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

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Overview of Invited Talks and Sessions

(Lecture halls H2 and H6; Poster P)

Invited Talks

DY 2.1	Tue	10:00–10:30	H6	**Local Versus Global Two-Photon Interference in Quantum Networks** — •Sonja Barkhofen, Thomas Nitsche, Syamsundar De, Evan Meyer-Scott, Johannes Tiedau, Jan Sperling, Aurél Gábris, Igor Jex, Christine Silberhorn
DY 9.1	Wed	13:30–14:00	H6	**Nanofriction in Ion Coulomb Systems** — •Tanja Mehlstäubler
DY 10.1	Wed	15:00–15:30	H6	**Effect of fibrosis on propagation on non-linear waves and onset of arrhythmias in cardiac tissue** — •Alexander Panfilov, Timur Nezlobinsky, Farhad Pashakhanloo
DY 10.4	Wed	16:00–16:30	H6	**Chaos and nonlinear dynamics in the heart: Experiments and simulations of arrhythmias and defibrillation** — •Flavio fenton
DY 13.1	Thu	13:30–14:00	H2	**Multi-scale modeling of dyadic structure-function relation in ventricular cardiac myocytes** — •Martin Falcke, Filippo G. Cosi, Wolfgang Giese, Wilhelm Neubert, Stefan Luther, Nagaiah Chmakuri, Ulrich Parlitz
DY 13.4	Thu	14:45–15:15	H2	**Cardiac repolarization dynamics and arrhythmias in healthy and diseased hearts** — •Esther Pueyo
DY 13.7	Thu	15:45–16:15	H2	**Dynamics of paroxysmal tachycardias** — •Gil Bub
DY 18.1	Fri	13:30–14:00	ESS	**Network-Induced Multistability Through Lossy Coupling** — •Jürgen Kurths
DY 18.2	Fri	14:00–14:30	ESS	**Control of synchronization in two-layer power grids** — •Simona Olmi, Carl Totz, Eckehard Schöll
DY 18.3	Fri	15:00–15:30	ESS	**Relay and complete synchronization of chimeras and solitary states in heterogeneous networks of chaotic maps** — Elena Rybalova, Eckehard Schöll, •Galina Strelkova
DY 18.4	Fri	15:30–16:00	ESS	**A bridge between the fractal geometry of the Mandelbrot set and partially synchronized dynamics of chimera states.** — •Ralph G Andrejzak

Invited talks of the joint symposium Topological constraints in biological and synthetic soft matter (SYSM)

See SYSM for the full program of the symposium.

SYSM 1.1	Mon	10:00–10:30	Audimax 1	**Interphase Chromatin Undergoes a Local Sol-Gel Transition Upon Cell Differentiation** — •Alexandra Zidovska
SYSM 1.2	Mon	10:30–11:00	Audimax 1	**Topological Tuning of DNA Mobility in Entangled Solutions of Supercoiled Plasmids** — •Jan Smrek, Jonathan Garamella, Rae Robertson-Anderson, Davide Michieletto
SYSM 1.3	Mon	11:15–11:45	Audimax 1	**Dynamics of macromolecular networks under topological and environmental constraints: some outstanding challenges** — •Dimitris Vlassopoulos
SYSM 1.4	Mon	11:45–12:15	Audimax 1	**Supercoiling in a Protein Increases its Stability** — •Joanna Sulkowska, Szymon Niewieczerzał
SYSM 1.5	Mon	12:15–12:45	Audimax 1	**Topology for soft matter photonics** — •Igor Musevic

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen, Roderich Moessner, Frank Pollmann
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert
SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Invited talks of the joint symposium The Physics of CoViD Infections (SYCO)

See SYCO for the full program of the symposium.

SYCO 1.1	Mon	13:30–14:00	Audimax 1	**A Tethered Ligand Assay to Probe SARS-CoV-2:ACE2 Interactions** — Magnus Bauer, Sophia Gruber, Adina Hausch, Lukas Milles, Thomas Nicolaus, Leonard Schendel, Pilar Lopez Navajas, Erik Procko, Daniel Lietha, Rafael Bernadi, Hermann Gaub, •Jan Lipfert
SYCO 1.2	Mon	14:00–14:30	Audimax 1	**From molecular simulations towards antiviral therapeutics against COVID-19** — •Rebecca Wade
SYCO 1.3	Mon	14:45–15:15	Audimax 1	**The physical phenotype of blood cells is altered in COVID-19** — Markéta Kubánková, Martin Kräter, Bettina Hohberger, •Jochen Guck
SYCO 1.4	Mon	15:15–15:45	Audimax 1	**Extended lifetime of respiratory droplets in a turbulent vapor puff and its implications on airborne disease transmission** — •Detlef Lohse, Kai Leong Chong, Chong Shen Ng, Naoki Hori, Morgan Li, Rui Yang, Roberto Verzicco
SYCO 1.5	Mon	15:45–16:15	Audimax 1	**Beyond the demographic vaccine distribution: Where, when and to whom should vaccines be provided first?** — •Benno Liebchen, Jens Grauer, Fabian Schwarzendahl, Hartmut Löwen

Invited talks of the joint symposium Amorphous materials: structure, dynamics, properties (SYAM)

See SYAM for the full program of the symposium.

SYAM 1.1	Tue	13:30–14:00	Audimax 1	**Glassy dynamics of vitrimers** — •Liesbeth Janssen
SYAM 1.2	Tue	14:00–14:30	Audimax 1	**Liquid-Liquid Phase Transition in Thin Vapor-Deposited Glass Films** — •Zahra Fakhraai
SYAM 1.3	Tue	14:30–15:00	Audimax 1	**Connection between structural properties and atomic motion in ultraviscous metallic liquids close to the dynamical arrest** — •Beatrice Ruta, Nico Neuber, Isabella Gallino, Ralf Busch
SYAM 1.4	Tue	15:15–15:45	Audimax 1	**Signatures of the spatial extent of plastic events in the yielding transition in amorphous solids** — •Celine Ruscher, Daniel Korchinski, Joerg Rottler
SYAM 1.5	Tue	15:45–16:15	Audimax 1	**Constitutive law for dense agitated granular flows: from theoretical description to rheology experiment** — •Olfa D'Angelo, W. Till Kranz

Invited talks of the joint symposium Facets of many-body quantum chaos (SYQC)

See SYQC for the full program of the symposium.

SYQC 1.1	Tue	13:30–14:00	Audimax 2	**Holographic interpretation of SYK quantum chaos** — •Alexander Altland
SYQC 1.2	Tue	14:00–14:30	Audimax 2	**Non-Fermi liquids and the lattice** — •Sean Hartnoll

SYQC 1.3	Tue	14:30–15:00	Audimax 2	**Dual-unitary circuits: non-equilibrium dynamics and spectral statistics** — •Bruno Bertini
SYQC 1.4	Tue	15:15–15:45	Audimax 2	**Post-Ehrenfest many-body quantum interferences in ultracold atoms** — •Steven Tomsovic
SYQC 1.5	Tue	15:45–16:15	Audimax 2	**Dynamics in unitary and non-unitary quantum circuits** — •Vedika Khemani

Invited talks of the joint symposium Advanced neuromorphic computing hardware: Towards efficient machine learning (SYNC)

See SYNC for the full program of the symposium.

SYNC 1.1	Wed	10:00–10:30	Audimax 1	**Equilibrium Propagation: a Road for Physics-Based Learning** — •Damien Querlioz
SYNC 1.2	Wed	10:30–11:00	Audimax 1	**Machine Learning and Neuromorphic Computing: Why Physics and Complex Systems are Indispensable** — •Ingo Fischer
SYNC 1.3	Wed	11:00–11:30	Audimax 1	**Photonic Tensor Core Processor and Photonic Memristor for Machine Intelligence** — •Volker Sorger
SYNC 1.4	Wed	11:45–12:15	Audimax 1	**Material learning with disordered dopant networks** — •Wilfred van der Wiel
SYNC 1.5	Wed	12:15–12:45	Audimax 1	**In-memory computing with non-volatile analog devices for machine learning applications** — •John Paul Strachan

Prize talks of the joint Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

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

See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Invited talks of the joint symposium Diversity on the Device Scale (SYHN)

See SYHN for the full program of the symposium.

SYHN 1.1	Thu	10:00–10:30	Audimax 1	**Scaling behavior of stiffness and strength of hierarchical network nanomaterials** — •Shan Shi
SYHN 1.2	Thu	10:30–11:00	Audimax 1	**Functional and programmable DNA nanotechnology** — •Laura Na Liu
SYHN 1.3	Thu	11:15–11:45	Audimax 1	**Multivalent nanoparticles for targeted binding** — •Stefano Angioletti-Uberti
SYHN 1.4	Thu	11:45–12:15	Audimax 1	**Programming Nanoscale Self-Assembly** — •Oleg Gang
SYHN 1.5	Thu	12:15–12:45	Audimax 1	**Achieving Global Tunability via Local Programming of a Structure's Composition** — •Jochen Mueller

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

See SYCE for the full program of the symposium.

SYCE 1.1	Thu	13:30–14:00	Audimax 1	**The challenge of anthropogenic climate change - Earth system analysis can guide climate mitigation policy** — •Matthias Hofmann
SYCE 1.2	Thu	14:00–14:30	Audimax 1	**Towards a carbon-free energy system: Expectations from R&D in renewable energy technologies** — •Bernd Rech, Rutger Schlatmann
SYCE 1.3	Thu	14:30–15:00	Audimax 1	**Decarbonizing the Heating Sector - Challenges and Solutions** — •Florian Weiser
SYCE 1.4	Thu	15:15–15:45	Audimax 1	**A carbon-free Energy System in 2050: Modelling the Energy Transition** — •Christoph Kost, Philip Sterchele, Hans-Martin Henning
SYCE 1.5	Thu	15:45–16:15	Audimax 1	**The transition of the electricity system to 100% renewable energy: agent-based modeling of investment decisions under climate policies** — •Kristian Lindgren

Invited talks of the joint symposium Active nematics: From 2D to 3D (SYAN)

See SYAN for the full program of the symposium.

