SGs) are disordered magnetic systems which provide prototypical models for complex systems, including systems outside physics such as neural networks and machine-learning problems. For the two-dimensional (2d) case, exact numerical ground states (GSs) of large sizes can be obtained by polynomial-time graph-matching algorithms. Using these methods it was shown that 2d SGs exhibit a spin-glass ordered phase only at zero temperature, see e.g. [1]. Results from applying a modified version of the GS algorithm indicate that this phase is well described [2] by the so-called "droplet" theory, i.e., it has a simple structure. Here, we consider the *metastate* approach, which was introduced [3] to deal with the chaotic size-dependence of the spin-glass state. By studying a large range of sizes, we show convincingly that, in the thermodynamic limit, spin correlations in a local region are unaffected by the bonds far away, which is one of the main assumptions of the droplet picture.

[1] A.K. Hartmann and A.P. Young, Phys. Rev. B 64, 180404 (2001).
[2] A.K. Hartmann and M.A. Moore, Phys. Rev. Lett. 90, 127201 (2003).
[3] C.M. Newman and D.L. Stein, J. Phys.: Condens. Matter 15, R1319 (2003).

DY 49.2 Thu 15:15 ZEU 160

On the criticality of structurally disordered magnets — Maxym Dudka[1,2], Mariana Krasnytska[1,2,3], Juan Ruiz-Lorenzo[4,5], and •Yurij Holovatch[1,2,6] — [1]ICMP, NAS of Ukraine, Lviv, Ukraine — [2]L4 Collaboration Leipzig-Lorraine-Lviv-Coventry, Europe — [3]Université de Lorraine, Nancy, France — [4]Universidad de Extremadura, Badajoz, Spain — [5]BIFI, Zaragoza, Spain — [6]Coventry University, Coventry, UK

We discuss the problem of influence of structural disorder on criticality. As a case study, we consider an impact of a weak quenched disorder on a magnetic phase transition. Usually, such an impact is analyzed for a two-component mixture (e.g. a solid solution of a magnet with its non-magnetic counterpart). A distinct feature of our analysis is consideration of changes in the magnetic phase transition when both components are magnets. To this end, we make use of a generalized Ising model suggested recently [M. Krasnytska et al., J.Phys.: Complexity 1 (2020) 035008] in a context of complex systems. We apply the field theoretical renormalization group approach to analyze its effective and asymptotic critical behaviour. We show that this is the structural disorder itself that causes changes in the universal critical behaviour, regardless of whether it has a form of a random mixture of magnetic and non-magnetic constituents or of two different magnetic compounds [M. Dudka et al., arXiv:2207.13655].

DY 49.3 Thu 15:30 ZEU 160

Non-Hermitian PT-symmetric Ising spin chains: novel quantum phases and quantum phase transitions — •Grigory Starkov, Mikhail Fistul, and Ilya Eremin — Ruhr-Universität Bochum, Bochum, Germany

A theoretical study of quantum phases and quantum phase transitions occurring in non-Hermitian PT-symmetric transverse-field Ising spin model. A non-Hermitian part of the Hamiltonian is implemented via imaginary staggered longitudinal magnetic field corresponding to a local staggered gain and loss terms, γ.

Using a numerical diagonalization of the Hamiltonian for spin chains of a finite size N accompanied by a scaling procedure for the coherence length ξ, a complete quantum phase diagram γ-J (J is an adjacent spins interaction strength) is established. We obtain two quantum phases for $J < 0$, i.e., PT-symmetry broken antiferromagnetic state and PT-symmetry preserved paramagnetic state, and the quantum phase transition line is the line of exception points. For $J > 0$ the PT-symmetry of the ground state is retained in a whole region of parameter space of J and γ, and a system shows two intriguing quantum phase transitions between ferromagnetic and paramagnetic states for a fixed parameter $\gamma > 1$.

The qualitative quantum phase diagram is derived in the framework of the Bethe-Peierls approximation that is in a good accord with numerically obtained results. The quantum phase diagram can be verified in the microwave transmission experiments allowing to identify the transitions between the first excited and the ground states.

DY 49.4 Thu 15:45 ZEU 160

Predictive percolation: assessing fire connectivity in California — Olivia Hemond[1], •Diego Rybski[1,2,3], Ariani C. Wartenberg[1,4], Katherine J. Siegel[5], and Van Butsic[1] — [1]Department of Environmental Science, Policy, and Management, University of California, Berkeley, Berkeley, CA, United States — [2]Potsdam Institute for Climate Impact Research - PIK, Member of Leibniz Association, P.O. Box 601203, 14412 Potsdam, Germany — [3]Complexity Science Hub Vienna, Josefstädterstrasse 39, A-1090 Vienna, Austria — [4]Leibniz Centre for Agricultural Landscape Research, Eberswalder Str. 84, 15374 Müncheberg, Germany — [5]Department of Ecology & Evolutionary Biology, University of Colorado, Boulder, CO, USA

Damages from wildfire are increasing globally. Analyzing historical California fire data from 1950-2019, we propose a new method to estimate the percolation threshold, which represents statewide connectivity of fire-affected habitats. We create grid realizations of burnt areas over various time spans, measure the critical distances, and explore analogies with continuum percolation to predict the percolation threshold. Fires within our study period trend towards but do not yet reach percolation. We calculate the percolation threshold to be 45.8%

of the state?s burnable area. Assuming fire patterns similar to the past seventy years, it would take 146.5 years, starting from 1950, to reach percolation across California. Within time periods shorter than 146 years, wildfire-affected areas are fragmented.

DY 49.5 Thu 16:00 ZEU 160

Determination of the nearest-neighbor interaction strength in VO2 via fractal dimension analysis — •Jacob Holder, Daniel Kazenwadel, Peter Nielaba, and Peter Baum — Universität Konstanz, Konstanz, Deutschland

The Ising model is one of the simplest and well-established models to simulate phase transformations in complex materials. However, its most central constant, the interaction strength J between two nearest neighbors, is not directly related to any macroscopic material property and is therefore hard to obtain. Here we report how to obtain this basic constant by a fractal dimension analysis of measured domain structures. In the example of VO_2, a strongly correlated material with first-order metal-to-insulator transition close to room temperature, we obtain an interaction strength of 11 meV. In a two dimensional simplification, we find an effective value of 17 meV due to the reduced number of nearest neighbors. These results link the fundamental constants in the Ising model to measured quantities of bulk materials.

15 min. break

DY 49.6 Thu 16:30 ZEU 160

Global Speed Limit for Finite-Time Dynamical Phase Transition in Nonequilibrium Relaxation — •Kristian Blom and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

The nearest-neighbor interacting Ising model is a paradigm for classical many-body physics. Recent works unraveled an intriguing finite-time dynamical phase transition in the thermal relaxation of a mean field Curie-Weiss Ising model. This phase transition reflects a sudden switch in the dynamics, and manifests as a cusp in the probability density of magnetization. Its existence in systems with a finite range of interaction, however, remained unclear.

Employing the Bethe-Guggenheim approximation, which is exact on Bethe lattices, we demonstrate the finite-time dynamical phase transition in nearest-neighbor Ising systems for arbitrary quenches, including those within the two-phase coexisting region. Strikingly, for any given initial condition we prove and explain the existence of non-trivial speed limits for the dynamical phase transition and the relaxation of magnetization, which are absent in the mean field setting. Pair correlations, which are neglected in mean field theory, and trivial in the Curie-Weiss model, account for kinetic constraints due to frustrated local configurations, that give rise to a global speed limit.

Our findings may be relevant for optimizing ultrafast optical-switching ferromagnetic materials.

DY 49.7 Thu 16:45 ZEU 160

Crossover in the phase-coexistence between models with discrete and continuous variables — •Florian Kischel, Nils Caci, and Stefan Wessel — RWTH Aachen University, Aachen, Germany

The relative weight of the distinct phases that coexist at a first-order phase transition in systems with discrete degrees of freedom is well understood. For example, in the q-state Potts model, it is characterized by a ratio $R = 1 : q$ of the disordered vs. ordered regions. In models with continuous variables on the other hand, this ratio is generally unknown. Several recent instances however suggest that it equals $R = 1 : I_O$, where I_O denotes the integral measure of the space of extremal states of the ordered phase. In order to explore the emergence of this integral measure, we examine a system that realizes a crossover from discrete to continuous variables and study the behavior of R at its phase-coexistence points. In particular, we consider a generalized n-state clock-model on a three-dimensional simple cubic lattice with both bilinear and biquadratic exchange interactions. In the large-n (XY) limit, this model is known to harbor a first-order thermal phase transition, as does the 3-state Potts model, to which the model reduces in the limit of $n = 3$. Here, we explore the phase-coexistence over the range of intermediate values of n using large-scale Monte Carlo simulations.

DY 49.8 Thu 17:00 ZEU 160

Partition function zeros in the 3D Blume-Capel model — •Leïla Moueddene — Laboratoire de Physique et Chimie Théoriques, Université de Lorraine, Vandoeuvre-lès-Nancy, France

The phase diagram of the three-dimensionnal Blume Capel model shows an ordered ferromagnetic phase and a disordered paramagnetic phase, separated by a transition line from second order to first order at the tricritical point (TCP). The universality class of the second-order line is the Ising class, while the tricritical universality class governs the behaviour of the critical exponents at the tricritical point. It is well known that the upper critical dimension is $d_{uc} = 3$ at the TCP, thus Mean Field exponents are expected, modified by logarithmic correction factor. We determine analytically the logarithmic-correction exponents - also universal - using RG for ϕ_6 model. The knowledge of the partition function zeros is a quite fundamental and powerful approach to study a phase transition. While the Fisher zeros and Lee-Yang zeros are well known to study the thermal exponent y_t and magnetic exponent y_h, we build a new type of zeros from the complex plane of the crystal field which leads to the crystal exponent y_2: the crystal field zeros. We study the leading and logartihmic-corrections exponents numerically from the partition function zeros and compare with the analytical results, and check if the scaling relations are verified.

DY 49.9 Thu 17:15 ZEU 160

Boundary critical behavior of the three-dimensional O(N) universality class — •Francesco Parisen Toldin[1] and Max A. Metlitski[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

It was recently realized that the three-dimensional O(N) model exhibits an extraordinary surface universality class for a finite range of $N \geq 2$. We investigate the boundary critical behavior by means of high-precision Monte Carlo simulations of an improved model, where leading scaling corrections are suppressed. Contrary to simplified arguments on the bulk-surface phase diagram, and in line with a recent field-theoretical analysis, we find a special surface transition for $N = 3$, with unusual exponents, and an extraordinary phase with logarithmically decaying correlations. For a general N, the existence and universal properties of extraordinary phase are predicted to be controlled by certain amplitudes of the normal universality class, where one applies an explicit symmetry breaking field to the boundary. We extract these universal amplitudes by Monte Carlo simulations for $N = 2, 3$. Our results are in good agreement with direct Monte Carlo studies of the extraordinary universality class serving as a nontrivial quantitative check of the connection between the normal and extraordinary classes.

Ref.: F. Parisen Toldin, Phys. Rev. Lett. 126, 135701 (2021); F. Parisen Toldin, M. A. Metlitski, Phys. Rev. Lett. 128, 215701 (2022)

DY 49.10 Thu 17:30 ZEU 160

Critical phenomena in the two-dimensional dilute Baxter-Wu model — •Alexandros Vasilopoulos[1], Nikolaos G. Fytas[1], Michail Akritidis[1], and Martin Weigel[2] — [1]Centre for Fluid and Complex Systems, Coventry University, Coventry CV1 5FB, United Kingdom — [2]Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany

We study the question of universality in the two-dimensional spin-1 Baxter-Wu model in the presence of a crystal field Δ. We employ extensive numerical simulations consisting of various types, providing us with complementary results: Wang-Landau sampling at fixed values of Δ and a parallelized variant of the multicanonical approach performed at constant temperature T. A detailed finite-size scaling analysis in the regime of second-order phase transitions in the (Δ, T) phase diagram indicates that the transition belongs to the universality class of the four-state Potts model. Previous controversies with respect to the nature of the transition are discussed and attributed to the presence of strong finite-size effects, especially as one approaches the pentacritical point of the model. Lastly, to facilitate the study of $\Delta > 0$, where the two previous methods become increasingly inhibitory, a hybrid algorithm consisting of both a cluster and a single-spin-flip update was implemented and tested.

DY 50: Evolutionary Game Theory (joint session SOE/DY)

Time: Thursday 15:00–15:30 Location: ZEU 260

DY 50.1 Thu 15:00 ZEU 260

Bet hedging in populations evolving in fluctuating environments — Rubén Calvo[1] and •Tobias Galla[2] — [1]Instituto Carlos I de Física Téorica y Computaciona, and Departamento de Electromagnetismo y Física de la Materia, Facultad de Ciencias, Universidad de Granada, 18071 Granada, Spain — [2]Instituto de Física Interdisciplinar y Sistemas Complejos IFISC (CSIC-UIB), Campus Universitat de les Illes Balears, E-07122 Palma de Mallorca, Spain

Bet-hedging strategies are strategies aimed at reducing risk in the face of uncertainty. For example, biological organisms face uncertain time-varying environmental conditions, such as dry years versus wet years. Similarly, future conditions in financial markets or other social systems are often unknown. Traditional bet-hedging theory shows that a reduction of the variance of an agent's payoff may increase their success even when their mean payoff is also reduced. Bet-hedging strategies are often built on maximum growth. Here instead, we ask how a mutant invading a resident wildtype population can maximise its chances of taking over the population (i.e., the fixation probability of the mutant). We consider a birth-death dynamics in fluctuating environments, and show that, depending on the distribution of payoffs across environmental states, a reduction in variance can either be beneficial or detrimental to the mutant. We establish conditions for either scenario to be realised, and show how this is related to the skewness of the payoff distribution.

DY 50.2 Thu 15:15 ZEU 260

Hawk Dove Game on Networks with Continuous Populations — •Lennart Gevers[1,2], Tobias Wand[1,2], and Svetlana V. Gurevich[1,2] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Straße 9, D-48149 Münster, Germany — [2]Center for Nonlinear Science (CeNoS), University of Münster, Corrensstrasse 2, D-48149 Münster, Germany

Evolutionary game theory is a population-based approach to game theoretical scenarios by analyzing the evolution of populations resembling competing strategies.
We expand the classical model analysed by (1), which assumes that no spatial or social segregation of populations occurs, with a network-based approach to the hawk-dove game which models the ability of contestants to migrate between neighboring realizations of the game by adapting different migratory behaviors.
Our model reveals that competitive and cooperative populations can show preferred strategies on how to spatially organize on such territories.
Furthermore, we find that the resulting outcomes of the participating species diverge from the original model with increasing mobility of species.

(1) F. Stollmeier and J. Nagler, Phys. Rev. Lett. 120, 058101, 2018.

DY 51: Members' Assembly

Agenda:

Report

Elections

Future Activities of DY

Any other bussiness

Time: Thursday 18:00–19:00 Location: ZEU 160

All members of the Dynamics and Statistical Physics Division are invited to participate.

DY 52: Statistical Physics of Biological Systems II (joint session BP/DY)

Time: Friday 9:30–12:00 Location: BAR Schö

DY 52.1 Fri 9:30 BAR Schö

Evolutionary optimization of multicomponent phase separation — •David Zwicker[1] and Liedewij Laan[2] — [1]MPI-DS, Göttingen, Germany — [2]TU Delft, The Netherlands

Biological cells use passive phase separation to segregate different biomolecules into various condensates. Since the molecular interactions determine the number of distinct condensates and their composition, they have likely been optimized evolutionarily for robust segregation. To study this, I will present a numerical method that efficiently determines coexisting phases in multicomponent liquids and use it in evolutionary optimization experiments. I will demonstrate that the optimized interactions lead to a precise number of different condensates, even if the overall composition varies. Consequently, adjusting microscopic interactions leads to stable emergent behaviors in these complex systems.

DY 52.2 Fri 9:45 BAR Schö

Kinetics of droplet sizes in non-conserved emulsions — •Jacqueline Janssen[1], Frank Jülicher[1], and Christoph A. Weber[2] — [1]Max Planck Institute for the Physics of Complex Systems — [2]University of Augsburg

Droplets form via phase separation and coexist with a dilute phase that is composed of droplet material of lower concentration. Many droplets in an emulsion undergo coarsening to the thermal equilibrium state that corresponds to a single droplet in a finite system. In passive emulsions, where the total amount of droplet material is conserved, the average radius grows as a function $t^{1/3}$ in time, and the droplet size distribution function broadens. Here we consider emulsions for which the total droplet material is not conserved, e.g. material is supplied by a chemical reaction or external reservoirs. We calculate the kinetics of droplet sizes and show that there is a switch from coarsening to narrowing of the size distribution upon material supply. Regulation of droplet sizes by material supply could be relevant for biomolecular condensates in living cells.

DY 52.3 Fri 10:00 BAR Schö

Dynamics of vesicle clusters studied by passive x-ray microrheology — •Titus Czajka[1], Charlotte Neuhaus[1], Jette Alfken[1], Moritz Stammer[1], Yuriy Chushkin[2], Diego Pontoni[2], Christian Hoffmann[3], Dragomir Milovanovic[3], and Tim Salditt[1] — [1]Institut for X-ray Physics, Georg-August-Universität Göttingen, Germany — [2]ESRF, Grenoble, France — [3]Laboratory of Molecular Neuroscience, DZNE, Berlin, Germany

Inferring the viscoelastic properties of a complex fluid from the dynamics of suspended tracer particles is a common method to perform rheological measurements where a direct measurement of the constituents of the system is not possible or impractical. The previously observed pool formation of vesicles induced by divalent salts or the protein synapsin I is a case in point. One would like to know how the mobility of a single (tracer) particle changes in a dense pool as compared to a homogeneous vesicle suspension. Here we used x-ray correlation spectroscopy (XPCS) to measure silica nanoparticles im-

mersed in a complex biomolecular fluid composed of small unilamellar vesicles and $CaCl_2$, or SUVs and Synapsin-Ia protein, both in buffer solution. While the former system leads to irregular clusters, the latter has been observed to form protein induced vesicle pools, suggesting a liquid-liquid phase separation. Analysis of the photon correlation functions reveals the presence of different timescales, which we attribute to the free diffusive motion of the tracer particles and the motion of the tracer particles that interact with the cluster.

DY 52.4 Fri 10:15 BAR Schö

A stereotypical sequence of condensation and dispersal of RNA polymerase II clusters during stem cell differentiation — •Tim Klingberg[1], Irina Wachter[2], Agnieszka Pancholi[2], Roshan Prizak[2], Priya Kumar[3], Yomna Gohar[3], Marcel Sobucki[2], Elisa Kämmer[2], Süheyla Eroğlu-Kayikçi[2], Sylvia Erhardt[2], Carmelo Ferrai[3], Vasily Zaburdaev[1], and Lennart Hilbert[2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Karlsruher Institut für Technologie — [3]Universitätsmedizin Göttingen

Most eukaryotic genes are transcribed by RNA polymerase II (Pol II). In stem cells, recruited Pol II forms prominent, long-lived clusters, which gradually disappear during differentiation, so that only smaller clusters remain. Here, we ask whether the loss of large Pol II clusters is a stereotypical transition that can be explained by changes in the Pol II transcriptional state during differentiation. We assess clusters by super-resolution microscopy in three different experimental models of differentiation. In all cases, Pol II clusters first become larger and rounder, then unfold, and finally split into small clusters. These shape changes are accompanied by changes of transcriptional activity of Pol II. Previous work suggests a surface-condensate model, where enhancer regions support Pol II cluster formation, and transcriptional activity disperses clusters. Using this theoretical model, we propose that the developmental changes in enhancer marks and transcriptional activity during differentiation are sufficient to define a stereotyped trajectory through a cluster shape space.

DY 52.5 Fri 10:30 BAR Schö

Anomalous dynamics of differentiated droplets — •Xi Chen[1], Frank Jülicher[2], Jens-Uwe Sommer[1], and Tyler Harmon[1] — [1]Leibniz-Institut für Polymerforschung Dresden, Institut Theory der Polymere 01069 Dsden — [2]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden

Membraneless compartments formed by liquid-liquid phase separation in cells behave like droplets and take part in various biological processes. The function of these droplets are largely dependent on their components. We previously showed with a theoretical model that droplets can undergo a differentiation process where a homogeneous population of droplets converts into two coexisting types of droplets. We proposed this allows droplet specialization similar to cell differentiation.

These differentiated droplets exhibit new features and anomalous dynamics. Like a normal droplet system where droplets ripen and merge into one big droplet, this differentiation can significantly accelerate this Ostwald ripening. This happens with the caveat that instead of ripening into one droplet, it ripens into two droplets of different types with a competing reverse Ostwald ripening process. Unexpectedly, these differentiated droplets divide and repel each other over long distances.