SYAN 1.1	Fri	10:00–10:30	Audimax 1	**Corrugated patterns made from an active nematic sheet** — •Anis Senoussi, Shunichi Kashida, Raphaël Voituriez, Jean-Christophe Galas, Ananyo Maitra, Estevez-Torres André
SYAN 1.2	Fri	10:30–11:00	Audimax 1	**Wrinkling instability in 3D active nematics** — •Isabella Guido
SYAN 1.3	Fri	11:15–11:45	Audimax 1	**Three-dimensional active nematic defects and their energetics** — •Miha Ravnik
SYAN 1.4	Fri	11:45–12:15	Audimax 1	**Liquid-crystal organization of liver tissue** — •Benjamin M Friedrich, Hernan Morales-Navarrete, Andre Scholich, Hidenori Nonaka, Fabian Segovia Miranda, Steffen Lange, Jens Karschau, Yannis Kalaidzidis, Frank Jülicher, Marino Zerial
SYAN 1.5	Fri	12:15–12:45	Audimax 1	**Machine learning active nematic hydrodynamics** — •Vincenzo Vitelli

Sessions

DY 1.1–1.4	Mon	10:00–11:15	H1	**Statistical physics of biological systems (joint session BP/DY)**
DY 2.1–2.7	Tue	10:00–12:15	H6	**Quantum Chaos**
DY 3.1–3.11	Tue	17:30–19:30	P	**Poster Sesssion I: Quantum Chaos and Many-Body Quantum Dynamics**
DY 4.1–4.10	Tue	17:30–19:30	P	**Poster Session II: Nonlinear Dynamics, Simulations and Machine Learning**
DY 5.1–5.15	Tue	17:30–19:30	P	**Poster Session III: Statistical Physics, Complex Fluids and Soft Matter**
DY 6.1–6.8	Wed	10:00–12:45	H3	**Soft Matter (joint session CPP/DY)**
DY 7.1–7.11	Wed	10:00–13:00	H6	**Focus Session: Facets of Many-Body Quantum Chaos (organised by Markus Heyl and Klaus Richter) (joint session DY/TT)**

DY 8.1–8.7	Wed	11:15–13:00	H7	**Quantum Computing (joint session TT/DY)**
DY 9.1–9.4	Wed	13:30–14:45	H6	**Many-Body Quantum Dynamics I (joint session DY/TT)**
DY 10.1–10.4	Wed	15:00–16:30	H6	**Focus session: Nonlinear Dynamics of the Heart I (organized by Markus Bär, Stefan Luther and Ulrich Parlitz)**
DY 11.1–11.6	Thu	10:00–11:30	H2	**Many-Body Quantum Dynamics II (joint session DY/TT)**
DY 12.1–12.5	Thu	11:45–13:00	H2	**Active Matter (joint session DY/BP/CPP)**
DY 13.1–13.7	Thu	13:30–16:15	H2	**Focus session: Nonlinear Dynamics of the Heart II (organized by Markus Bär, Stefan Luther and Ulrich Parlitz)**
DY 14	Thu	18:00–19:00	MVDY	**Mitgliederversammlung Fachverband DY**
DY 15.1–15.4	Fri	10:00–11:00	H2	**Condensed-Matter Simulations augmented by Advanced Statistical Methodologies (joint session DY/CPP)**
DY 16.1–16.5	Fri	11:15–12:30	H2	**Machine Learning in Dynamical Systems and Statistical Physics (joint session DY/BP)**
DY 17.1–17.5	Fri	13:30–15:00	H3	**Theory and Simulation (joint session CPP/DY)**
DY 18.1–18.4	Fri	13:30–16:00	ESS	**Symposium: Synchronization Patterns in Complex Dynamical Networks (organized by Jakub Sawicki, Sabine Klapp, Markus Bär and Jens Christian Claussen) (joint session DY/SOE)**
DY 19.1–19.6	Fri	13:30–15:00	H6	**Transport (joint session TT/DY)**

Annual General Meeting of the Dynamics and Statistical Physics Division

Donnerstag, 30. September 2021 18:00–19:00 MVDY

- Bericht DY Aktivitäten und Entwicklung 2020 - 21
- Planung Frühjahrstagung Regensburg 2022
- Verschiedenes

DY 1: Statistical physics of biological systems (joint session BP/DY)

Time: Monday 10:00–11:15 Location: H1

Invited Talk DY 1.1 Mon 10:00 H1

Physics-Informed Deep Learning for Characterizing Perturbed Cell Growth — •Robert Endres[1], Henry Cavanagh[1], Rob Lind[2], Andreas Mosbach[3], and Gabriel Scalliet[3] — [1]Imperial College London, UK — [2]Syngenta International Research Centre, UK — [3]Syngenta Crop Protection AG, Switzerland

The morphodynamical analysis of cells can be a powerful and cost-effective way of understanding the phenotypic effects of perturbations, but current techniques often only work for stationary cell behaviour. Here, we introduce a novel framework that extends the morphodynamic analysis to nonstationary dynamics during early-stage growth of the soybean rust P. pachyrhizi. At its core, our approach learns the 2-dimensional feature space of cell shape using variational autoencoders from deep learning, and subsequently models how populations of cells develop over this space using two simple differential equations, each capturing complementary aspects of the dynamics with parameters depending on the perturbations. First, a Fokker-Planck model to describe the diffusive development on a Waddington-type energy landscape, providing a global perspective on the dynamics, and second, a cell-mechanical model describing local growth as a persistent random walk. Informative perturbation-dependent parameters are found by fitting simulations to the shape-space embeddings, representing a powerful tool for linking machine-learning and biophysical modelling.

DY 1.2 Mon 10:30 H1

Collisions increase self-diffusion in odd-diffusive systems — •Erik Kalz[1,2], Iman Abdoli[1], Hidde Derk Vuijk[1], Jens-Uwe Sommer[1,2], and Abhinav Sharma[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Institut Theory der Polymere, 01069 Dresden — [2]Technische Universität Dresden, Institut für Theoretische Physik 01069 Dresden

It is generally believed that collisions of particles reduce the self-diffusion coefficient. We show that in odd-diffusive systems, which are characterized by diffusion tensors with anti-symmetric elements, collisions surprisingly can enhance the self-diffusion. In these systems, due to an inherent curving effect, the motion of particles is facilitated, instead of hindered by collisions. We refer to this as an overdamped swing-by effect. Consistent with this we find that the collective diffusion remains unaffected. We demonstrate this counterintuitive behavior in a system of Brownian particles under Lorentz force. Using a geometric model, we theoretically predict a magnetic-field governed crossover from a reduced to an enhanced self-diffusion. The physical interpretation is quantitatively supported by the force-autocorrelation function, which turns negative with increasing magnetic field. Using Brownian dynamic simulations, we show that the predictions are also valid for active chiral particles as another odd-diffusive system.

DY 1.3 Mon 10:45 H1

How is anomalous diffusion compatible with thermodynamics in biophysical systems? — •David Hartich and Aljaz Godec — Mathematical bioPhysics Group, MPI-BPC, Göttingen, Germany

In a finite system driven out of equilibrium by a constant external force the thermodynamic uncertainty relation (TUR) bounds the variance of the conjugate current variable by the thermodynamic cost of maintaining the non-equilibrium stationary state. Here we highlight a new facet of the TUR by showing that it also bounds the time-scale on which a finite system can exhibit anomalous kinetics. In particular, we demonstrate that the TUR bounds subdiffusion in a single file confined to a ring as well as a dragged Gaussian polymer chain even when detailed balance is satisfied. Conversely, the TUR bounds the onset of superdiffusion in the active comb model. Remarkably, the fluctuations in a comb model evolving from a steady state behave anomalously as soon as detailed balance is broken. Our work establishes a link between stochastic thermodynamics and the field of anomalous dynamics that will fertilize further investigations of thermodynamic consistency of anomalous diffusion models.

[1] DH, A. Godec, Phys Rev. Lett. (in press), arXiv:2102.06678.

DY 1.4 Mon 11:00 H1

Maximum likelihood estimates of diffusion coefficients from single-particle tracking experiments — •Jakob Tómas Bullerjahn[1] and Gerhard Hummer[1,2] — [1]Department of Theoretical Biophysics, MPI of Biophysics, Frankfurt am Main, Germany — [2]Institute of Biophysics, Goethe University, Frankfurt am Main, Germany

Single-molecule localization microscopy allows practitioners to locate and track labeled molecules in biological systems. When extracting diffusion coefficients from the resulting trajectories, it is common practice to perform a linear fit on mean-squared-displacement curves. However, this strategy is suboptimal and prone to errors. Recently, it was shown that the increments between the observed positions provide a good estimate for the diffusion coefficient, and their statistics are well-suited for likelihood-based analysis methods. Here, we revisit the problem of extracting diffusion coefficients from single-particle tracking experiments subject to static noise and dynamic motion blur using the principle of maximum likelihood. Taking advantage of an efficient real-space formulation, we extend the model to mixtures of subpopulations differing in their diffusion coefficients, which we estimate with the help of the expectation-maximization algorithm. This formulation naturally leads to a probabilistic assignment of trajectories to subpopulations. We employ the theory to analyze experimental tracking data that cannot be explained with a single diffusion coefficient, and test how well the data conform to the model assumptions. https://doi.org/10.1063/5.0038174

DY 2: Quantum Chaos

Time: Tuesday 10:00–12:15 Location: H6

Invited Talk DY 2.1 Tue 10:00 H6

Local Versus Global Two-Photon Interference in Quantum Networks — •Sonja Barkhofen[1], Thomas Nitsche[1], Syamsundar De[1], Evan Meyer-Scott[1], Johannes Tiedau[1], Jan Sperling[1], Aurél Gábris[2,3], Igor Jex[2], and Christine Silberhorn[1] — [1]Applied Physics, University of Paderborn, Warburger Strasse 100, 33098 Paderborn, Germany — [2]Department of Physics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Brehová 7, 115 19 Praha 1-Stare Mesto, Czech Republic — [3]Wigner Research Centre for Physics, Konkoly-Thege M. út 29-33, H-1121 Budapest, Hungary

We devise an approach to characterizing the intricate interplay between classical and quantum interference of two-photon states in a network, which comprises multiple time-bin modes. By controlling the phases of delocalized single photons, we manipulate the global mode structure, resulting in distinct two- photon interference phenomena for time-bin resolved (local) and time-bucket (global) coincidence detection. This coherent control over the photons' mode structure allows for synthesizing two-photon interference patterns, where local measurements yield standard Hong-Ou-Mandel dips while the global two-photon visibility is governed by the overlap of the delocalized single-photon states. Thus, our experiment introduces a method for engineering distributed quantum interferences in networks.

DY 2.2 Tue 10:30 H6

Interplay between coherent and incoherent decay processes in chaotic systems: the role of quantum interference — •Camilo Alfonso Moreno Jaimes and Juan-Diego Urbina — Regensburg University, Regensburg, Germany

The population decay due to a small opening in an otherwise closed cavity supporting chaotic classical dynamics displays a quantum correction on top of the classical exponential form, a pure manifestation of quantum coherence that acquires a universal form and can be explained by path interference. Being coherent, such enhancement is prone to decoherence effects due to the coupling of the system to an external environment. We study this interplay between incoherent and coherent quantum corrections to decay by evaluating, within a Caldeira-Leggett scenario, off-diagonal contributions to the decoherence functional com-

ing from pairs of correlated classical paths in the time regime where dissipative effects are neglected and decoherence does not affect the classical dynamics, but quantum interference must be accounted for. We find that the competing effects of interference and decoherence lead to a universal nonmonotonic form for the survival probability depending only on the coupling strength and macroscopic parameters of the cavity.

DY 2.3 Tue 10:45 H6

Geometry of complex instability in four-dimensional symplectic maps — •Jonas Stöber and Arnd Bäcker — TU Dresden, Institut für Theoretische Physik

In four-dimensional symplectic maps complex instability of periodic orbits is possible, which cannot occur for the two-dimensional case. We investigate the transition from stable to complex unstable dynamics of a fixed point under parameter variation. The change in the geometry of regular structures is visualized using three-dimensional phase-space slices and in frequency space using the example of two coupled standard maps. The chaotic dynamics is studied using escape time plots and two-dimensional invariant manifolds associated with the complex unstable fixed point. Based on a normal-form description, we investigate the underlying transport mechanism by visualizing the escape paths and the long-time confinement in the surrounding of the complex unstable fixed point.

15 min. break.

DY 2.4 Tue 11:15 H6

Chaos induced by interface produces universal Hong-Ou-Mandel correlations in topological insulators — •Andreas Bereczuk, Juan Diego Urbina, Cosimo Gorini, and Klaus Richter — Institut of Theoretical Physics, University Regensburg, Germany

The celebrated Hong-Ou-Mandel (HOM) effect [1] is a known coherent manifestation of the indistinguishable-distinguishable transition that is experimentally accessible through measurements of the transmission probability for two-body fermionic states propagating through a quantum point contact in electron quantum optics [2]. As shown in [3, 4], universal HOM correlations are visible by substituting the quantum point contact by a chaotic cavity in a mesoscopic regime [3] where universal correlations of the scattering matrix entries at different energies enter. We present here a numerical analysis of this correlators for a HOM setup with normal cavities playing the role of complex beam splitters and edge states of a topologiocal insulator instead of waveguides. Our main observation is the emergence of universal HOM correlations in this setup where chaotic dynamics is driven by the high reflectivity due to mode mismatch at the interfaces.