15 min. break

DY 52.6 Fri 11:00 BAR Schö

Microrheology of red blood cell cytosol — •Thomas John and Christian Wagner — Universität des Saarlandes, Saarbrücken

Tracking of small particles undergoing a Brownian motion is a widespread method in passive microrheology. Washed human red blood cells (RBC) are destroyed by ultrasound treatment to extract the cytosol, the hemoglobin and protein solution inside the cells. We use microrheology with sub-micrometer-sized particles to determine the viscosity of the cytosol. Since the cytosol is always diluted with an unknown amount of water due to the treatment, this small dilution has a huge impact on the viscosity. To circumvent this problem, we measured very accurately the mass density of every sample. However, the resulting density-viscosity relation is a strong monotonic increasing relation. In a separate experiment we determined the mass density distribution of individual intact RBCs in a continuous density gradient by centrifugation. Finally, we can present the probability density distribution of the viscosity in naturally distributed human RBCs.

DY 52.7 Fri 11:15 BAR Schö

Clonal dynamics at tissue interfaces — •Ruslan Mukhamadiarov[1,2], Matteo Ciarchi[1,2], Fabrizio Olmeda[1,2], and Steffen Rulands[1,2] — [1]Ludwig Maximilian University of Munich, München, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Tissue morphogenesis relies on the spatial separation of different cell types. Understanding how cells regulate the positions of such interfaces is key to understanding the processes that occur during dysregulation, such as in cancer. Genetic tracing has become an important experimental tool in studying the regulation of cell behaviour. However, its use in both homeostatic and growing tissues is limited by the emergence of universal size distributions. Here, we show that the mechanisms of tissues interface regulation is reflected in cell-fate specific size distributions of genetically labelled cells, termed clones. Specifically, we show how interface fluctuations affect the size distributions of labelled clones and derive theoretical predictions for a range of biologically relevant scenarios that can be tested experimentally. We test our theoretical framework by stochastic simulations and analysis of live imaging experiments. By relating interface fluctuations to clone size distributions our work paves the way for using genetic tracing experiments to understand the mechanisms underlying tissue compartmentalization.

DY 52.8 Fri 11:30 BAR Schö

Multivalent binding proteins can drive collapse and reswelling of chromatin in confinement — •Sougata Guha and Mithun K. Mitra — Department of Physics, IIT Bombay, India

Collapsed conformations of chromatin have been long suspected of being mediated by interactions with multivalent binding proteins, which can bring together distant sections of the chromatin fiber. In this study, we use Langevin dynamics simulation of a coarse grained chromatin polymer to show that the role of binding proteins can be more nuanced than previously suspected. In particular, for chromatin polymer in confinement, entropic forces can drive reswelling of collapsed chromatin with increasing binder concentrations, and this reswelling transition happens at physiologically relevant binder concentrations. Both the extent of collapse, and also of reswelling depends on the strength of confinement. We also study the kinetics of collapse and reswelling and show that both processes occur in similar timescales. We characterise this reswelling of chromatin in biologically relevant regimes and discuss the non-trivial role of multivalent binding proteins in mediating the spatial organisation of the genome.

DY 52.9 Fri 11:45 BAR Schö

A possible application of the Physics of topological defects to oncology — •Andy Manapany, Leïla Moueddenne, Sébastien Fumeron, Bertrand Berche, and Loriane Didier — Université de Lorraine

We propose a numerical study of the thermal diffusion process in non-Euclidian geometry applied to biological active matter. Thanks to the similarities displayed by both nematic and cells in biological tissue, we aim to apply results derived from the study of diffusion processes around topological defects found in liquid crystals, in order to highlight the thermal response in the vicinity of certain disclination defects found in epithelial tissues. This work is motivated by the fact that these types of disclination defects, mainly "comet" and "trefoil" systematically appear during metastatic phases in some forms of aggressive cancers. Thus, a study of the thermal footprint in such mediums may give us information on the most efficient ways to perform thermal ablation targeted towards aforementioned cells while preserving healthy surrounding tissue.

DY 53: Active Matter V (joint session BP/CPP/DY)

Time: Friday 9:30–12:00 Location: TOE 317

Invited Talk DY 53.1 Fri 9:30 TOE 317

Experiments on Active Polymer-Like Worms — •Antoine Deblais[1], Daniel Bonn[1], and Sander Woutersen[2] — [1]Van der Waals-Zeeman Institute, Institute of Physics, University of Amsterdam, 1098XH Amsterdam, The Netherlands — [2]Van't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, 1098XH Amsterdam, The Netherlands

We propose a new 'active particle' system in which the particles are in fact polymer-like: the Tubifex tubifex or 'sludge' worm. I will discuss three recent experiments that highlight the richness of this active system. In the first experiment, we perform classical rheology experiments on this entangled polymer-like system. We find that the rheology is qualitatively similar to that of usual polymers, but, quantitatively, the (tunable) activity of the particle changes the flow properties. In a second experiment, we disperse the worm in a quasi-2D aquarium and observe their spontaneous aggregation to compact, highly entangled blobs; a process similar to polymer phase separation, and for which we observe power-law growth kinetics. We find that the phase separation of active polymer-like worms occurs through active motion and coalescence of the phase domains. This leads to a fundamentally different phase-separation mechanism, that may be unique to active polymers. Finally, in the remaining time, I will briefly show that we can efficiently separate by size and activity these living polymers using hydrodynamic chromatography technics.

DY 53.2 Fri 10:00 TOE 317

Filamentous Cyanobacteria Aggregate at Light Boundaries — •Maximilian Kurjahn[1], Leila Abbaspour[1], Philip Bittihn[1], Ramin Golestanian[1,2], Benoît Mahault[1], and Stefan Karpitschka[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, OX1 3PU, Oxford, UK

Filamentous cyanobacteria are among the oldest, yet still most abundant phototrophic prokaryotes on Earth, fixing vast amounts of atmospheric carbon by photosynthesis. Gliding motility, coupled to photophobic responses (direction reversals in response to light intensity gradients), are believed to drive accumulation in suitable light conditions. Here, we demonstrate that photosensitivity goes beyond simple accumulation: Super-filamentous aggregates, capable of collective mechanical action, form at the boundaries of illuminated regions and may, for instance, contract and detach from the substrate, once grown to a critical mass. We explore how the light pattern, in particular its boundary curvature, impacts aggregation. A minimal model of active rods captures the behavior qualitatively. The ecological impact of such behavior is still unclear, but may enable colonies to escape from saturated habitats by switching to a planktonic state.

DY 53.3 Fri 10:15 TOE 317

Odd dynamics of living chiral crystals — •Tzer Han Tan[1,2,3,4], Alexander Mietke[4,5], Junang Li[4], Yuchao Chen[4], Hugh Higinbotham[4], Peter Foster[4], Shreyas Gokhale[4], Jorn Dunkel[4], and Nikta Fakhri[4] — [1]MPI-PKS, Dresden, Germany — [2]MPI-CBG, Dresden, Germany — [3]CSBD, Dresden, Germany — [4]MIT, Cambridge, USA — [5]University of Bristol, Bristol, UK

Active crystals are highly ordered structures that emerge from the self-organization of motile objects, and have been widely studied in synthetic and bacterial active matter. Whether persistent crystalline order can emerge in groups of autonomously developing multicellular organisms is currently unknown. Here we show that swimming starfish embryos spontaneously assemble into chiral crystals that span thousands of spinning organisms and persist for tens of hours. Combining experiments, theory and simulations, we demonstrate that the formation, dynamics and dissolution of these living crystals are controlled by the hydrodynamic properties and the natural development of embryos. Remarkably, living chiral crystals exhibit self-sustained chiral oscillations as well as various unconventional deformation response behaviours recently predicted for odd elastic materials. Our results provide direct experimental evidence for how non-reciprocal interactions between autonomous multicellular components may facilitate non-equilibrium phases of chiral active matter.

DY 53.4 Fri 10:30 TOE 317

Optimal collective durotaxis through active wetting — Macià-Esteve Pallarès[1], Irina Pi-Jaumà[2], Isabela Corina Fortunato[1], Valeria Grazu[3], Manuel Gómez-González[1], Pere Roca-Cusachs[1], Jesus de la Fuente[3], •Ricard Alert[4], Raimon Sunyer[1], Jaume Casademunt[2], and Xavier Trepat[1] — [1]Institute for Bioengineering of Catalonia — [2]University of Barcelona — [3]Instituto de Nanociencia y Materiales de Argón — [4]Max Planck Institute for the Physics of Complex Systems

The directed migration of cell clusters enables morphogenesis, wound healing and collective cancer invasion. Gradients of substrate stiffness are known to direct migration of cell clusters in a process called collective durotaxis, but underlying mechanisms remain unclear. Combining theory and experiments, we reveal a connection between collective durotaxis and the wetting properties of cell clusters. Our experiments show that durotaxis is non-monotonic with substrate stiffness, being optimal at intermediate stiffness. Modeling the cell clusters as active droplets, we explain this non-monotonic durotaxis in terms of a balance between active traction, tissue contractility, and surface tension. Finally, we show that the distribution of cluster displacements has a heavy tail, with infrequent but large cellular hops that contribute to durotactic migration. Our study demonstrates a physical mechanism of collective durotaxis based on the wetting properties of active droplets.

15 min. break

DY 53.5 Fri 11:00 TOE 317

Chlamydomonas axonemes twist during the beat — •Martin Striegler[1,2], Benjamin M. Friedrich[3], Stefan Diez[1,2,3], and Veikko F. Geyer[1] — [1]B CUBE - Center for Molecular Bioengineering, TU Dresden, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany

Motile cilia are slender cell appendages that drive single cell locomotion and fluid transport across surfaces. The motility of cilia is generated by its inner core, the axoneme, which bends by the activity of dynein motor proteins. Generation of bending requires antagonistic dynein activity on opposing sides of the axoneme. How dyneins are activated antagonistically is unknown. Theoretical models propose dynein regulation by mechanical feedback, which entails structural deformations of the axoneme, but direct experimental evidence is missing. To study axonemal deformations during the beat, we purify and reactivate Chlamydomonas reinhardtii axonemes. Using defocused-high-speed-darkfield microscopy, we resolve the 3D waveforms with nanometer resolution on millisecond timescales. We find that asymmetric waveforms have a non-planar component, which is most pronounced during the recovery stroke. To generate non-planarity within the geometric constraints of the axoneme, twist is thought to be required. Using gold-nano-particles as probes attached to the outside of reactivated axonemes, we, for the first time, measure dynamic twisting deformations in reactivated axonemes. We hypothesize that these deformations are involved in controlling dynein motors generating the axonemal beat.

DY 53.6 Fri 11:15 TOE 317

Curvotaxis - the effect of curvature on cells and tissue — Lea Hppel, Jan Sischka, and •Axel Voigt — Institute of Scientific Computing, Technische Universität Dresden, Germany

How do cells respond to curvature? Does curvature has an influence on cell shape and movement? What are the consequences for collective behaviour of interacting cells in tissue? We address these questions using a multiphase field model on different curved surfaces and compare the results with experimental data on pillars, in tubes and other surfaces. The results show a significant influence of curvature and the possibility to effectively model the observed phenomena with classical models and additional curvature terms.

DY 53.7 Fri 11:30 TOE 317

Onset of Homochirality in Cell Monolayers — •Ludwig A. Hoffmann and Luca Giomi — Universiteit Leiden, Leiden, Netherlands

Chirality is a feature of many biological systems and much research has been focused on understanding the origin and implications of this

property. Most famously, sugars and amino acids that are found in nature are homochiral, meaning that chiral symmetry is broken and only one of the two possible chiral states is ever observed. Perhaps less well-know, something similar is the case for certain types of cells too. They show chiral behavior and only one of the two possible chiral states is observed in nature. Understanding the origin of cellular chirality and what, if any, use or function it has in tissues and cellular dynamics is still an open problem and subject to much (recent) research. For example, cell chirality has already been shown to play an important role in drosophila morphogenesis.

DY 53.8 Fri 11:45 TOE 317

Dynamic instability of cytoplasmic compartments — •Melissa Rinaldin[1,2] and Jan Brugués[1,2] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [2]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany

Early embryos are the epitome of self-organization. Following the cell cycle oscillator, their internal structure is continuously reorganized into precise patterns at remarkable speeds. For example, the mm-sized egg of the frog Xenopus Laevis divides every 30 minutes into equally-sized cells. Physical processes such as autocatalytic growth, active transport, and reaction-diffusion can allow these embryos to keep up with fast cell cycle times, however, their understanding in early development remains largely elusive. Here, we present recent data from experiments of in vitro cytoplasmic extract obtained from frog eggs and exhibiting cell-free division. We show that the properties of the cell cycle oscillator regulate the pattern of cytoplasmic compartments. Specifically, by perturbing the oscillator, we establish that the interface of cytoplasmic compartments is unstable. We demonstrate that such instability arises from competing waves of autocatalytic microtubule growth, and can generate compartment fusion, strongly affecting the early embryonic pattern formation. Altogether, our results propose that the cell cycle oscillator plays a critical role in partitioning the cytoplasm of early embryos, keeping the dynamic instability of cytoplasmic compartments at bay.

DY 54: Complex Fluids and Colloids, Micelles and Vesicles (joint session CPP/DY)

Time: Friday 9:30–13:00 Location: MER 02

Invited Talk DY 54.1 Fri 9:30 MER 02

Chiral transport of active and passive colloids — •Anke Lindner[1], Andreas Zöttl[2], Olivia du Roure[1], Eric Clement[1], Francesca Tesser[1], and Guangying Jing[3] — [1]PMMH-ESPCI, 10, rue Vauquelin, 75011 Paris, France — [2]Faculty of Physics, University of Vienna, Kolingasse 14-16, 1090 Wien, Austria — [3]School of Physics, Northwest University, Xi'an, 710127, China

Chirality-induced effects are at the origin of bacterial rheotaxis and particle drift in shear flows. Here we investigate such effects using a combination between experiments and theoretical modeling for two systems: E-coli bacteria and 3D printed micro-particles.

The micro-particles consist of a spherical head and a helical tail of different pitch and handedness. We investigate the chirality-induced reorientation dynamics using microfluidics and observe asymmetric orientation bistability perpendicular to the flow direction. We quantitatively explain our findings through a theoretical model without adjustable parameters considering particle elongation, chirality and head-heaviness, in very good agreement with experiments.

We then present a study of the transport of motile bacteria in shear flows. Experimentally, we obtain with high accuracy and for a large range of flow rates, the spatially resolved velocity and orientation distributions. They are in excellent agreement with the simulations of a kinematic model accounting for stochastic and microhydrodynamic properties and flagella chirality. In contrast to the micro-printed particles Brownian rotational noise plays a crucial role in bacterial rheotactic drift.

DY 54.2 Fri 10:00 MER 02

Active and driven colloids interacting with vesicles — •Antonio Stocco, Vaibhav Sharma, Florent Fessler, and Carlos Marques — Institut Charles Sadron, CNRS University of Strasbourg

When a colloid is close to a lipid giant vesicle, the interaction between the Brownian particle and the fluctuating soft membrane affects not only the particle motion but also the membrane properties. The membrane may change its shape to accommodate the particle and partial or complete engulfment may occur as a function of the energy of adhesion, membrane tension and bending. Furthermore, the interaction between a micrometric solid particle and a giant vesicle membrane may lead to complex dynamics when the system is driven out of equilibrium. Here, we report our efforts with self-propelled Janus colloids and with bare colloids under optical trapping to mimic complex dynamics such as particle endocytosis, the motion of a self-propelled particle confined to a spherical membrane, or the physics of particle engulfment by a membrane. In a wide range of experimental conditions, we have observed that a self-propelled Janus colloid is able to perform orbital motion around a giant vesicle remaining in a non-engulfment state. Still, the active particle is able to impart a force of the order of 0.01 pN on the vesicle, which is however too small to trigger particle engulfment. By applying external forces in the 1-100 pN range, we were able to observe engulfment of bare and Janus colloids by a giant vesicle.

DY 54.3 Fri 10:15 MER 02

Universal Casimir interaction and its relevance for colloidal and biophysical systems — •Tanja Schoger[1], Benjamin Spreng[2], Gert-Ludwig Ingold[1], Paulo A. Maia Neto[3], and Serge Reynaud[4] — [1]Universität Augsburg, Germany — [2]University of California at Davis, USA — [3]Universidade Federal do Rio de Janeiro, Brazil — [4]Laboratoire Kastler Brossel, France

Colloidal systems and biophysical interfaces involve electrolytic environments where the Debye screening is extremely efficient. Therefore, it was thought that the interaction induced by electromagnetic fluctuations could not give rise to long-range forces in such systems. It has now been shown and experimentally verified [1] that the contribution to the Casimir force or retarded van der Waals force induced by low-frequency transverse magnetic fluctuations is not screened. There thus exists a contribution to the long-range interaction between two objects in an electrolyte two orders of magnitude larger than previously thought at distances as small as one hundred nanometres.

For two dielectric microspheres in salted water at room temperature, the force becomes universal for sufficiently large distances, in that it depends solely on the geometrical parameters and not on dielectric functions. While in general, a significant numerical effort is required to determine the Casimir interaction [2], we have also derived approximate simple expressions [3] accurate enough for most practical applications. - [1] L. B. Pires et al., Phys. Rev. Res. 3 033037, (2021); [2] B. Spreng et al. J. Chem. Phys. 153, 024115 (2020); [3] T. Schoger et al., Phys. Rev. Lett. 128, 230602 (2022)

DY 54.4 Fri 10:30 MER 02

Interparticle forces between real cement surfaces across aqueous and non-aqueous solvents — •Simon Becker and Regine von Klitzing — Soft Matter at Interfaces, TU Darmstadt, 64289 Darmstadt, Germany

Concrete and cement are highly abundant construction materials. Therefore, their flow behavior in early stages of processing is of great interest. By using chemical admixtures such as superplasticizers (e.g. polycarboxylate ethers - PCEs) their rheological performance can be enhanced. The rheology is governed by the forces between the particles and the forces between particles and the liquid phase.

The aim of this work is to map the force between cement surfaces across an electrolyte via colloidal probe atomic force microscopy (CP-AFM). Since cement hydrates in aqueous solutions the surface changes with time. The challenge is to disentangle different effects like hydration and roughness of the cement surfaces on the interaction. To prevent hydration of the cement the force measurements are conducted in ethanol solutions. For comparison the force measurements are carried out between two silica particles, between cement and silica as well as between cement and cement.

Furthermore, the time dependence of the cement surface due to hydration in water is mapped using tapping mode AFM. Moreover, the hydration time dependent interparticle force between cement surfaces is investigated in aqueous electrolyte solution with and without PCE to approach application related conditions.

DY 54.5 Fri 10:45 MER 02

Structure and interaction of surface charged polymeric micelles — Lingsam Tea, Lutz Willner, •Jörg Stellbrink, and Stephan Förster — JCNS-1, Forschungszentrum Jülich, 52425 Jülich, Germany

Soft colloids are ubiquitous in synthetic and biological matter and display macroscopically interesting structural and dynamical properties resulting from its hybrid microscopic structure. We established micelles formed by amphiphilic block copolymers as an easy and elegant model system to tailor colloidal softness [1].

In the present work, we introduce surface charges on n-alkyl-PEO-OH micelles resulting in electrostatic interactions in addition to the inherently present steric repulsion. These charges are precisely implemented by oxidation of only the terminal hydroxy group of the PEO block into a carboxy group. We studied intra- and interparticle structure by SANS over a broad range of concentrations, pH and ionic strength and demonstrate that the micellar form factor remains the same independent of the number of charges. However, in contrast to neutral micelles, the charged micelles typically reveal structure factor contributions even at very dilute concentration, arising from the here dominating long-range electrostatic repulsion. Structure factors in the liquid state are analyzed using competing effective interaction potentials. By increasing the concentration a liquid to crystal transition is observed for all systems, but for charged micelles at a much lower concentration compared to the uncharged micelles.

[1] S. Gupta et al., Nanoscale, 7 (2015) 13924.

DY 54.6 Fri 11:00 MER 02

Structure and dynamics of concentrated suspensions of PMMA-PDMS core-shell particles — •Joel Diaz Maier, Paul Tümmler, and Joachim Wagner — Institut für Chemie, Universität Rostock, 18051 Rostock, Germany

Sterically stabilized polymer particles with silicone based stabilizers find increasing interest as a novel colloidal model system with hard-sphere interactions. In this contribution, the largely unknown behavior of concentrated suspensions of PMMA-PDMS core-shell particles was investigated over a wide range of volume fractions employing static and dynamic light scattering experiments. Static structure factors extracted from scattered intensities are analyzed using integral equation theory. The wavevector-dependent short-time diffusion of the systems can be accurately described using $\delta\gamma$-expansion, based on interpolated experimental structure factors as a direct input. All investigated structural and dynamical properties closely follow theoretical predictions for hard-sphere systems, proving the suitability of these colloidal particles as an easily accessible model system for hard spheres.