[1] C. K. Hong, Z. Y. Ou and L. Mandel, Phys. Rev. Lett. 59, 2044 (1987)
[2] E. Bocquillon et al., Annalen der Physik 526, 1 (2014)
[3] J. D. Urbina et al., Phys. Rev. Lett. 116, 100401 (2016)
[4] A. Bereczuk et al., Phys. Rev. E 103, 052209 (2021)

DY 2.5 Tue 11:30 H6

Dirac fermion optics and directed emission from single- and bilayer graphene cavities — •Jule Katharina Schrepfer[1], Szu-Chao Chen[2], Ming-Hao Liu[2], Klaus Richter[3], and Martina Hentschel[4] — [1]Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]National Cheng Kung University, Tainan 70101, Taiwan — [3]Universität Regensburg, 93040 Regensburg, Germany — [4]Technische Universität Chemnitz, 09107 Chemnitz, Germany

High-mobility graphene hosting massless charge carriers with linear dispersion provides a promising platform for electron optics phenomena. Inspired by the physics of dielectric optical micro-cavities where the photon emission characteristics can be efficiently tuned via the cavity shape, we study corresponding mechanisms for trapped Dirac fermionic resonant states in deformed micro-disk graphene billiards and directed emission from those. In such graphene devices a backgatevoltage provides an additional tunable parameter to mimic different effective refractive indices and thereby the corresponding Fresnel laws at the boundaries. Moreover, cavities based on single-layer and double-layer graphene exhibit Klein- and anti-Klein tunneling. Moreover,we find a variety of different emission characteristics depending on the position of the source where charge carriers are fed into the cavites. Combining quantum mechanical simulations with optical ray tracing and a corresponding phase-space analysis, we demonstrate strong confinement of the emitted charge carriers in the mid field of single-layer graphene systems and can relate this to a lensing effect. For bilayer graphene, trapping of the resonant states is more efficient.

DY 2.6 Tue 11:45 H6

Optical microcavities in a ray picture with phase information — •Lukas Seemann — TU Chemnitz

Ray-wave correspondence has proven a useful tool to describe various aspects of optical microcavities, for example the far-field emission of deformed microdisk resonators. However, for more complicated settings such as coupled microcavities, interference effects will become important [1]. To this end we expand the ray description by the phase information and include the phase collected by the light ray along its trajectory [2] into the model. We explore the chances as well as possible limitations of this approach in various examples and investigate to what extent a ray model with phase information can deepen ray-wave correspondence.

[1] J. Kreismann, J. Kim, M. Bosch, M. Hein, S. Sinzinger, and M. Hentschel, Super-directional light emission and emission reversal from micro cavity arrays, Phys. Rev. Res. 1, 033171(1-5) (2019).
[2] M. Hentschel and M. Vojta, Multiple beam interference in a quadrupolar glass fiber, Opt. Lett. 26, 1764-1766 (2001).

DY 2.7 Tue 12:00 H6

Emergent fractal phase in energy stratified random models — •Anton Kutlin and Ivan Khaymovich — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187-Dresden, Germany

We study the effects of partial correlations in kinetic hopping terms of long-range disordered random matrix models on their localization properties. We consider a set of models interpolating between fully-localized Richardson's model and the celebrated Rosenzweig-Porter model (with implemented translation-invariant symmetry). In order to do this, we propose the energy-stratified spectral structure of the hopping term, allowing one to gradually decrease the range of correlations. We show both analytically and numerically that any deviation from the completely correlated case leads to the emergent non-ergodic delocalization in the system unlike the predictions of localization of cooperative shielding. In order to describe the models with correlated kinetic terms, we develop the generalization of the Dyson Brownian motion and cavity approaches basing on stochastic matrix process with independent rank-one matrix increments and examine its applicability to the above set of models

DY 3: Poster Sesssion I: Quantum Chaos and Many-Body Quantum Dynamics

Time: Tuesday 17:30–19:30 Location: P

DY 3.1 Tue 17:30 P

Drift-induced Delocalization Transition in Resonance Channels — •Jan Robert Schmidt, Arnd Bäcker, and Roland Ketzmerick — TU Dresden, Institut für Theoretische Physik, Dresden

In higher-dimensional Hamiltonian systems resonance channels play a prominent role. Transport is typically slow due to Arnold diffusion, leading quantum mechanically to dynamical localization. Resonance channels widen as they approach the chaotic sea. We show that this induces (i) classically a drift and (ii) quantum mechanically leads to delocalization if the drift is strong enough. We propose a scaling of the delocalization transition by a single transition parameter. These phenomena are confirmed in a 4D symplectic map with a large resonance channel.

DY 3.2 Tue 17:30 P

Dynamics of NV centers interacting with background spins — •Lukas Voss and Jürgen Stockburger — Institute for Complex Quantum Systems, Ulm University

The nitrogen vacancy (NV) center in diamond is considered to be one of the most promising physical systems for application in emerging quantum technologies such as quantum sensing and quantum computing [1]. The corresponding protocols are highly sensitive to the interactions of NV centers with either ^{13}C background spins or other NV centers.

The number of spins typically involved is too large for direct methods of propagation (curse of dimensionality). As a remedy, we modify a stochastic jump method for coherent quantum dynamics introduced by Breuer [2], which greatly reduces the dimension of the state space of the propagation (sum vs. product spaces).

We demonstrate this technique for an NV center and several nuclear background spins and find attractive performance characteristics. Further investigations are aimed at clustering a large number of background spins. Treating intra-cluster interactions by unitary propagation while applying the jump approach to inter-cluster interactions will further improve simulation performance.

[1] MW Doherty et al., *Physics Reports* **528**, 1 (2013)
[2] H-P Breuer *Physical Review A* **69**, 122 (2004)

DY 3.3 Tue 17:30 P

Quantum signatures of partial barriers in 4D symplectic maps — •Jonas Stöber, Arnd Bäcker, and Roland Ketzmerick — TU Dresden, Institut für Theoretische Physik

Partial transport barriers in the chaotic sea of Hamiltonian systems restrict classical chaotic transport, as they only allow for a small flux between phase-space regions. Quantum mechanically for 2D symplectic maps one has a universal quantum localizing transition. The scaling parameter is the ratio of flux to the Planck cell of size h, such that quantum transport is suppressed if h is much greater than the flux, while mimicking classical transport if h is much smaller.

In a higher-dimensional 4D map one naively expects that the relevant scaling parameter is the same, but now with a Planck cell of size h squared. We show that due to dynamical localization along resonance channels the localization length modifies the scaling parameter. This is demonstrated for coupled kicked rotors for a partial barrier that generalizes a cantorus to higher dimensions.

DY 3.4 Tue 17:30 P

Enhanced state transfer by complex instability in coupled kicked tops — •Maximilian Kieler and Arnd Bäcker — Technische Universität Dresden, Institut für Theoretische Physik and Center for Dynamics, 01062 Dresden, Germany

By considering coupled kicked tops we provide a mechanism for a fast transfer between two specific states representing bits. This crucially relies on that fact that the semiclassical limit corresponds to a higher-dimensional system which allows for more types of stability of fixed points than the two-dimensional case. Tuning the parameters, the coupled kicked tops have fixed points with complex instability. Quantum mechanically this allows for a rapid transfer between coherent states located at these points, which is much faster than the coexisting dynamical tunneling.

DY 3.5 Tue 17:30 P

Fermionic duality beyond weak coupling: General simplifications of open-system dynamics — •Valentin Bruch[1], Konstantin Nestmann[1], Jens Schulenborg[2], and Maarten Wegewijs[1,3] — [1]Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany and JARA-FIT, 52056 Aachen — [2]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen — [3]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

A large class of fermionic open systems obeys a powerful dissipative analogue of the "symmetry" of hermitian conjugation in closed quantum systems. This *fermionic duality relation* applies to quantum-impurity transport models with strong interactions and hybridization exhibiting many-body and memory effects. Here we extend this relation from the time-nonlocal memory-kernel approach (Nakajima-Zwanzig) to prominent quantum-information inspired approaches in their exact formulation [arXiv:2104.11202]. These include the Kraus-operator decomposition of the dynamical map as well as the time-convolutionless quantum master equation with a time-local generator and generalized Lindblad jump-operators. Whereas in some of these formulations this yields a strong restriction on the involved quantities, in others it can be exploited to partially by-pass nontrivial time-evolution calculations. Fermionic duality also offers new insights into the divisibility and causal structure of the dynamics and applied to nonperturbative semigroup approximations [Phys. Rev. X 11, 021041 (2021)] it provides a new way to construct initial-slip corrections.

DY 3.6 Tue 17:30 P

Quantum dynamics and thermodynamics in nanosystems with strong electronic-vibrational coupling under external driving — •Jakob Bätge[1], Wenjie Dou[2], Amikam Levy[3], and Michael Thoss[1] — [1]Institute of Physics, University of Freiburg, Freiburg, Germany — [2]School of Science, Westlake University, Hangzhou, China — [3]Department of Chemistry, Bar-Ilan University, Ramat-Gan, Israel

The development and optimization of quantum devices increase the interest in dynamics and thermodynamics of systems on the scale of single atoms and molecules. In this contribution, we investigate the nonequilibrium quantum dynamics of a time-dependent driven nanosystem with interacting electronic and vibrational degrees of freedom utilizing the numerically exact hierarchical equations of motion approach for multiple fermionic and bosonic environments [1]. We analyze the role of vibrations in the electronic friction induced by electronic-vibrational coupling and identify the adiabatic and nonadiabatic contributions to thermodynamic quantities[2].

[1] J. Bätge *et al.*, Phys. Rev. B **103**, 235413 (2021)
[2] W. Dou *et al.*, Phys. Rev. B **101**, 184304 (2020)

DY 3.7 Tue 17:30 P

Floquet prethermalization and Rabi oscillations in optically excited Hubbard clusters — •Junichi Okamoto[1,2] and Francesco Peronaci[3] — [1]Institute of Physics, University of Freiburg, Germany — [2]EUCOR Centre for Quantum Science and Quantum Computing, University of Freiburg, Germany — [3]Max Planck Institute for the Physics of Complex Systems, Germany

Floquet engineering is a growing field of study to realize exotic many-body quantum states beyond the conventional material science in equilibrium. The Floquet picture in terms of effective Hamiltonians is valid in the limit of high-frequency drive, where the heating rate is suppressed. In contrast, when the drive frequency is comparable to the energies of the system, the effect of heating is non-negligible, and the analysis becomes intricate. However, even in this case, the existence of quasi-steady states, so-called Floquet prethermal states (FPSs), has been demonstrated, which expands the boundary of Floquet engineering to a realistic drive range. In this work, we have investigated the optically excited Hubbard clusters by exact diagonalization. We show that FPSs emerge not only off resonance but also for resonant excitation, provided a small field amplitude. Notably, FPSs at resonance occur with Rabi oscillations. At stronger fields, thermalization to infinite temperature is observed. We elucidate the origin of the FPSs using time-dependent perturbation theory and the two-site Hubbard model. A finite-size analysis substantiates the main findings.