15 min. break

DY 54.7 Fri 11:30 MER 02

Inverse ISAsomes in biocompatible oils - formulation and characterisation — •Florian Trummer[1], Otto Glatter[2], and Angela Chemelli[2] — [1]Universität Stuttgart, Institut für Physikalische Chemie, Pfaffenwaldring 55, 70569 Stuttgart, Deutschland — [2]Technische Universität Graz, Institut für Anorganische Chemie, Stremayrgasse 9, 8010 Graz, Österreich

In contrast to their more common counterparts in aqueous solutions, inverse ISAsomes (internally self-assembled somes/particles) are formulated as kinetically stabilised dispersions of hydrophilic, lyotropic liquid-crystalline phases in non-polar oils. This contribution reports on their formation in bio-compatible oils and their structural characterisation with Small Angle X-Ray Scattering (SAXS), Dynamic Light Scattering (DLS) and optical microscopy [1]. By using these methods, we were able to demonstrate the presence of inverse hexosomes, inverse micellar cubosomes (Fd3m) and an inverse emulsified microemulsion in squalane with a polyethylene glycol (PEG) alkyl ether as the primary surfactant forming the internal self-assembled phase, which was stabilised by hydrophobised silica nanoparticles. Furthermore, an emulsified L_1-phase and inverse hexosomes were formed in triolein with the triblock-copolymer Pluronic P94 as the primary surfactant. In this case, stabilisation was achieved with a molecular stabiliser of type PEG-dipolyhydroxystearate. Finally, triolein was replaced with olive oil which also led to the successful formation of inverse hexosomes.

[1] Trummer, F., Glatter, O. & Chemelli, A. *Nanomaterials* **12**, 1133 (2022)

DY 54.8 Fri 11:45 MER 02

Anomalous Screening Behavior of Nanometer-Sized Ions — •Thomas Tilger and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

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

Therefore, it is of special interest to gain an understanding of which interparticle forces govern the stability of colloidal dispersions and how this stability can be tailored. The DLVO theory is a powerful framework to describe these interactions. While this description provides a good agreement with experimental data for small 1:1 electrolytes, larger deviations emerge for ions of higher valency and of larger dimensions. For a detailed examination of these border cases, we directly measure the forces between colloidal silica particles in aqueous electrolyte solutions containing nanometer-sized ions by the colloidal probe AFM (atomic force microscopy) technique.

Two different types of nano-ions were chosen as model systems, Keggin ions (silicotungstic acid, STA, a 1:4 system) and Terpyridine-Nickel-complexes with variable charge. Their electrostatic screening behavior reveals significant deviations between the calculated and measured ionic strengths, which indicates some unexpected phenomena.

DY 54.9 Fri 12:00 MER 02

Charged, screened-charged and hard-sphere fluids studied by confocal microsopy, analytical theory and simulation. — Sahana Kale, Martin Oettel, and •Hans Joachim Schöpe — Universität Tübingen, Institut für angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

We present a joint experimental and theoretical study investigating the fluid structure in direct and reciprocal space of PMMA particles dispersed in various solvents. Using decaline and CHB alone the structure can be well-described using PB-RMSA-Theory for monodisperse systems. Upon adding TBAB we observe that the surface charge can't be screened entirely. To model the fluid structure we use Monte Carlo simulations for a polydisperse hard core Yukawa System. Thus we get meaningful data for the effective charge and salt concentration. The results indicate behavior that is significantly different from HS. Surprisingly the situation is fundamentally different for particles dispersed in a mixture of decaline and TCE. Here all measured observables follow polydisperse Percus-Yevick theory.

DY 54.10 Fri 12:15 MER 02

Bicontinuous Microemulsion in Porous Materials — •Margarethe Dahl[1], René Haverkamp[2], Larissa Doll[1], Thomas Hellweg[2], and Stefan Wellert[1] — [1]Institut für Chemie, Technische Universität Berlin, Germany — [2]Physikalische und Biophysikalische Chemie, Universität Bielefeld, Germany

While the bulk phase behavior of microemulsions has been intensively studied, the influence of a geometrical confinement has been widely neglected. Understanding the influence of geometrical restrictions yields both, fundamental insights and importance for applications, e.g. decontamination and enhanced oil recovery. In our study, controlled-pore silica glasses (CPGs) serve as confining matrices for bicontinuous microemulsions. Effects of the pore network and surface chemistry on phase behavior and structure of a model microemulsion are studied by using various CPGs with pore diameter between 75 – 1000 Å and ternary bicontinuous microemulsions (water/octane/$C_{10}E_4$). The naturally hydrophilic surfaces of the CPGs were hydrophobically modified to analyze the influence of the surface polarity. We use imaging techniques (cryo-SEM), small angle scattering (SANS, SAXS) with measurements of the advancing contact angles inside the hydrophilic and hydrophobically modified pores (Washburn approach) to explore the microemulsion phase structure in bulk and inside the pores. In this talk, the results of these combined experiments will be presented and discussed.

DY 54.11 Fri 12:30 MER 02

Diffusion and thermodiffusion of polymers in mixed solvents — •Daniel Sommermann, Jannik Kantelhardt, and Werner Köhler — Physikalisches Institut, Universität Bayreuth, Germany

We present experiments on diffusion and thermodiffusion of polymers in mixed solvents. So far, most works on thermodiffusion have dealt with binary systems or ternary mixtures of small molecules. Binary samples with polymers in solvents have been studied over both a broad concentration and polymer molar mass range. Only a few very recent

experiments measured polymers in a binary solvent. In this work, samples made of polystyrene ($M_w = 4880\,g/mol$), toluene and cyclohexane have been analysed using multi-color optical beam deflection (OBD) and supporting single-color thermal diffusion forced Rayleigh scattering (TDFRS). While binary mixtures are readily characterized by one diffusion and one thermodiffusion coefficient, the number of coefficients increases to four plus two for ternaries. The measured signals show three well separated modes that can be assigned to the thermal diffusivity and the two eigenvalues of the mass diffusion matrix. We are particularly interested in the question, to what extent the dynamics of the large entity, the polymer, is coupled to the solvent-solvent dynamics, both with respect to diffusion and thermodiffusion. A first analysis supports the picture of an effective solvent whose internal dynamics is decoupled from the one of the polymer.

DY 54.12 Fri 12:45 MER 02

Dynamic susceptibility of magnetic nanoplatelet suspensions — •Margaret Rosenberg[1], Sofia S. Kantorovich[1], and Philip J. Camp[2] — [1]Department of Physics, University of Vienna, Vienna, 1090, Austria — [2]School of Chemistry, The University of Edinburgh, David Brewster Road, Edinburgh EH9 3FJ, UK

Particle anisometry and anisotropy provide valuable control parameters to alter the self-assembly, and thermodynamic, rheological, and phase behaviour, of colloidal suspensions. This work is concerned with the dynamic magnetic susceptibility (DMS) of a ferrofluid with platelet-shaped anisotropic particles, which have a fixed out-of-plane dipole moment providing additional, magnetic anisometry. Such a colloidal suspensions is of particular interest as, above a threshold concentration, it exhibits a ferromagnetic nematic phase. Recent experimental work [1] has shown that the DMS spectrum exhibits multiple dynamical modes, suggesting that there might be clusters of particles with distinct rotational timescales. Using Brownian dynamics simulations, we explore the effects of varying nanoparticle concentration - and therefore microstructure - on the DMS, and explain the gap in relaxation times, and changes in the spectrum, that are observed experimentally.

[1] M. Küster et al., "Magnetic dynamics in suspensions of ferrimagnetic platelets", Journal of Molecular Liquids, Vol. 360, (2022), 119484

DY 55: Dynamics and Chaos in Many-Body Systems II (joint session DY/TT)

Time: Friday 9:30–12:30 Location: MOL 213

DY 55.1 Fri 9:30 MOL 213

Towards a more fundamental understanding of eigenstate thermalization — •Tobias Hofmann, Tobias Helbig, Ronny Thomale, and Martin Greiter — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

We explore several venues how eigenstate thermalization may be understood on a more fundamental level. In particular, we report on extensive numerical work in spin systems with random interactions, where a small subsystem is subject to thermalization. We discuss possible directions towards an understanding of our numerical results.

DY 55.2 Fri 9:45 MOL 213

Spectral Response of Disorder-Free Localized Lattice Gauge Theories — •Nilotpal Chakraborty[1], Markus Heyl[1,2], Petr Karpov[1], and Roderich Moessner[1] — [1]Max Planck Institute for Physics of Complex Systems, Dresden — [2]University of Augsburg

We show that certain lattice gauge theories exhibiting disorder-free localization have a characteristic response in spatially averaged spectral functions: a few sharp peaks combined with vanishing response in the zero frequency limit. This reflects the discrete spectra of small clusters of kinetically active regions formed in such gauge theories when they fragment into spatially finite clusters in the localized phase due to the presence of static charges. We obtain the transverse component of the dynamic structure factor, which is probed by neutron scattering experiments, deep in this phase from a combination of analytical estimates and a numerical cluster expansion. We also show that local spectral functions of large finite clusters host discrete peaks whose positions agree with our analytical estimates. Further, information spreading, diagnosed by an unequal time commutator, halts due to real space fragmentation. Our results can be used to distinguish the disorder-free localized phase from conventional paramagnetic counterparts in those frustrated magnets which might realize such an emergent gauge theory.

DY 55.3 Fri 10:00 MOL 213

Chaos in the three-site Bose-Hubbard model - classical vs quantum — •Goran Nakerst[1] and Masudul Haque[1,2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany

We consider a quantum many-body system - the Bose-Hubbard system on three sites - which has a classical limit, and which is neither strongly chaotic nor integrable but rather shows a mixture of the two types of behavior. We compare quantum measures of chaos (eigenvalue statistics and eigenvector structure) in the quantum system, with classical measures of chaos (Lyapunov exponents) in the corresponding classical system. As a function of energy and interaction strength, we demonstrate a strong overall correspondence between the two cases. In contrast to both strongly chaotic and integrable systems, the largest Lyapunov exponent is shown to be a multi-valued function of energy.

DY 55.4 Fri 10:15 MOL 213

Many-Body Dwell-time and Density of States — •Georg Maier, Carolyn Echter, Juan-Diego Urbina, and Klaus Richter — Universität Regensburg, Regensburg, Germany

Many body systems with a large number of degrees of freedom are usually described by statistical physics on the theoretical side while experiments usually relay on scattering (e.g. particle physics). Is it possible to relate scattering and statistical physics, or to measure scattering-related observables which directly relate to quantities of statistical physics? At least for single particle systems a close relation exists between the well known Wigner-Smith delay time in scattering theory and the density of states of the scattering system.

I will present a novel ansatz relating a many-body version of dwell-/Wigner-Smith delay time and many body density of states based on the famous Birman-Krein-Friedel-Loyd formula connecting scattering theory and statistical observales in the many-body context. This formalism could provide answers to a wide variety of interesting questions, e.g. can we observe the effect of interactions (or even the emergence of chaos) through the lens of the dwell-time? Another interesting point is the roll of particle statistics on dwell-time meaning e.g. does it take longer for a particle to leave a fermionic or bosonic system?. I will present our analytical and numerical results on these questions.

DY 55.5 Fri 10:30 MOL 213

Dynamical correlations and domain wall relocalisation in transverse field Ising chains — •Philippe Suchsland[1], Benoît Douçot[2], Vedika Khemani[3], and Roderich Moessner[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]LPTHE, UMR 7589, CNRS and Sorbonne Université, 75252 Paris Cedex 05, France — [3]Department of Physics, Stanford University, Stanford, California 94305, USA

We study order parameters and out-of-time-ordered correlators (OTOCs) for a wide variety of transverse field Ising chains: classical and quantum, clean and disordered, integrable and generic. The setting we consider is that of a quantum quench. We find a remarkably rich phenomenology, ranging from stable periodic to signals decaying with varying rates. This variety is due to a complex interplay of dynamical constraints (imposed by integrability and symmetry) which thermalisation is subject to. In particular, a process we term dynamical domain wall relocalisation provides a long-lived signal in the clean, integrable case, which can be degraded by the addition of disorder even without interactions. Our results shed light on a proposal to use an OTOC specifically as a local dynamical diagnostic of a quantum phase transition even when evaluated in a state with an energy density corresponding to the paramagnetic phase.

15 min. break

DY 55.6 Fri 11:00 MOL 213

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

It is known for the antiferromagnetic sawtooth chain with Heisenberg interactions to develop a flat band at the quantum-critical point of $J_1 = 2J_2$, where J_1 is the exchange interaction between nearest neighbors and J_2 the interaction at the base of the triangles [1]. We investigate the time evolution of several observables of the sawtooth chain, especially near that point and in particular in view of their equilibration properties. [1] J. Schulenburg, A. Honecker, J. Schnack, J. Richter, H.-J. Schmidt, Phys. Rev. Lett. 88 (2002) 167207

DY 55.7 Fri 11:15 MOL 213

Quantum Noise as a Symmetry-Breaking Field — •Paul McClarty[1], Beatriz Dias[2], Domagoj Perkovic[3], Masudul Haque[4], and Pedro Ribeiro[5] — [1]MPI PKS, Dresden, Germany — [2]TU Munich, Garching, Germany — [3]Cavendish Lab, University of Cambridge, UK — [4]TU Dresden, Germany — [5]IST, Lisbon, Portugal

We investigate the effect of quantum noise on the measurement-induced quantum phase transition in monitored random quantum circuits. Using the efficient simulability of random Clifford circuits, we find that the transition is broadened into a crossover and that the phase diagram as a function of projective measurements and noise exhibits several distinct regimes. We show that a mapping to a classical statistical mechanics problem accounts for the main features of the random circuit phase diagram. The bulk noise maps to an explicit permutation symmetry breaking coupling; this symmetry is spontaneously broken when the noise is switched off. These results have implications for the realization of entanglement transitions in noisy quantum circuits.

DY 55.8 Fri 11:30 MOL 213

Finite-size prethermal behavior at the chaos-to-integrable transition — •Johannes Dieplinger[1] and Soumya Bera[2] — [1]Institute of Theoretical Physics, University of Regensburg, D-93040 Germany — [2]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India

We investigate the dynamics of the complex Sachdev-Ye-Kitaev model complemented with a single particle hopping term, leading to a chaos-to-integrable transition of the eigenstates. We determine the dynamics close to the transition via the density-density correlator, where we observe a prethermal plateau in the ergodic phase. This indicates a finite time localised behavior up to an interaction-dependent thermalization time scale. This time scale is quantified as $t_{th} \propto 2^{\alpha/\sqrt{\lambda}}$ as a function of the relative interaction strength λ. The results are validated by investigating the time-dependent structure of the time-evolved wave functions in the Fock space.

DY 55.9 Fri 11:45 MOL 213

Quasiparticle Description of Entanglement Growth — •Molly Gibbins, Bruno Bertini, and Adam Smith — University of Nottingham

The quasiparticle picture of entanglement is a novel way to describe a feature unique to quantum many-body systems. Recent research has found excellent agreement of this description with numeric results: a description that had been shown to hold for the general family of Rényi entanglement entropies, for different classes of quench and different geometries of the boundary across which entanglement develops.

The aim of this project is to develop a quasiparticle description of the entanglement growth in free-fermionic systems with translational invariance in both 1D and 2D. The propagation of quasiparticles across this cut will respect this translational invariance and it is expected that the entanglement generated between these particles will be in very good agreement with the exact solution for these systems.

DY 55.10 Fri 12:00 MOL 213

Excitation Transport in Molecular Aggregates with Thermal Motion — •Ritesh Pant and Sebastian Wüster — Indian institute of science education and research, Bhopal, India

Molecular aggregates can under certain conditions transport electronic excitation energy over large distances due to the long range dipole-dipole interactions. These interactions are also the characteristics of Rydberg aggregates which have been proved as the quantum simulators for molecular aggregates. An idea that naturally arises in Rydberg aggregates, is adiabatic excitation transport through atomic motion, where slow motion of the atoms combined with excitation transport can result in efficient and guided transport of the excitation from one end of an atomic chain to the other. Based on the analogy between Rydberg and Molecular aggregates, in ref. [1] we explore whether the adiabatic excitation transport can play a functional role in molecular aggregates in the absence of intra-molecular vibrations. But because the transport is partially adiabatic and because it involves transitions between non-eigenstates, it is challenging to estimate the adiabaticity of transport in molecular aggregates. Hence, in ref [2] we established a measure to quantify the adiabatic character of quantum transitions in general. Next, the effect of intramolecular vibrations is included by extending our calculation for excitation transport to an open-quantum-system technique [3].

[1] R. Pant and S. Wüster, Physical Chemistry Chemical Physics 22, 21169 (2020). [2] R. Pant, et al., https://arxiv.org/abs/2007.10707. [3] R. Pant, et al., (Manuscript in preparation)

DY 55.11 Fri 12:15 MOL 213

Tailoring the Phonon Environment of Embedded Rydberg Aggregates — •Sidharth Rammohan[1], Sebastian Wüster[1], and Alexander Eisfeld[2] — [1]IISER Bhopal, Madhya Pradesh, India — [2]MPIPKS, Dresden, Germany

State-of-the-art experiments can controllably create Rydberg atoms inside a Bose-Einstein condensate (BEC) such that the Rydberg electron orbital volume contains many neutral atoms, which can be tuned, resulting in electron-atom scattering events [1]. In my talk, I will discuss the physics of the interaction and corresponding dynamics of a single or multiple Rydberg atoms in two internal electronic states embedded inside a BEC, to assess their utility for controlled studies of decoherence and quantum simulations of excitation transport similar to photosynthetic light-harvesting. We initially developed a theoretical framework to calculate the open quantum system input parameters for a single Rydberg atom, possibly in two internal states, in BEC and then for a chain of Rydberg atoms, forming an aggregate [2]. The electron-atom interactions lead to Rydberg-BEC coupling, creating phonons in the BEC. Using the spin-boson model with the calculated parameters, we then examine the decoherence and the Non-Markovian features of a Rydberg atom in a superposition, resulting from the interaction with the environment [3]. The scenario with a single Rydberg atom is then extended to the aggregate case, allowing us to set up dynamics similar to those found in light-harvesting complexes. Ref:1. J. B. Balewski, et.al; Nature 502 664 (2013).2. S. Rammohan, et.al; PRA 103, 063307 (2021).3. S. Rammohan, et.al; PRA 104, L060202 (2021).

DY 56: Brownian Motion and Anomalous Diffusion

Time: Friday 9:30–12:45 Location: ZEU 160

DY 56.1 Fri 9:30 ZEU 160

Odd Diffusion of Interacting Particles — •Erik Kalz[1], Hidde Derk Vuijk[2], Iman Abdoli[2], Jens-Uwe Sommer[2,3], Hartmut Löwen[4], Ralf Metzler[1], and Abhinav Sharma[2,3] — [1]Universität Potsdam, Institut für Physik und Astronomie — [2]Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere — [3]Technische Universität Dresden, Institut für Theoretische Physik — [4]Heinrich Heine-Universität Düsseldorf, Institut für Theoretische Physik II: Weiche Materie

It is generally believed that collisions of particles reduce the self-diffusion coefficient, closely related to autocorrelation functions, which are assumed to decay monotonously in the overdamped limit. We show that these beliefs are only limiting cases in odd-diffusive systems, which are characterized by diffusion tensors with antisymmetric offdiagonal elements. We show that in the dilute limit, particle interactions can reduce, unalter and even enhance the self-diffusion. The underlying particle dynamics thereby can be captured by the force autocorrelation function. We show that this autocorrelation function exhibits a variety of behaviour: (a) even in the dilute limit where collisions are rare, the correlation can become negative, (b) despite the overdamped dynamics, the force autocorrelation can exhibit temporal oscillations and (c) the long-time power-law decay of the force autocorrelation depends on the odd-diffusion parameter. Odd diffusivity, therefore, shines new light on fundamental beliefs in overdamped systems.

Kalz, Erik, et al. Collisions enhance self-diffusion in odd-diffusive systems. Physical Review Letters 129.9 (2022): 090601.

DY 56.2 Fri 9:45 ZEU 160

Bounding Uncertainty of Empirical First-Passage Times of Reversible Markov Processes — •Rick Bebon and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

First-passage phenomena are ubiquitous in nature and are at the heart of, e.g. reaction kinetics, cell signaling, gene regulation, foraging behavior of animals, and stock option dynamics. Whereas theoretical studies typically focus on predicting statistics for a given process, practical applications often aim at inferring, e.g. mean first-passage times (i.e. inverse kinetic rates) from experimental or simulation data. The inference of mean first-passage times is challenging because only a small number of realizations is usually available, in turn leading to high uncertainties and non-Gaussian errors. We derive universal concentration inequalities for first-passage times of ergodic reversible Markov processes on discrete and continuous-state spaces. For a sample of $n \geq 1$ independent realizations of the first-passage process, we prove a Cramér-Chernoff-type bound on the probability that the inferred sample mean deviates from the true mean first-passage time by more than any given amount. We further construct reliable non-asymptotic estimation guarantees, such as confidence intervals valid for all sample sizes n. Our findings allow for a rigorous uncertainty quantification of inferred first-passage times and lay grounds for a systematic understanding of finite-sample effects avoiding asymptotic approximations or biases due to prior-distribution assumptions.