DY 3.8 Tue 17:30 P

Transmission through three-terminal microwave graphs with orthogonal, unitary and symplectic symmetry — Felipe de Jesús Castañeda-Ramírez[1], Angel M. Martínez-Argüello[2], •Tobias Hofmann[3], Aimaiti Rehemanjiang[3], Moisés Martínez-Mares[1], José A. Méndez-Bermúdez[4], Ulrich Kuhl[5], and Hans-Jürgen Stöckmann[3] — [1]Departamento de Física, Universidad Autónoma Metropolitana-Iztapalapa, Apartado Postal 55-534, 09340 Ciudad de México, Mexico — [2]Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Apartado Postal 48-3, 62210 Cuernavaca, Mor., Mexico — [3]Fachbereich Physik der Philipps-Universität Marburg, D-35032 Marburg, Germany — [4]Instituto de Física, Benemérita Universidad Autónoma de Puebla, Apartado Postal J-48, 72570 Puebla, Pue., Mexico — [5]Université Côte d'Azur, CNRS, Institut de Physique de Nice (INPHYNI), 06108 Nice, France

Transmission measurements through three-port microwave graphs are performed, in analogy to three-terminal voltage drop devices, with orthogonal, unitary, and symplectic symmetry. The terminal used as a probe is symmetrically located between two different chaotic subgraphs of the same mean density of states. Each subgraph is connected to one port, the input and the output, respectively. We find a good agreement with theoretical predictions, provided the effects of dissipation and imperfect coupling to the ports is considered. This extends previous studies using an asymmetric probe position [1].

[1] A. M. Martínez-Argüello et.al, Phys. Rev. B **98** (7) (2018) 075311.

DY 3.9 Tue 17:30 P

Heat transport through a superconducting artificial atom — •Meng Xu, Juergen Stockburge, and Joachim Ankerhold — ICQ and IQST, Ulm University, Germany

Theoretical studies of photonic heat transport and rectification in superconducting platforms play an important role not only in understanding current experimental findings but also in designing and potentially improving future architectures to control heat, for example in circuit Quantum Electrodynamics (cQED). Moreover, fundamental questions regarding signatures of quantum mechanics in thermodynamic properties of devices at nanoscales have not been answered yet and require advanced simulation techniques beyond conventional perturbative treatments

Quantum heat transfer through a generic superconducting set-up consisting of a tunable transmon qubit placed between resonators that are terminated by thermal reservoirs is explored. Applying the numerical exact hierarchical equation of motion (HEOM) approach, steady-state properties are revealed, and experimentally relevant parameter sets are identified. Benchmark results are compared with predictions based on approximate treatments to demonstrate their failure in broad ranges of parameter space. These findings may allow improving future designs for heat control in superconducting devices.

DY 3.10 Tue 17:30 P

Interaction-driven dynamical quantum phase transitions in a strongly correlated bosonic system — •Sebastian Stumper[1], Michael Thoss[1,2], and Junichi Okamoto[1,2] — [1]Institute of Physics, University of Freiburg — [2]EUCOR Centre for Quantum Science and Quantum Computing, University of Freiburg

We investigate the dynamical quantum phase transitions (DQPTs) in the one-dimensional extended Bose-Hubbard model after a sudden quench of the nearest-neighbor interaction strength. We show that interaction-driven DQPTs can appear after quenches between two topologically trivial insulating phases based on extensive matrix-product-states simulations. The threshold value of the quench parameter for the DQPTs does not coincide with the equilibrium phase boundaries, which is contrary to the DQPTs between topologically distinct phases. Furthermore, we define a new set of string and parity order parameters to characterize the dynamics and find a close connection between DQPTs and these order parameters for both types of quenches. Finally, the timescales of DQPTs are also studied, revealing different kinds of power laws for the topological and interaction-driven cases.

DY 3.11 Tue 17:30 P

A particle conserving framework to transport in AC-driven quantum dots contacted to superconducting leads — •Julian Siegl[1], Jordi Pico-Cortes[1,2], and Milena Grifoni[1] — [1]Universität Regensburg — [2]Universidad Autónoma de Madrid

Transport through an interacting quantum dot coupled to superconducting leads and subject to DC and AC-bias is studied within a particle conserving framework. In this formulation, charge conservation during tunneling of an electron out of the dot includes processes where a quasiparticle is destroyed in the superconductor and simultaneously a Cooper pair is created. This possibility gives rise to non vanishing coherences of the density matrix involving Cooper pairs and states with zero or double occupancy in the quantum dot. In the sequential tunneling regime (second order in the tunneling), the *anomalous* contribution to the current due to the coherences is negligible and quasiparticle transport dominates. Here, the combination of AC and DC bias gives rise to stability diagrams whose features cannot be explained within the simple Tien-Gordon theory. At higher orders the coherences are responsible for the supercurrent in the junction.

DY 4: Poster Session II: Nonlinear Dynamics, Simulations and Machine Learning

Time: Tuesday 17:30–19:30 Location: P

DY 4.1 Tue 17:30 P

Memory effects and stochastic forces on a passive particle in an active bath — •Jeanine Shea[1], Friederike Schmid[1], and Gerhard Jung[2] — [1]Johannes Gutenberg University — [2]University of Innsbruck

Implicit models of passive, equilibrium systems have been used for many years to study and understand the physical behavior of these systems. Given the success of understanding equilibrium systems through models, recent studies have focused on mapping non-equilibrium systems onto modified equilibrium models to better understand non-equilibrium behavior. In particular, active systems are non-equilibrium systems which are highly pertinent to biological studies and which exhibit vastly different behavior than strictly passive systems. These distinctive dynamics are not limited to purely active systems, but can also be transferred to passive particles in active systems. As such, the behavior of passive particles immersed in active systems can significantly differ from that in a passive system. We investigate the dissipative and stochastic forces which act on one fundamental example of such a system, that of a colloid in a bath of active particles.

DY 4.2 Tue 17:30 P

Epidemic modeling with delay-differential equations including saturation effects by isolation and contact restriction — •Susanne Kiefer and Edeltraud Gehrig — RheinMain University of Applied Science, Germany

Delay differential equation enable a realistic modeling of epidemics since they allow the inclusion of incubation periods, recovery times or the influence of a quarantine. A systematic modelling of the influence of parameters and their mutual dependence is of high importance when analyzing the behavior of the numbers of infected, susceptible and recovered persons. In this work we present and compare epidemic models with variable delays and saturation parameters. Thereby we consider both, a delay term describing the influence of incubation time as well as a delay for an inclusion of recovery. Our stability analysis and modeling of the temporal behavior allow for a determination of critical regimes where, depending on model approach, a delay may turn the system into instable behavior. A rise in amplitude of the characteristic oscillations shows a strong dependence on delay. This behavior may be controlled by parameters describing quarantine rules. Results of our simulations reveal an influence of parameters describing isolation of infected persons and contact restrictions on the dynamics and particularly on the transition to unstable behavior. A thorough adjustment of contact restriction and isolation may allow to shift the onset of instability and to adjust restriction rules. Thereby the range of control options of each of these parameters critically depends on initial values, infection and recovery rates as well on the delays.

DY 4.3 Tue 17:30 P

Interplay of viscosity and surface tension for ripple formation by external laser melting — •Klaus Morawetz[1,2], Sarah Trinschek[1], and Evgeny Gurevich[1] — [1]Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

A model for ripple formation on liquid surfaces exposed to an external laser or particle beam and a variable ground is developed. Starting from the Navier Stokes equation the coupled equations for the velocity potential and the surface height are derived with special attention to viscosity. Linear stability analysis provides the formation of a damped gravitation wave modified by an interplay between the external beam, the viscosity, and the surface tension. The resulting wavelengths are in the order of the ripples occurring in laser welding experiments hinting to their hydrodynamical origin. The stability due to the periodic time-dependence of the external beam is discussed with the help of Floquet multipliers showing that the ripple formation could be triggered by an external excitation with frequencies in the order of the repetition rate of the laser. The weak nonlinear stability analysis provides ranges where hexagonal or stripe structures can appear. The orientation of stripe structures and ripples are shown to be dependent on the incident angle and a minimal angle is reported. Two models are presented to couple the external current to the gradient of the surface. Numerical simulations confirm the findings. arXiv:2107.02651

DY 4.4 Tue 17:30 P

Observation of phase synchronization and alignment during free induction decay of quantum spins with Heisenberg interactions — •Patrick Vorndamme[1], Heinz-Jürgen Schmidt[2], Christian Schröder[1,3], and Jürgen Schnack[1] — [1]Bielefeld University, 33615 Bielefeld, Germany — [2]Osnabrück University, Barbarastraße 7, 49076 Osnabrück, Germany — [3]Bielefeld Institute for Applied Materials Research, 33619 Bielefeld, Germany

Equilibration of observables in closed quantum systems that are described by a unitary time evolution is a meanwhile well-established phenomenon. Here we report the surprising theoretical observation that spin rings with nearest-neighbor or long-range isotropic Heisenberg interaction not only equilibrate but moreover also synchronize the directions of the expectation values of the individual spins. Here, we observe mutual synchronization of local spin directions in closed systems under unitary time evolution. This synchronization is independent of whether the interaction is ferro- or antiferromagnetic. In our numerical simulations, we investigate the free induction decay of an ensemble of quantum spins by solving the time-dependent Schrödinger equation numerically exactly. The synchronization is very robust against for instance random fluctuations of the Heisenberg couplings and inhomogeneous magnetic fields. Synchronization is not observed with strong enough symmetry-breaking interactions such as the dipolar interaction. We also compare our results to closed-system classical spin dynamics which does not exhibit phase synchronization due to the lack of entanglement. (arxiv:2104.05748)

DY 4.5 Tue 17:30 P

Neural Network-Based Approaches for Multiscale Modelling of Topological Defects — •Kyra Klos[1], Karin Everschor-Sitte[2], and Friederike Schmid[1] — [1]Johannes Gutenberg University, Mainz, Germany — [2]University of Duisburg-Essen, Duisburg, Germany

Topological defects and their dynamics are a heavily researched topic in a wide range of physics fields.[1]

Due to the multiscale character of those defect structures, numerically simulating a large number of them in full microscopic detail gets highly complicated, as the large size of associated deformation fields around each core leads to a complex interaction pattern.

To give a possible insight into the connection between the macroscopic (particle) description of a model with topological defects and the underlying microscopic true structure, the use of neural networks is proposed. Starting with a spin-dynamic simulated microscopic model as input [2,3], a fully convolutional network (FCN)[4] is used to simplify the complex defect structure of the microscopic theory without loss of valuable information. This allows the extraction of the configuration and location of the topological defects.

[1] Mermin, N. D., Rev. Mod. Phys. 51, 591, (1979)
[2] Leoncini, X. et. al., Phys. Rev. E 57(6), 6377, (1998)
[3] Cerruti-Sola, M. et. al., Phys. Rev. E 61(5A), 5171, (2000)
[4] Long, J. et. al., IEEE, 39(4), 640, (2017)

DY 4.6 Tue 17:30 P

Nonlinear dynamics in intra-cavity pumped thin-disk lasers — •Sarah Trinschek, Christian Vorholt, and Ulrich Wittrock — Münster University of Applied Sciences, Germany

For an intra-cavity pumped Yb:YAG thin-disk laser, complex dynamics of the laser output power can be observed. The gain medium of this laser is residing in the resonator of a conventional, diode-pumped Yb:YAG thin-disk laser. We present illustrative experimental results and a detailed analysis of the nonlinear dynamics of the laser in the framework of a rate-equation model. Despite stable continuous-wave pumping, periodic pulse trains and chaotic fluctuations of the optical power of both lasers occur. The dynamics is not driven by external perturbations but arises naturally in this laser system due to cross-saturation effects of the two gain media. The qualitative type of dynamics can be controlled by the resonator length of the diode-pumped laser but the detailed behaviour of the laser is complex and also shows hysteresis and multistability.