DY 56.3 Fri 10:00 ZEU 160

Single-trajectory spectral analysis as a criterion of anomalous diffusion — •Vittoria Sposini — University of Vienna, Austria

The departure of the spreading dynamics of diffusing particles from the traditional law of Brownian-motion is a signature feature of a large number of complex soft-matter and biological systems. This anomalous diffusion can emerge due to a variety of physical mechanisms, e.g., trapping interactions or the viscoelasticity of the environment. Demonstrating that a system exhibits normal- or anomalous-diffusion is highly desirable for a vast host of applications. In this talk I will present a criterion for anomalous-diffusion based on the method of power-spectral analysis of single trajectories. The robustness of this criterion is studied for trajectories of fractional-Brownian-motion, a ubiquitous stochastic process for the description of anomalous-diffusion, in the presence of two types of measurement errors. In particular, I will report results from various tests on surrogate data in absence or presence of additional positional noise demonstrating the efficacy of this method in practical contexts.

[1] V Sposini, D Krapf, E Marinari, R Sunyer, F Ritort, F Taheri, C Selhuber-Unkel, R Benelli, M Weiss, R Metzler & G Oshanin, Comms. Phys. 5, 305 (2022).

DY 56.4 Fri 10:15 ZEU 160

Apparent anomalous diffusion and non-Gaussian distributions in a simple mobile-immobile transport model with poissonian switching — •Timo J. Doerries[1], Aleksei V. Chechkin[1,2,3], and Ralf Metzler[1] — [1]Institute of Physics & Astronomy, University of Potsdam, Germany — [2]Faculty of Pure and Applied Mathematics, Hugo Steinhaus Center, Wrocław University of Science and Technology, Wrocław, Poland — [3]Akhiezer Institute for Theoretical Physics National Science Center "Kharkiv Institute of Physics and Technology", Kharkiv, Ukraine

We analyse mobile-immobile transport of particles that switch between mobile and immobile states with finite rates. Despite this seemingly simple assumption of Poissonian switching we unveil rich transport dynamics including significant transient anomalous diffusion and non-Gaussian displacement distributions. Our discussion is based on experimental parameters for tau proteins in neuronal cells, but the results obtained here are expected to be of relevance for a broad class of processes in complex systems. Concretely, we obtain that when the mean binding time is significantly longer than the mean mobile time, transient anomalous diffusion is observed at short and intermediate time scales, with a strong dependence on the fraction of initially mobile and immobile particles. We unveil a Laplace distribution of particle displacements at relevant intermediate time scales and the mean squared displacement of mobile tracers displays a plateau. Adding advection to the mobile phase, corresponding to a biosensor with flow, generates a cubic regime of the MSD for high Péclet numbers.

Invited Talk DY 56.5 Fri 10:30 ZEU 160

Transport and self-organization in living fluids — •Matthias Weiss — Experimental Physics I, University of Bayreuth, Bayreuth, Germany

Intracellular fluids, e.g. the eukariotic cytoplasm, are crowded with a plethora of macromolecules, bearing similarities to semidilute polymer solutions. Since many of the macromolecules are actively driven by ATP hydrolysis, these crowded living fluids are also equipped with genuine non-equilibrium properties. Using model systems from culture cells to extracts, we have explored fluctuation-driven transport and the self-organized formation of compartments in living fluids. As a result, we have observed via extensive single-particle tracking experiments that the generic mode of motion in the cytoplasm appears to be a driven, anti-persistent, and partially intermittent fractional Brownian motion process. On larger length scales, we have observed that a spontaneous, ATP-driven compartmentalization in cell extracts without priming template structures, features geometric properties and a dynamic coarse-graining like two-dimensional foams. Altogether, our experimental observations suggest that fluctuation-driven transport and self-organized space compartmentalization in living biofluids are well captured by few but robust physico-chemical principles.

15 min. break

DY 56.6 Fri 11:15 ZEU 160

Brownian solitons in periodic structures — •Alexander P. Antonov[1], Artem Ryabov[2], and Philipp Maass[1] — [1]Fachbereich Physik, Universität Osnabrück, Osnabrück, Germany — [2]Charles University, Faculty of Mathematics and Physics, Department of Macromolecular Physics, Prague, Czech Republic

Solitons are known in systems with inertia as waves propagating without dispersion due to nonlinear effects. We show that solitons can occur in the absence of inertia for fully overdamped Brownian dynamics of hard spheres in periodic potentials at high particle densities [1,2]. The solitons manifest themselves as periodic sequences of different particle assemblies moving even in the zero-noise limit, where transport of single particles is not possible. To uncover the hard sphere dynamics at zero noise, a new simulation technique has been developed that can be applied for arbitrary external force fields [3]. At low temperature, the solitons give rise to particle currents appearing in band-like structures around certain particle diameters. At high temperatures, currents occur for all particle diameters. The variation of the current magnitudes

with particle diameter and driving force reflects the inherent soliton formation.

[1] A. P. Antonov, A. Ryabov, P. Maass, Phys. Rev. Lett. 129, 080601 (2022).
[2] A. P. Antonov, D. Voráč, A. Ryabov, P. Maass, New J. Phys 24, 093020 (2022).
[3] A. P. Antonov, S. Schweers, A. Ryabov, P. Maass, Phys. Rev. E 106, 054606 (2022).

DY 56.7 Fri 11:30 ZEU 160

Large beam X-ray Photon Correlation Spectroscopy — •Fabian Westermeier, Nimmi Das A, Vijay Kartik, Zhe Ren, Wojciech Roseker, Rustam Rysov, Daniel Weschke, Han Xu, and Michael Sprung — Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

The Coherence Applications Beamline P10 at PETRA III is dedicated to coherent X-ray scattering experiments such as X-ray Photon Correlation Spectroscopy (XPCS) and Coherent Diffraction Imaging (CDI). In an XPCS experiment, either the speckle visibility or the temporal changes of a series of scattering patterns are used to measure the dynamics of a sample.

At beamline P10, two 12 m long experimental hutches (EH1 and EH2) house various experimental setups. Among them, two setups are optimized to perform XPCS experiments. One of them is a SAXS/WAXS instrument, where the detector can be translated between 0° and 30° at a sample to detector distance of 5 m. This setup also offers the possibility to use a range of different focal sizes to adjust to the needs of the experiment. The other configuration is an ultra-small angle X-ray scattering (USAXS) setup, where the detector is positioned at a sample to detector distance of around 21 m. This long pathway allows it to use a large fraction of the coherent flux in an unfocused X-ray beam, while providing a fairly strong speckle visibility. Exemplary experimental results obtained at both setups will be shown illustrating the possibilities of XPCS at the beamline.

DY 56.8 Fri 11:45 ZEU 160

Dynamic finite size correction reveals the long-time hydrodynamic tail of liquid water from molecular dynamics simulations — •Laura Scalfi, Domenico Vitali, and Roland R. Netz — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Finite-size effects in molecular dynamics simulations with periodic boundary conditions have significant effects on computed static and dynamic properties. We study the effect of periodic boundary conditions on the friction memory function and on velocity autocorrelation functions of a particle in a liquid using hydrodynamic theory and molecular dynamics simulations. We show that for liquid water, the long-time decay of these functions is significantly affected by hydrodynamic finite-size effects so that the long-time power law tails are not visible for standard simulation box sizes. We develop an analytical correction scheme that corrects for hydrodynamic finite-size effects. Using this correction scheme, the long-time power-law tails of the friction memory and the velocity autocorrelation functions are clearly revealed even for relatively small simulation box sizes. Our developed method generally allows the accurate determination of the long-time behavior of time-dependent response functions from molecular dynamics simulations.

DY 56.9 Fri 12:00 ZEU 160

Fractional anomalous diffusion and Non-Darcian flow in geological system — •Qing Wei — Institute for Physics and Astronomy, University of Potsdam, 14476 Potsdam-Golm,Germany

With the non-Darcian flow and anomalous diffusion in low-permeability porous media as research subjects, the analytical models of non-Darcian flow as well as diffusive transport in low-permeability porous media was in- vestigated by invoking the fractional calculus theory. Using the fractional derivatives with different kernel, fractional diffusion models are proposed to describe radionuclide anomalous transport in geological repository sys- tems. On the basis of Darcy*s law, the memory effectiveness deduced by solid-fluid interaction is depicted by fractional derivative approach, and a fractional Swartzendruber model is proposed for the description of low velocity non-Darcian flow in porous media.

DY 56.10 Fri 12:15 ZEU 160

Universal hyper-scaling relations, power-law tails, and data analysis for strong anomalous diffusion — •Jürgen Vollmer[1], Lamberto Rondoni[2], Claudio Giberti[3], and Carlos Mejía-Monasterio[4] — [1]Inst. Theor. Physik, Univ. Leipzig, 04103 Leipzig, Germany — [2]Dept. Math. Sc., Politecnico di Torino, 10129 Torino, Italy — [3]Dept. Scienze e Metodi dell Ingegneria, Univ. Modena e Reggio E., 42100 Reggio E., Italy — [4]School of Agric. Food and Biosys. Eng., Techn. Univ. Madrid, 28040 Madrid, Spain

Strong anomalous diffusion is often characterized by a piecewise-linear spectrum of the moments of displacement. The spectrum is characterized by slopes ξ and ζ for small and large moments, respectively, and by the critical moment α of the crossover. Higher moments are asymptotically dominated by ballistic excursions; lower moments correspond to weak anomalous diffusion. We argue that ξ and ζ characterize the asymptotic scaling of the bulk and the tails of the distribution, respectively. Asymptotic theory is adopted to match the behaviors at intermediate scales. The resulting constraint entails that strong anomalous diffusion emerges if the distribution has algebraic tails, and it relates α to the corresponding power law. Our theory provides the leading-order corrections to the asymptotic power-law behavior. This insight allows us to point out sources of (at times) severe systematic errors in numerical estimates of the moments of displacement. Rather than fitting exponents we devise a robust scheme to determine ξ, ζ and α. The findings are supported by numerical and analytical results on different models exhibiting strong anomalous diffusion.

DY 56.11 Fri 12:30 ZEU 160

Bio-hybrid colloidal transport of beads on cell monolayers — Lara Bort, Setareh Sharifi Panah, •Robert Grossmann, and Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany

The erratic motion of Brownian particles at the mesoscale, driven by collisions with the surrounding fluid particles, is the paradigm of random colloidal transport within a passive environment. In this work, we describe the transport of polystyrene micro-beads whose motion is driven by a monolayer of motile cells. We use cells of the social amoeba *Dictyostelium discoideum*, which is a widely used model organism for actin-driven motility of adherent eukaryotic cells, including neutrophils and cancer cells. Given the non-specific adhesion of our model organism, the binding of such micro-cargo to the cell membrane does not require any surface-functionalization – the physical link between cargo and carrier is established spontaneously. As a particle gets in contact with a cell, it adheres to the cell membrane and is then subjected to active forces exerted by cells. The dynamics of micro-beads reveals linear scaling of the ensemble-averaged mean-square displacement and, notably, non-Gaussian displacement distributions. We rationalize these findings by assuming that each colloidal particle effectively performs normal Brownian motion, but the diffusion coefficients vary within the ensemble due to cell-to-cell variability. This superstatistics allows to reproduce the statistical features of the long-time dynamics of colloids, subject to the active cellular forces. It serves as a first step to better understand the targeted transport of foreign objects in dense tissues.

DY 57: Networks: From Topology to Dynamics IV (joint session DY/SOE)

Time: Friday 9:30–11:45 Location: ZEU 250

DY 57.1 Fri 9:30 ZEU 250

Efficient integration of short-range models on complex networks — •Jeffrey Kelling[1,2], Géza Ódor[3], Lilla Barancsuk[3], Shengfeng Deng[3], Bálint Hartmann[3], and Sibylle Gemming[2] — [1]Chemnitz University of Technology, Chemnitz, Germany — [2]Helmholtz-Zentrum Dresden - Rossendorf, Dresden, Germany — [3]Centre for Energy Research, Budapest, Hunguary

Complex, hierarchical or random network topolgies can give rise to unique behavior in many physical models. We study dynamical synchronization behavior in Kuramoto models on power grids and brain connectomes with millons of connections and $\mathcal{O}(100k)$ nodes. At these scales it is crucial to use the sparsity when computing derivatives, which, due to the random network structure, makes employing modern parallel hardware tricky. Here, we present our approach to numerically solving large systems ordinary differential equations on random directed graphs, where we focus on the computationally expensive task of computing derivatives and leave the common integration step to the `boost::odeint` library. Our application can utilize both parallel CPUs and GPUs. We also provide an overview of our results on human and fly brain connectomes as well as failure cascades in power grids and provide a measure of the advantage gained from our computational optimization efforts.

DY 57.2 Fri 9:45 ZEU 250

Discovering hidden layers in quantum graphs — Łukasz Gajewski, •Julian Sienkiewicz, and Janusz Hołyst — Faculty of Physics, Warsaw University of Technology, Warsaw, Poland

Finding hidden layers in complex networks is an important and nontrivial problem in modern science. We explore the framework of quantum graphs to determine whether concealed parts of a multilayer system exist and, if so, their extent, i.e., how many unknown layers are there. Assuming that the only information available is the time evolution of wave propagation on a single layer of a network, it is indeed possible to uncover that which is hidden by merely observing the dynamics. We present evidence on both synthetic and real-world networks that the frequency spectrum of the wave dynamics can express distinct features in the form of additional frequency peaks. These peaks exhibit dependence on the number of layers taking part in the propagation and thus allowing for the extraction of said number. We show that, in fact, with sufficient observation time, one can fully reconstruct the row-normalized adjacency matrix spectrum. We compare our propositions to a machine learning approach using a wave packet signature method modified for the purposes of multilayer systems.

DY 57.3 Fri 10:00 ZEU 250

Dynamic network modelling of tumor disease and sepsis — •Eckehard Schöll[1,2,3], Jakub Sawicki[1,2], Rico Berner[1,4], Fenja Drauschke[1], Moritz Alkofer[1], Eckhardt Schneider[5], and Thomas Löser[5] — [1]Institut für Theoretische Physik, TU Berlin — [2]Potsdam Institute for Climate Impact Research — [3]Bernstein Center for Computational Neuroscience Berlin — [4]Institut für Physik, HU Berlin — [5]Institut LOESER, Wettiner Straße 6, 04105 Leipzig

We introduce a novel functional model for tumor disease and sepsis within the framework of complex networks [1,2]. Both diseases are treated in a unified way centered on their effect on the innate immune system. We propose an adaptively coupled two-layer network model of phase oscillators based upon the interaction of parenchymal cells (organ tissue) and immune cells, respectively, and the co-evolutionary dynamics of parenchymal, immune cells, and cytokines. The interaction and information exchange via cytokines between the cells of the parenchyma and the innate immune system is modeled by adaptive coupling weights. The emergent complex collective dynamics is represented with a few fundamental control parameters. Concepts and methods of nonlinear dynamical systems and networks theory, such as partial synchronization and clustering, as well as numerical and statistical methods are applied to describe physiological and pathological states. [1] Sawicki, J., Berner, R., Löser, T., and Schöll, E., Front. Netw. Physiol. 1, 730385 (2022). [2] Berner, R., Sawicki, J., Thiele, M., Löser, T. and Schöll, E., Front. Netw. Physiol. 2, 904480 (2022).

DY 57.4 Fri 10:15 ZEU 250

Automated chemical reaction network discovery for the simulation of long-timescale degradation of materials — •Joe Gilkes[1], Mark Storr[2], Reinhard J. Maurer[1], and Scott Habershon[1] — [1]University of Warwick, United Kingdom — [2]AWE plc, United Kingdom

Degradation of organic materials such as polymers occurs over time scales of years and involves rare reaction events over an expansive network of elementary processes. Building such networks in order to predict the degradation pathways of these materials requires tackling combinatorially large chemical spaces, and propagating these networks in time becomes considerably more difficult as network size increases. Predicting overall rates by which materials break down requires accurate calculations of the energetic barriers of thousands of elementary reaction steps, which also comes with a substantial computational cost. We present a software framework written in the Julia language for automatically traversing chemical reaction space with an approach that iteratively expands the reaction network through successive re-evaluation of degradation products. We couple this with a machine learning model to predict activation energies. The result is a workflow that can swiftly sample reaction space to create computationally efficient molecular breakdown networks, and then run simulations to predict the long-term stability of these species under a range of environmental conditions. We demonstrate this approach for the example of polyethylene degradation.

15 min. break

DY 57.5 Fri 10:45 ZEU 250

Exact statistical mechanics of spin models on networks — •Konstantin Klemm — IFISC (CSIC-UIB), Mallorca, Spain

Biological, social, and technical systems are modeled as discrete entities interacting through a network. Predicting these systems' behaviour thus involves the computationally difficult task of solving dynamics on a given complex network. Although networks of interest typically have an abundance of short cycles influencing dynamics, existing computational methods build on the assumption that short cycles are small structural corrections, thus making a *locally tree-like* approximation. Here we show that exact and efficient prediction, exemplified by the Ising and spin glass models, is possible for many networks. We exploit *globally tree-like* structure in the sense of small tree-width. The full manuscript is available at https://arxiv.org/abs/2111.04766 .

DY 57.6 Fri 11:00 ZEU 250

Network meta-analysis: A statistical physics perpective — Annabel L. Davies[1] and •Tobias Galla[2] — [1]Bristol Medical School, University of Bristol, Bristol BS8 2PS, UK — [2]IFISC, Instituto de Física Interdisciplinar y Sistemas Complejos (CSIC-UIB), Campus Universitat de les Illes Balears, 07122 Palma de Mallorca, Spain

Network meta-analysis (NMA) is a technique used in medical statistics to combine evidence from multiple medical trials. In particular it allows one to compare treatments that have not been tested directly against each other in a trial. NMA defines an inference and information processing problem on a network of treatment options and trials connecting the treatments. In this talk I will briefly outline the 'NMA problem', and I will then describe how statistical physics can offer useful ideas and tools for this area, including from the theory of complex networks, stochastic modelling and simulation techniques [1]. In particular I will present an analogy we recently established between NMA and random walks on networks [2], and which improves existing algorithms for the estimation of 'proportion contributions' – that is the importance of any one element in the network for the comparison of any two given treatment options. One main aim of the talk is to attract physicists to this timely, interesting and worthwhile area of research.

[1] Annabel L Davies and Tobias Galla, J. Stat. Mech. (2022) 11R001

[2] Annabel L Davies, Theodoros Papakonstantinou, Adriani Nikolakopoulou, Gerta Rücker, Tobias Galla, Statistics in Medicine, 41 (2022) 2091

DY 57.7 Fri 11:15 ZEU 250

Controlling the coarsening dynamics of ferrogranular networks by means of a vertical magnetic field — •Oksana

Bilous[1], Pedro Sánchez[1], Matthias Biersack[2], Ali Lakkis[2], Reinhard Richter[2], and Sofia Kantorovich[1] — [1]University of Vienna — [2]University of Bayreuth

In nature, phase transitions of various nature are significant and often lead to abrupt changes in the macroscopic properties of the material. Here, we address the question if a viscoelastic phase separation (VPS), proposed in 2000 by Hajime Tanaka for dynamically asymmetric mixtures, scales up for a shaken mixture of steel and glass spheres, i.e. for a so-called ferrogranulate when an external magnetic field is applied perpendicular to the plane in which the system is confined. In this contribution we focus on computer simulation. We calculated magnetization, dipolar and steric energies, radial distribution functions, the average number of neighbours and the efficiency of the emerging networks as functions of the simulation time and the values of the external vertical magnetic fields. Our results demonstrate that the network formation can be inhibited by the field perpendicular to the sample via dipole-dipole repulsion the field. These results are qualitatively confirmed by the experimental data.

DY 57.8 Fri 11:30 ZEU 250

Controlling the coarsening dynamics of ferrogranular networks by means of a vertical magnetic field — •Oksana Bilous[1], Pedro Sánchez[1], Matthias Biersack[2], Ali Lakkis[2], Reinhard Richter[2], and Sofia Kantorovich[1] — [1]Computational and Soft Matter Physics, Faculty of Physics, University of Vienna, 1090 Vienna, Austria — [2]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany

In nature, phase transitions of various nature are significant and often lead to abrupt changes in the macroscopic properties of the material. Here, we address the question if a viscoelastic phase separation (VPS), proposed in 2000 by Hajime Tanaka for dynamically asymmetric mixtures, scales up for a shaken mixture of steel and glass spheres, i.e. for a so-called ferrogranulate when an external magnetic field is applied perpendicular to the plane in which the system is confined. In this contribution we focus on computer simulation. We calculated magnetization, dipolar and steric energies, radial distribution functions, the average number of neighbours and the efficiency of the emerging networks as functions of the simulation time and the values of the external vertical magnetic fields. Our results demonstrate that the network formation can be inhibited by the field perpendicular to the sample via dipole-dipole repulsion the field. These results are qualitatively confirmed by the experimental data.