DY 4.7 Tue 17:30 P

Quantitative Waveform Sampling on Atomic Scales — Dominik Peller[1], Carmen Roelcke[1], •Lukas Kastner[1], Thomas Buchner[1], Alexander Neef[1], Johannes Hayes[1], Franco Bonafé[2], Dominik Sidler[2], Michael Ruggenthaler[2], Angel Rubio[2,3,4], Rupert Huber[1], and Jascha Repp[1] — [1]University of Regensburg, Germany — [2]MPSD, MPG, Hamburg, Germany — [3]CCQ, Flatiron Institute, New York, USA — [4]UPV/EHU, San Sebastían, Spain

Using a single molecule as a local field sensor, we precisely sample the absolute field strength and temporal evolution of tip-confined near-field transients in a lightware-driven scanning tunnelling microscope. To develop a comprehensive understanding of the extracted atomic-scale nearfield, we simulated the far-to-near-field transfer with classical electrodynamics and include time-dependent density functional theory to validate our calibration and conclusions.

DY 4.8 Tue 17:30 P

Calculating Raman Spectra using Kernel-Based Machine Learning — •Manuel Grumet[1], Karin S. Thalmann[1], Tomáš Bučko[2,3], and David A. Egger[1] — [1]Technical University of Munich, Germany — [2]Comenius University in Bratislava, Slovakia — [3]Slovak Academy of Sciences, Slovakia

First-principles theoretical predictions of Raman spectra are possible using either a phonon-based approach or molecular dynamics (MD) simulations. In both cases, the polarizability tensor of the system, α, is the central quantity. Specifically, the Raman spectrum is obtained from Fourier-transformed velocity autocorrelation functions (VACs) of tensor invariants of α in the MD method [1]. This requires a large number of evaluations of α and thus leads to high computational cost.

We use kernel-based machine learning (ML) to reduce the number of polarizability calculations needed. In this approach, a subset of all configurations serves as a training data set, and polarizabilities for all other configurations are predicted using ML methods. In particular, we obtain the polarizabilites using kernel ridge regression with descriptors based on the atomic neighbourhood density around each atom [2,3].

We apply these methods to a number of test systems, consisting of small molecules and simple solids. We compare different descriptors with regard to the size of the training data set required to obtain accurate predictions for polarizabilties and Raman spectra.

[1] M. Thomas et al., Phys. Chem. Chem. Phys. **15**, 6608 (2013)
[2] N. Raimbault et al., New J. Phys. **21**, 105001 (2019)
[3] A. P. Bartók et al., Phys. Rev. B **87**, 184115 (2013)

DY 4.9 Tue 17:30 P

Machine learning generators of open system Lindblad dynamics — •Francesco Carnazza[1], Dominik Zietlow[2], Federico Carollo[1], Sabine Andergassen[1], Georg Martius[2], and Igor Lesonovsky[1,3] — [1]Institut für Theoretische Physik and Center for Quantum Science, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany — [2]Max Planck Institute for Intelligent Systems, Max-Planck-Ring 4, 72076 Tübingen, Germany — [3]School of Physics and Astronomy, University of Nottingham, Nottingham, NG7 2RD, UK

In recent years artificial neural network methods have established themselves as a versatile tool to encode the state of both closed and open quantum systems. We are interested in the ques-

tion whether they can learn the generator of an effective open quantum dynamics which governs a small system of interest that is embedded within a larger one (Paolo Mazza et al. 2020 https://doi.org/10.1103/PhysRevResearch.3.023084). The model we consider is a spin chain where the system of interest is formed by two spins which are coupled to a "bath" consisting of the rest of the chain. The whole chain is evolved according to an transverse field Ising Hamiltonian. From the reduced density matrix, obtained by tracing out the bath degrees of freedom, the two-body correlations are determined, which are subsequently used to train the network. A simple architecture is adopted in order to have the possibility to "look inside" the network and to see whether the learned dynamics is indeed governed by a time-local Lindblad generator.

DY 4.10 Tue 17:30 P

Modelling a highly adaptive, nonlinear acoustic sensor — •Philipp Hövel[1], Thomas Meurer[2], Martin Ziegler[3], and Claudia Lenk[3] — [1]University College Cork, Ireland — [2]Kiel University, Germany — [3]Technische Universität Ilmenau, Germany

Hearing is a remarkable sense both in terms of physiology and signal processing. In biology, hearing exhibits amazing sensing properties, in particular for low-volume sounds and noisy environments, which is known as the "cocktail party effect". For many state-of-the-art technological implementations, speech recognition remains a challenging task in these hard-to-hear situations and varying surroundings.

In this contribution, we present a mathematical model of a novel, adaptive, bio-inspired acoustic sensor with integrated signal processing functionality, whose sensing and processing properties can be widely tuned using real-time feedback. We show that dynamical switching between linear and nonlinear characteristics improves detection of signals in noisy conditions, increases the dynamic range of the sensor, and enables adaptation to changing acoustic environments. We demonstrate that the dynamical switching can be attributed to a Hopf bifurcation, and its dependence of sensor and feedback parameters is validated in experiments, and highlight the applicability and conceptual advantages of the acoustic sensor.

DY 5: Poster Session III: Statistical Physics, Complex Fluids and Soft Matter

Time: Tuesday 17:30–19:30 Location: P

DY 5.1 Tue 17:30 P

Correlational entropy by nonlocal quantum kinetic theory — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

The nonlocal kinetic equation unifies the achievements of the transport in dense quantum gases with the Landau theory of quasiclassical transport in Fermi systems. Large cancellations in the off-shell motion appear which are hidden usually in non-Markovian behaviors [1]. The remaining corrections are expressed in terms of shifts in space and time that characterize the non-locality of the scattering process [2]. In this way quantum transport is possible to recast into a quasi-classical picture [3]. The balance equations for the density, momentum, energy and entropy include besides quasiparticle also the correlated two-particle contributions beyond the Landau theory [4]. The medium effects on binary collisions are shown to mediate the latent heat, i.e., an energy conversion between correlation and thermal energy. For Maxwellian particles a sign change of the latent heat is reported at a universal ratio of scattering length to the thermal De Broglie wavelength. This is interpreted as a change from correlational heating to cooling [5]. [1] Ann. Phys. 294 (2001) 135, [2] Phys. Rev. C 59 (1999) 3052, [3] "'Interacting Systems far from Equilibrium -Quantum Kinetic Theory"' Oxford University Press, (2017) ISBN 9780198797241, [4] Phys. Rev. E 96 (2017) 032106, [5] Phys. Rev. B 97 (2018) 195142

DY 5.2 Tue 17:30 P

Toolbox for quantifying memory in dynamics along reaction coordinates — Alessio Lapolla and •Aljaz Godec — Mathematical bioPhysics Group, Max Planck Institute for Biophysical Chemistry

Memory effects in time series of experimental observables are ubiquitous and may have important consequences for the interpretation of kinetic data. They may even affect the function of biomolecular nanomachines such as enzymes. We propose a set of complementary methods for quantifying conclusively the magnitude and duration of memory in a time series of a reaction coordinate [1]. The toolbox is general, easy to use, and does not rely on any underlying microscopic model. As a proof of concept we apply it to the analysis of memory in the dynamics of the end-to-end distance of the analytically solvable Rouse-polymer model, an experimental time series of extensions of a single DNA hairpin measured by optical tweezers, and the fraction of native contacts in a small protein probed by atomistic molecular dynamics simulations.

[1] A. Lapolla and A. Godec, Phys. Rev. Research 3, L022018 (2021)

DY 5.3 Tue 17:30 P

Depinning of confined colloidal dispersions under oscillatory shear — •Marcel Hülsberg and Sabine H.L. Klapp — ITP, Technische Universität Berlin, Germany

Strongly confined colloidal dispersions under shear exhibit a variety of dynamical phenomena, including a depinning transition similar to single particles that are driven over a periodic substrate potential [1].

Here, we investigate the depinning behavior of these systems under pure oscillatory shearing with shear rate $\dot{\gamma}(t) = \dot{\gamma}_0 \cos(\omega t)$, as it is a common scenario in rheological experiments [2].

The colloids' depinning behavior is assessed from a microscopic level based on particle trajectories, which are obtained from overdamped Brownian Dynamics simulations. The numerical approach is complemented by an analytic one based on a single-particle model in the limit of weak driving.

Investigating a broad spectrum of shear rate amplitudes $\dot{\gamma}_0$ and frequencies ω, we observe complete pinning as well as temporary depinning behaviour. We discover that temporary depinning occurs for shear rate amplitudes above a frequency-dependent critical amplitude $\dot{\gamma}_0^{\mathrm{crit}}(\omega)$, for which we attain a functional expression. This allows us to identify the dominant system-intrinsic time scale that dictates the scaling behavior of $\dot{\gamma}_0^{\mathrm{crit}}$ with driving frequency ω.

Finally, we discuss the connection between depinning and structural changes in the system.

[1] S. Gerloff and S.H.L. Klapp, Phys. Rev. E **94**(6), 062605 (2016)
[2] J.M. Brader, et al., Phys. Rev. E **82**(6), 061401 (2010)

DY 5.4 Tue 17:30 P

Emergence of collective motion in two-dimensional colloidal systems with delayed feedback — •Robin A. Kopp and Sabine H. L. Klapp — ITP, TU Berlin, Berlin, Germany

In recent years, delayed feedback (dFB) in colloidal systems has become an active and promising field of study [1,2,3], 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. To this end we perform overdamped Brownian dynamics simulations, where the particles interact through a Weeks-Chandler-Andersen (WCA) potential. Furthermore, each particle is subject to a Gaussian, repulsive feedback potential (cf. [1]), that depends on the difference of the particle position at the current time, $\mathbf{r}_i(t)$ and the particle position at an earlier time, $\mathbf{r}_i(t - \tau_{\mathrm{delay}})$. We observe the emergence of collective motion characterized by a nonzero mean velocity. After quantitatively studying this phenomenon, we also provide a possible explanation combining single-particle and mean-field-like effects.

[1] S. Tarama, S. U. Egelhaaf, and H. Löwen, Physical Review E **100**, 022609 (2019)
[2] R. Gernert and S. H. L. Klapp, Physical Review E **92**, 022132 (2015)
[3] S. A. M. Loos, and S. H. L. Klapp, Scientific Reports **9**, 2491 (2019)

DY 5.5 Tue 17:30 P

Brownian magneto-gyrator as a tunable microengine — •Iman Abdoli[1], René Wittmann[2], Joseph Michael Brader[3], Jens-Uwe Sommer[1,4], Hartmut Löwen[2], and Abhinav Sharma[1,4] — [1]Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, Dresden, 01069, Germany — [2]Institut für Theoretische

Physik II, Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Düsseldorf, 40225, Germany — [3]Department de Physique, Université de Fribourg, CH-1700 Fribourg, Switzerland — [4]Technische Universität Dresden, Institut für Theoretische Physik, Dresden, 01069, Germany

A Brownian particle performs gyrating motion around a potential energy minimum when subjected to thermal noises from two different heat baths. Here, we propose a magneto-gyrator made of a single charged Brownian particle that is steered by an external magnetic field. Key properties, such as the direction of gyration, the torque exerted by the engine on the confining potential and the maximum power delivered by the microengine can be tuned by varying the strength and direction of the applied magnetic field. Further tunability is obtained with a potential that couples the spatial degrees of freedom. We show that in this generic scenario, the microengine can be stalled and even reversed by the magnetic field. Finally, we highlight a property of the magneto-gyrator that has no counterpart in the overdamped approximation–the heat loss from the hot to cold bath requires explicit knowledge of the mass of the particle. Consequently, the efficiency of the microengine is mass-dependent even in the overdamped limit.

DY 5.6 Tue 17:30 P

Broadband frequency filters with quantum dot chains — •Tilmann Ehrlich[1] and Gernot Schaller[1,2] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany

Two-terminal electronic transport systems with a rectangular transmission can violate standard thermodynamic uncertainty relations. This is possible beyond the linear response regime and for parameters that are not accessible with rate equations obeying detailed-balance. Looser bounds originating from fluctuation theorem symmetries alone remain respected. We demonstrate that optimal finite-sized quantum dot chains can implement rectangular transmission functions with high accuracy and discuss the resulting violations of standard thermodynamic uncertainty relations as well as heat engine performance.

[1] arXiv:2103.04322, to appear in PRB

DY 5.7 Tue 17:30 P

Cosmological and Elementary Particles Explained by Phase Transitions Derived by Quantum Gravity — •Hans-Otto Carmesin — Gymnasium Athenaeum, Harsefelder Straße 40, 21680 Stade — Studienseminar Stade, Bahnhofstr. 5, 21682 Stade — Universität Bremen, Fachbereich 1, Postfach 330440, 28334 Bremen

In the early universe, the density was very high. As a consequence, there occurred gravitational instabilities and corresponding dimensional phase transitions, see Carmesin, Hans-Otto (March 2021): Quanta of Spacetime Explain Observations, Dark Energy, Graviton and Nonlocality. Berlin, Dr. Köster Verlag. These transitions are very robust, as they occur in three very different physical systems.

Based on the quantum states corresponding to these dimensional transitions, we derive many excitation modes that include the formation of neutrinos, of the Higgs boson, of the quanta of dark energy, and of many novel elementary particles, see Carmesin, Hans-Otto (August 2021): Cosmological and Elementary Particles Explained by Quantum Gravity. Berlin, Dr. Köster Verlag. These particles range form the Planck scale to the lightest particles, and so they solve the hierarchy problem of particle physics.

All results are derived by quantum gravity and are in precise accordance with observation. I emphasize that the only numerical input used in my theory is the present day time after Big Bang combined with the universal constants G, c, k_B and h.

DY 5.8 Tue 17:30 P

Dimensional Phase Transitions of a Bose Gas in the Early Universe — •Paul Sawitzki[1] and Hans-Otto Carmesin[1,2,3] — [1]Gymnasium Athenaeum, Harsefelder Straße 40, 21680 Stade — [2]Studienseminar Stade, Bahnhofstr. 5, 21682 Stade — [3]Universität Bremen, Fachbereich 1, Postfach 330440, 28334 Bremen

In the early universe, the density was very high. As a consequence, there occurred gravitational instabilities and corresponding dimensional phase transitions, see Carmesin, Hans-Otto (March 2021): Quanta of Spacetime Explain Observations, Dark Energy, Graviton and Nonlocality. Berlin, Dr. Köster Verlag. These transitions are very robust, as they occur in three very different physical systems. Here we derive these transitions for the case of a Bose gas.

These transitions are essential for various fields of cosmology, including the so-called era of 'cosmic inflation' and the solution of the horizon problem.

All results are derived by quantum gravity and are in precise accordance with observation. We emphasize that the only numerical input used in the theory is the present day time after Big Bang combined with the universal constants G, c, k_B and h.

DY 5.9 Tue 17:30 P

Diagrammatic expansion of the two-point effective action around non-Gaussian theories — •Tobias Kühn and Frédéric van Wijland — Laboratoire Matière et Systèmes Complexes, Université de Paris

Consider a many-body problem, such as one involving interacting spins, particles or the time series of a random signal, of which we know the corresponding one- and two-point correlation functions. We suppose that the distribution of the spin values (or particle positions,...) is written in a Boltzmann form with a Hamiltonian possessing one- and two-body interactions only. How does one choose the corresponding couplings so that the distribution generates the prescribed statistics? This so-called inverse problem is conveniently described by the second Legendre transform of the cumulant-generating function, the two-point effective action, whose arguments are means and correlations. The couplings we seek for are then explicitly given by its derivatives. Weak correlation approximations have been proven useful to compute the two-point effective action (Sessak & Monasson 2009). As long as the one-body problem is described by independent Gaussian distributions, they can be routinely derived using diagrammatic methods dating back to Feynman, Luttinger and Ward. Here we explain how similar diagrammatics can be extended to the case in which the one-body problem is not of a Gaussian nature. We discuss how this can prove useful in inference problems pertaining to neuroscience and other complex systems. Another possible application is the derivation of mean-field theories self-consistently taking into account pairwise correlations.

DY 5.10 Tue 17:30 P

Charged Liquid Bridges — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

A new solution of a charged catenary is presented which allows to determine the static and dynamical stability conditions where charged liquid bridges are possible. The creeping height, the bridge radius and length as well as the shape of the bridge is calculated showing an asymmetric profile in agreement with observations. The flow profile is calculated from the Navier Stokes equation leading to a mean velocity which combines charge transport with neutral mass flow and which describes recent experiments on water bridges. The velocity profile in a water bridge is reanalyzed. Assuming hypothetically that the bulk charge has a radial distribution, a surface potential is formed that is analogous to the Zeta potential. The Navier*Stokes equation is solved, neglecting the convective term; then, analytically and for special field and potential ranges, a sign change of the total mass flow is reported caused by the radial charge distribution. [Water 9 (2017) 353, Phys. Rev. E 86 (2012) 026302, errata Phys. Rev. 86 (2013) 069904, AIP Advances 2 (2012) 022146-1-6]

DY 5.11 Tue 17:30 P

Ornstein-Zernike relation in hypergraphs — •Christian Faber[1,2,3], Till Kranz[2,3], and Matthias Sperl[3,2] — [1]Jülich Supercomputing Centre, FZ Jülich — [2]Institut für Theoretische Physik, Uni Köln — [3]Institut für Materialphysik im Weltraum, DLR Köln

The pair correlation function is an important input to describe equilibrium phase transitions and the glass transitions [1]. An Ornstein-Zernike relation can be used to represent the pair correlation function in a form that is easy to approximate and that allows an intuitive representation in terms of graphs [2]. However, this graphical representation is limited to pairwise interactions between particles and recent analyses show that some systems, such as foams, cannot be adequately represented with pair interactions [3]. To be able to specify a meaningful Ornstein-Zernike relation for such systems, we have started from scratch and have introduced hypergraphs for multi-body interactions. With these we are able to represent the Ornstein-Zernike relation for multi-body interactions and to give a graphical meaning to the individual terms. We will discuss the similarities and differences between the relation for pair- and for multi-body interactions.

[1] W. Götze, *Zeitschrift f. Physik B Condensed Matter* **60**, 2 (1985).
[2] M. Wortis, "Linked Cluster Expansion" in *Phase Transitions and Critical Phenomena*, C. Domb, M.S. Green, Eds. (Academic Press, London, 1974), vol. 3.
[3] G. Ginot, R. Höhler, S. Mariot, A. Kraynik, W. Drenckhan, *Soft Matter* **15.22**, 4570-4582 (2019).

DY 5.12 Tue 17:30 P

Phase behaviour of a generalized chiral Lebwohl-Lasher model — •Anja Kuhnhold and Philipp Elsässer — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

The Lebwohl-Lasher (LL) model is a simple model to study the isotropic-nematic (IN) transition of liquid-crystalline systems. Particles are described by unit vectors that sit on a simple cubic lattice and only interact with nearest neighbours; the interaction potential has a minimum for parallel orientation of the particles' axes, which drives the IN transition.

Fish and Vink generalized the LL model so that the sharpness of the potential can be tuned and with that the type of phase transition in the 2D limit [1]. Memmer et al. added a chiral interaction to the LL model. They studied the resulting cholesteric phase (where the orientation of particles is parallel within a layer but is rotated between layers) and its behaviour when confined between aligning surfaces [2]. We combine both extensions to the generalized chiral Lebwohl-Lasher model and study the isotropic-cholesteric transition depending on the sharpness parameter, the chirality, and the dimensionality of the system. We use a Wang-Landau Monte-Carlo method to simulate the system and apply finite-size scaling to identify the type of phase transitions.

[1] J.M. Fish, R.L.C. Vink, PRE **81**, 021705 (2010).
[2] R. Memmer, O. Fliegans, PCCP **5**, 558 (2003).

DY 5.13 Tue 17:30 P

Microsecond XPCS on soft matter probed at the European XFEL — •Francesco Dallari and Felix Lehmkühler — Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany

Many soft-matter systems are composed of nanoparticles or macromolecules dispersed in water. The characteristic time at the relevant length-scales of few nanometers falls therefore in the (sub)microsecond time-scales, making the measurement of the dynamical properties for these system an extremely challenging (often impossible) task at third generation synchrotron light sources. With the recent development of hard X-ray free electron lasers (XFELs) and fourth generation light sources, time-resolved experiments in this time- and length-scale regimes have become accessible. Here we present the first results on prototypical charge-stabilized silica nanoparticles dispersed in water both in diluted [1] and concentrated [2] systems. Tuning the pulse fluence we are able to probe and describe with thermodynamical models the diffusion properties in stationary systems and in systems driven by the XFEL pulses.

Bibliography:

[1] F. Lehmkühler, F. Dallari, A. Jain, et al. (2020). PNAS, 117, 24110-24116. https://doi.org/10.1073/pnas.2003337117
[2] F. Dallari, ,A. Jain, F. Lehmkühler, et al. (2021). IUCrJ 8, https://doi.org/10.1107/S2052252521006333.

DY 5.14 Tue 17:30 P

Efficient Event-Driven Simulation of the Bubbling Instability in a Fluidised Bed — Raphael Biertz[1], •Till Kranz[1,2], and Matthias Sperl[2,1] — [1]Institut für Theoretische Physik, Uni Köln — [2]Institut für Materialphysik im Weltraum, DLR Köln

Two-phase flows, comprised of granular particles and an interstitial molecular fluid occur in many places in nature and industry. The prototypical setup for this kind of complex fluid is a fluidised bed. At sufficient fluidisation flow rates, the particulate phase displays a bubbling instability with close packed and very dilute regions [1].

While pure granular fluids are efficiently simulated by event-driven molecular dynamics algorithms, the two-phase flow problem is still a numerical challenge. Here, we discuss that an implicit model of the fluidising fluid in combination with a event-driven approach for the particles [2] can faithfully capture the bubbling instability [3].

[1] Jackson, R., *The Dynamics of Fluidized Particles*, Cambridge University Press, 2000
[2] Fiege, A., Zippelius, A., J. Phys.: Conf. Ser. **759**, 012001 (2016)
[3] Biertz, R., Sperl, M., Kranz, W. T., in preparation

DY 5.15 Tue 17:30 P

Topological optimization of microfluidic Tesla valves for applications with low Reynold numbers — •Sebastian Bohm[1], Hai Binh Phi[2], Ayaka Moriyama[3], and Erich Runge[1] — [1]TU Ilmenau, FG Theoretische Physik I, DE — [2]TU Ilmenau, FG Mikrosystemtechnik, DE — [3]Carleton College, Physics Department, USA

Passive Tesla valves represent a promising method for rectifying flows in microfluidic systems because no moving parts are needed. The efficiency of the valves is characterised by the diodicity which can be defined as the pressure drop ratio of the forward and the reverse flow direction. To obtain efficient valve designs, topological optimization has proven to be a particularly suitable method [1]. The challenge is the dependency of the diodicity on the Reynolds number. Normally, the valves are only efficient at Reynolds numbers much greater than 100. In microfluidics, Reynolds numbers are usually very low, which hitherto limits the applicability of Tesla valves. Therefore a novel approach for the topological optimization of valves that work at very small Reynolds numbers is presented: To ensure that the optimization yields meaningful designs, a customized objective function is introduced and a multi-stage optimization procedure is used. In addition, a method is presented to optimize the diodicity over a given range of Reynolds numbers simultaneously. The resulting valves achieve a diodicity of up to 2 already at Reynolds numbers smaller than 20. The simulated predictions are in close agreement to experimental results.

[1] S. Lin et al., *Topology Optimization of Fixed-Geometry Fluid Diodes*, J. Mech. Des., 137 **(8)**, (2015)

DY 6: Soft Matter (joint session CPP/DY)

Time: Wednesday 10:00–12:45 Location: H3

Invited Talk DY 6.1 Wed 10:00 H3

Chemically Fueled Out-Of-Equilibrium Self-Assemblies and Autonomous Material Systems — •Andreas Walther — Department of Chemistry, University of Mainz

Living self-organizing systems operate far-from-equilibrium and maintain functions by constant energy dissipation in feedback-regulated adaptive steady states. In stark contrast, man made self-assemblies are typically oriented towards equilibrium or deep metastable states.

Some of the next steps in self-assembling systems are to approach multicomponent co-assembling systems, and to master temporal behavior as well as complex adaptation mechanisms. The latter require new types of internal control mechanisms, such as kinetic control over opposing reactions (built-up/destruction), the integration of feedback mechanisms, or the use of energy dissipation to sustain structures only as long as a chemical fuel is available. This ultimately goes along with a transition towards out-of-equilibrium complex systems, in which multiple components self-assemble dynamically in a non-linear and adaptive fashion.

In this talk I will present two conceptual pathways towards out-of-equilibrium systems, (i) driven environments and (ii) driven structures, which allow to program self-assemblies and materials with lifetimes and programmable steady state dynamics using feedback mechanisms and conversion dynamics of chemical fuels. This will be showcased for different self-assembling systems (polymers, peptides, DNA), and the connection to hydrogels and photonic materials demonstrates possibilities for new horizons in materials science.

DY 6.2 Wed 10:30 H3

UV-light printing on APTES functionalized SiO2 surfaces: New approach for nanoparticle assembly — •Sergii Snegir[1], Olivier Plichery[2], Thomas Huhn[1], and Elke Scheer[1] — [1]University of Konstanz, Konstanz, Germany — [2]INSP, Sorbonne University, France

The 3-Aminopropyl)trimethoxysilane (APTES) terminated SiO2 surface allows creating self-assembled monolayers (SAMs) of gold nanoparticles (AuNPs). However, further functionalization of AuNPs with thiol-containing molecules leads to their strong aggregation due

to the appearance of uncompensated dipole moments on the AuNP. Therefore, we developed a UV-light fixation method, which anchors AuNPs on their initial positions on the APTES surface prior to the process of AuNP functionalization. Herein, we present detailed studies of the passivation efficiency as the function of UV light wavelength, time of exposure, the concentration of O2, N2, O3 gases (1). We have found that the combination of O3 and UV light under ambient atmospheric conditions lead to complete passivation of APTES terminated glass already after 2 min of UV exposure (26.1 mW/cm2). We have tested also the possibility to use the UV-light passivation for printing on APTES terminated surfaces by using different chromium masks. With this method, we can create SAMs of AuNP with different geometry and size (resolution limit several um) on a SiO2 surface (glass/quartz/silicon). 1. S.Snegir, T.Huhn,J. Boneberg, S.Haus, O.Pluchery, E.Scheer, J.Phys.Chem.C, 2020,124(35), 19259-19266.

DY 6.3 Wed 10:45 H3

In situ GISAXS analysis of printed hybrid diblock copolymer thin films containing mixed magnetic nanoparticles — •Christopher Everett[1], Xinyu Jiang[1], Manuel Scheel[1], Huaying Zhong[1], Martin Bitsch[2], Martina Plank[3], Markus Gallei[2], Matthias Schwartzkopf[4], Stephan V. Roth[4,5], and Peter Müller-Buschbaum[1,6] — [1]TU München, Physik-Department, LS Funktionelle Materialien, Garching, Germany — [2]Saarland University, LS Polymer Chemistry, Saarbrücken, Germany — [3]TU Darmstadt, Ernst-Berl-Institut, Darmstadt, Germany — [4]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [5]KTH Royal Institute of Technology, Stockholm, Sweden — [6]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Garching, Germany

Diblock copolymer (DBC) thin films that form periodic nanostructures are appropriate scaffolds for magnetic nanoparticles (NPs) and have potential for a variety of applications such as highly functional magnetic sensors and in high-density magnetic data storage. In this investigation, ultra-high molecular weight PS-b-PMMA films are used as templates for both ferrimagnetic magnetite NP and ferromagnetic Ni NPs. The thin films, containing up to 6 wt% NPs, are fabricated by a slot-die coating technique and the morphological evolution of the films during the deposition and drying process is monitored in situ with grazing incidence small-angle X-ray scattering (GISAXS). The dry thin films are subjected to solvent vapor annealing and ordered nanostructured hybrid films are obtained. Using a SQUID magnetometer, the resulting magnetic properties are measured.

15 min. break

Invited Talk DY 6.4 Wed 11:15 H3

The quest for robust superhydrophobic surfaces — •Robin Ras — Department of Applied Physics, Aalto University, Espoo, Finland

Nature offers various examples of extreme water-repellency, such as the leaves of Lotus plant and wings of cicada. The water repellency allows plants for efficient photosynthesis even in dusty environments, and allows large-wing insects to fly even in humid conditions. Likewise, our technological society could benefit from surfaces that stay clean and dry in challenging conditions. For example, solar cells on roof tops loose efficiency when they are covered with sand and dust.

The extreme water-repellency, also called superhydrophobicity, is attributed to the combination of micro/nanoscale topography and hydrophobic surface chemistry that allows trapping of a thin air film between the water and the solid substrate. The air film effectively shields the water from the solid by reducing the contact area, leading to very high contact angle and very low adhesion and friction. The required topography, however, also makes these surfaces very fragile.

Here I will present the progress made during previous decade, including different strategies for enhancing the mechanical durability. Recently, in collaboration with the group of Xu Deng, we developed an extremely durable superhydrophobic surface, by making use of a microstructured armor that protects the otherwise fragile nanostructures. I will present the concept, and steps that we are taking towards commercialization.

DY 6.5 Wed 11:45 H3

Calculating Magnetization Fields in Magnetoactive Elastomers: A Cascading Mean-Field Approach — •Dirk Romeis and Marina Saphiannikova — Leibniz Institute of Polymer Research Dresden, Germany

We consider the application of an external magnetic field to a composite of a non-magnetizable elastomer matrix with embedded magnetizable particle inclusions. The resulting interactions are determined by the magnetization field which is generated not only by the external magnetic field but also by the magnetic fields arising due to surrounding inclusions. A comprehensive description requires knowledge about the magnetization of individual particles and of macroscopic portions of the composite. Accordingly, a precise calculation becomes elaborate for a specimen comprising billions of particles. We present a greatly simplified, but accurate approximation for the computation of magnetization fields in such composites. Based on the dipole model, we introduce the cascading mean-field description [1] by separating the magnetization field into three contributions on the micro-, meso-, and macroscale. It is revealed that the contributions are nested into each other, as in the Matryoshka's toy. Our description allows for an efficient and transparent analysis of such composite materials under rather general conditions.

Financial support by DFG, SPP 1713, is gratefully acknowledged.

[1] D. Romeis and M. Saphiannikova: A cascading mean-field approach to the calculation of magnetization fields in magnetoactive elastomers. Polymers, 13(9):1372, 2021.

DY 6.6 Wed 12:00 H3

Magnetostrictive effects in soft magnetic gels and elastomers — •Lukas Fischer and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

Our work focuses on magnetic gels and elastomers, also known as magnetorheological elastomers or ferrogels, that feature a soft elastic matrix enclosing magnetizable particles. These materials react to an applied external magnetic field mainly in a twofold manner: by changing their overall mechanical properties (magnetorheological effect) and by overall macroscopic deformations (magnetostriction).

We have developed a mesoscopic theory to describe the latter effect. For this purpose, we analytically solve the linear elastic problem, linking the particle scale to the scale of overall deformation. To adjust the deformational response, we modify the initial positioning of the particles inside the material, relative to the magnetic field direction [1].

Specific spatial arrangements of the magnetizable particles inside the elastic medium favor specific magnetostrictive modes of deformation, for example torsion [2]. Targeted modification of the particle size can likewise serve to adjust the magnetostrictive response [3]. Our work supports the construction of magnetically controlled soft actuators that are tailored to requested deformational tasks.

[1] L. Fischer, A. M. Menzel, *J. Chem. Phys.* **151**, 114906 (2019).
[2] L. Fischer, A. M. Menzel, *Phys. Rev. Research* **2**, 023383 (2020).
[3] L. Fischer, A. M. Menzel, *Smart Mater. Struct.* **30**, 014003 (2021).

DY 6.7 Wed 12:15 H3

Perturbed Jamming transitions — Moumita Maiti[1] and •Michael Schmiedeberg[2] — [1]Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

By minimizing the interaction energy in a soft sphere system without crossing energy barriers the discontinuous athermal jamming transion can be observed at a packing fraction of about 0.64 in 3D [1]. However, if perturbations like thermal fluctuations [2] or an active self-propulsion [3] are added, the transition becomes continuous and the transition packing fraction might occur at a different density. For example, in case of thermal fluctuations, the transition packing fraction approaches 0.55 in case of small thermal fluctuations [2]. We show that the thermal jamming transition lies within the universality class of directed percolation. As a consequence, athermal jamming is a (singular) limit of a much wider class of perturbed jamming transitions that can also be understood as dynamical transitions [2,4]. Therefore, perturbed jamming transitions open up a large variety of amorphous packings and insights how these packings are related to glassy dynamics.

[1] C.S. O'Hern et al., Phys. Rev. Lett. 88, 075507 (2002), Phys. Rev. E 68, 011306 (2003).
[2] M. Maiti and M. Schmiedeberg, Scientific Reports 8, 1837 (2018).
[3] M. Maiti and M. Schmiedeberg, EPL 126, 46002 (2019).
[4] L. Milz and M. Schmiedeberg, Phys. Rev. E 88, 062308 (2013); S. Wilken et al., Phys. Rev. Lett. 127, 038002 (2021).

DY 6.8 Wed 12:30 H3

Fluidity models for amorphous glassy materials — •Robin Lautenschlager and Thomas Voigtmann — Institut für Materi-

alphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln

Different rheological models are proposed to describe the complex flow properties of amorphous glassy materials, such as granular materials or colloidal glasses, intermediate between a solid and liquid behavior. These systems show a strong non-linearity due to stresses and strain rates, as well as time-dependent ageing effects. The materials are hence described by a time-dependent local fluidity as a main rheological quantity. Spatial non-localities are quantified by a characteristic cooperativity length that describes the extent over which neighboring material regions influence their flow behavior.

We compare three different approaches of such fluidity models and discuss their key features regarding the complex flow properties and how they try to reproduce the time-dependent effects of such a flow. We probe the models in a pressure driven two-dimensional-channel-flow and compare their long-time numerical results to analytically estimated steady state solutions for this test case. We will discuss how the models respond to different flow properties to evaluate their usability in applications.

DY 7: Focus Session: Facets of Many-Body Quantum Chaos (organised by Markus Heyl and Klaus Richter) (joint session DY/TT)

This session covers the same topics as the TT-DY-MA symposium with the same name and five invited speakers on Tuesday, September 28th.

Time: Wednesday 10:00–13:00 Location: H6

DY 7.1 Wed 10:00 H6

Probing many-body quantum chaos with quantum simulators using randomized measurements — Lata K Joshi[1,2], •Andreas Elben[1,2,3], Amit Vikram[4,5], Benoit Vermersch[1,2,6], Victor Galitski[4], and Peter Zoller[1,2] — [1]Center for Quantum Physics, University of Innsbruck, Innsbruck A-6020, Austria — [2]Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, Innsbruck A-6020, Austria — [3]Institute for Quantum Information and Matter and Walter Burke Institute for Theoretical Physics, California Institute of Technology, Pasadena, CA 91125, USA — [4]Joint Quantum Institute, University of Maryland, College Park, MD 20742, USA — [5]Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, MD 20742, USA — [6]Univ. Grenoble Alpes, CNRS, LPMMC, 38000 Grenoble, France

Randomized measurements provide a novel toolbox to probe many-body quantum chaos in quantum simulators, utilizing observables such as out-of-time ordered correlators and spectral form factors (SFFs). Here, I will focus on a protocol to access the SFF, characterizing the energy eigenvalue statistics, in quantum spin models. In addition, I will introduce partial spectral form factors (pSFFs) which refer to subsystems of the many-body system and reveal unique insights into energy eigenstate statistics. I will show that our randomized measurement protocol allows to access both, SFF and pSFFs. It provides thus a unified testbed to probe many-body quantum chaotic behavior, thermalization and many-body localization in closed quantum systems.

DY 7.2 Wed 10:15 H6

Exploring the bound on chaos due to quantum criticality — •Mathias Steinhuber, Juan-Diego Urbina, and Klaus Richter — University of Regensburg, Regensburg, Germany

The 'bound on chaos' proposed by Maldacena, Shenker and Stanford [1] predicts a temperature-dependent upper bound on the initial exponential growth rate $\lambda_{\mathrm{OTOC}} \leq 2\pi T$ for out-of-time-order correlators (OTOCs) in quantum systems with chaotic classical limit. We explore the temperature dependence of the quantum Lyapunov exponent λ_{OTOC} in Bose-Hubbard systems near criticality of the ground state [2]. We find the conditions for a non-trivial temperature dependence satisfying the bound, indicating the requirement that the system shows signatures of classical instability at the ground state while reaching the semiclassical regime at the same time. This is guaranteed by many-body systems with a well defined mean-field limit close to a bifurcation [3].

[1] Maldacena J., Shenker S. H. & Stanford D. A bound on chaos. Journal of High Energy Physics 2016, 106 (2016).

[2] Hummel, Q., Geiger, B., Urbina, J. D. & Richter, K. Reversible Quantum Information Spreading in Many-Body Systems near Criticality. Phys. Rev. Let. 123, 160401 (2019).

[3] Eilbeck, J., Lomdahl, P. & Scott, A. The discrete self-trapping equation. Physica D: Nonlinear Phenomena 16, 318-338 (1985).

DY 7.3 Wed 10:30 H6

Critically slow operator dynamics in constrained many-body systems — •Johannes Feldmeier[1,2] and Michael Knap[1,2] — [1]Technical University of Munich — [2]Munich Center for Quantum Science and Technology (MCQST)

The far-from-equilibrium dynamics of generic interacting quantum systems is characterized by a handful of universal guiding principles, among them the ballistic spreading of initially local operators. Here, we show that in certain constrained many-body systems the structure of conservation laws can cause a drastic modification of this universal behavior. As an example, we study operator growth characterized by out-of-time-order correlations (OTOCs) in a dipole-conserving fracton chain. We identify a critical point with sub-ballistically moving OTOC front, that separates a ballistic from a dynamically frozen phase. This critical point is tied to an underlying localization transition and we use its associated scaling properties to derive an effective description of the moving operator front via a biased random walk with long waiting times. We support our arguments numerically using classically simulable automaton circuits.

DY 7.4 Wed 10:45 H6

Universal equilibration dynamics of the Sachdev-Ye-Kitaev model — •Soumik Bandyopadhyay, Philipp Uhrich, Alessio Paviglianiti, and Philipp Hauke — INO-CNR BEC Center and Department of Physics, University of Trento, Via Sommarive 14, I-38123 Trento, Italy

The Sachdev-Ye-Kitaev (SYK) model was introduced in the context of explaining the properties of "strange metals," and has been found to manifest the characteristics of a quantum theory which is holographically dual to extremal charged black holes with two-dimensional anti-de Sitter horizons. Being maximally chaotic, black holes are the best known scramblers of quantum information in nature. Same features are shared by the SYK model, which has triggered a massive interest in its chaotic dynamics. Yet, many questions about the dynamics of the SYK model remain open. In this presentation, we shall be discussing the equilibration process of a fermionic system under the SYK Hamiltonian evolution. Our study, based on a state-of-the-art exact diagonalization method, reveals that the system exhibits an universal equilibration process. By devising a master equation for disordered systems, we successfully explain some of the key features of this dynamics. We infer the universality from the spectral analysis of the corresponding Liouvillian. We expect our findings shed light on challenging questions for systems far from equilibrium, such as, thermalization of closed and disordered quantum many-body systems.

DY 7.5 Wed 11:00 H6

Periodic orbit sums and their relation to JT gravity correlators — •Fabian Haneder, Torsten Weber, Camilo Moreno, Juan Diego Urbina, and Klaus Richter — University of Regensburg, Germany

Jackiw-Teitelboim (JT) gravity is a two-dimensional dilaton gravity theory originally used to describe the near-horizon physics of charged, static black holes, but has recently garnered much attention due to its exact duality to a particular double-scaled Hermitian matrix model [1]. Applications are believed to be as a toy model for the black hole information paradox, the AdS/CFT correspondence, and holography

and quantum gravity more generally.

The duality with a matrix model suggests the existence of a classical chaotic system which, after semiclassical (periodic orbit) quantisation [2], leads to the same spectral correlations. Finding such a system would solve the long-standing problem of identifying a single dual, rather than an ensemble of theories, as expected from orthodox AdS/CFT.

In this contribution, we will give a very brief overview of the JT/matrix model duality and show the structural similarity of JT correlators and stochastically projected periodic orbit sums, at the level of the one-point function, as well as propose a candidate dual system.

[1] P. Saad, S. Shenker, D. Stanford, arXiv:1903.11115

[2] See e.g. M. Gutzwiller, *Chaos in classical and quantum mechanics*, Springer 2019

DY 7.6 Wed 11:15 H6

Entanglement entropy of fractal states — Giuseppe De Tomasi[1] and •Ivan Khaymovich[2] — [1]T.C.M. Group, Cavendish Laboratory, JJ Thomson Avenue, Cambridge CB3 0HE, United Kingdom — [2]Max Planck Institute for the Physics of Complex Systems

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

As a simple example we introduce a new class of *sparse* random pure states being fractal in the corresponding computational basis and show that their entropies reach the upper bound of Page value for fractal dimension larger than the subsystem size ($D_q > 0.5$ for equipartitioning) and grow linearly with D_q otherwise.

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

15 min. break.

DY 7.7 Wed 11:45 H6

Chaos for Interacting Bosons and Random Two-Body Hamiltonians — Lukas Pausch[1], Edoardo Carnio[1,2], Andreas Buchleitner[1,2], and •Alberto Rodríguez[3] — [1]Physikalisches Institut, Albert-Ludwigs-Universität-Freiburg, Hermann-Herder-Straße 3, D-79104, Freiburg, Germany — [2]EUCOR Centre for Quantum Science and Quantum Computing, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3, D-79104, Freiburg, Germany — [3]Departamento de Física Fundamental, Universidad de Salamanca, E-37008 Salamanca, Spain

We investigate the chaotic phase of the Bose-Hubbard model [1] in relation to the bosonic embedded random-matrix ensemble, which mirrors the dominant few-body nature of many-particle interactions, and hence the Fock space sparsity of quantum many-body systems. Within the chaotic regime, mean and fluctuations of the fractal dimensions of Bose-Hubbard eigenstates show clear fingerprints of ergodicity and are well described by the embedded ensemble, which is furthermore able to capture the energy dependence of the chaotic phase. Despite such agreement, the distributions of the fractal dimensions for these two models depart from each other and from the Gaussian orthogonal ensemble as Hilbert space grows.

[1] L. Pausch et al, Phys. Rev. Lett. **126**, 150601 (2021).

DY 7.8 Wed 12:00 H6

Orthogonal quantum many-body scars — •Hongzheng Zhao[1], Adam Smith Smith[2], Florian Mintert[1], and Johannes Knolle[1,3,4] — [1]Blackett Laboratory, Imperial College London, London, United Kingdom — [2]School of Physics and Astronomy, University of Nottingham, University Park, Nottingham, United Kingdom — [3]Department of Physics TQM, Technical University of Munich, Munich, Germany — [4]Munich Center for Quantum Science and Technology, Munich, Germany

Quantum many-body scars have been put forward as counterexamples to the Eigenstate Thermalization Hypothesis. These atypical states are observed in a range of correlated models as long-lived oscillations of local observables in quench experiments starting from selected initial states. The long-time memory is a manifestation of quantum non-ergodicity generally linked to a sub-extensive generation of entanglement entropy, the latter of which is widely used as a diagnostic for identifying quantum many-body scars numerically as low entanglement outliers. Here we show that, by adding kinetic constraints to a fractionalized orthogonal metal, we can construct a minimal model with orthogonal quantum many-body scars leading to persistent oscillations with infinite lifetime coexisting with rapid volume-law entanglement generation. Our example provides new insights into the link between quantum ergodicity and many-body entanglement while opening new avenues for exotic non-equilibrium dynamics in strongly correlated multi-component quantum systems. Reference: https://arxiv.org/abs/2102.07672

DY 7.9 Wed 12:15 H6

Genuine many-body quantum scarring in a periodic Bose-Hubbard ring — •Quirin Hummel and Peter Schlagheck — Université de Liège (Belgium)

Quantum scars have been known for decades to exist in quantum systems of low dimensionality (e.g. "quantum billiards"): While most eigenstates of a classically chaotic system are typically spread across the accessible phase space, individual states exist that are concentrated along unstable classical periodic orbits. On the other hand, recent studies in many-body quantum systems that admit no known meaningful classical limits have revealed eigenstates - now termed "quantum many-body scars" - that feature quantum mechanical properties reminiscent of scenarios of quantum scarring. An unambiguous classification as scars in the original sense, however, remains controversial, if not fundamentally impossible due to the lack of a classical limit. In order to bridge this gap, we investigate the phenomenon of quantum scarring in the prototypical Bose-Hubbard model, a many-body quantum system that combines both, a well-defined formally classical description and the typical high-dimensionality of many-body systems identified with the number of sites that constitute the one-body state space.

DY 7.10 Wed 12:30 H6

Quantum scars of bosons with correlated hopping — •Ana Hudomal[1,2], Ivana Vasić[2], Nicolas Regnault[3,4], and Zlatko Papić[1] — [1]School of Physics and Astronomy, University of Leeds, United Kingdom — [2]Institute of Physics Belgrade, University of Belgrade, Serbia — [3]Joseph Henry Laboratories and Department of Physics, Princeton University, USA — [4]Laboratoire de Physique de l'École Normale Supérieure, ENS, CNRS, Paris, France

Recent experiments have shown that preparing an array of Rydberg atoms in a certain initial state can lead to unusually slow thermalization and persistent density oscillations [1]. This type of non-ergodic behavior has been attributed to the existence of "quantum many-body scars", i.e., atypical eigenstates that have high overlaps with a small subset of vectors in the Hilbert space. Periodic dynamics and many-body scars are believed to originate from a "hard" kinetic constraint: due to strong interactions, no two neighbouring Rydberg atoms are both allowed to be excited. Here we propose a realization of quantum many-body scars in a 1D bosonic lattice model with a "soft" constraint: there are no restrictions on the allowed boson states, but the amplitude of a hop depends on the occupancy of the hopping site. We find that this model exhibits similar phenomenology to the Rydberg atom chain, including weakly entangled eigenstates at high energy densities and the presence of a large number of exact zero energy states [2].

[1] H. Bernien et al., Nature **551**, 579 (2017).

[2] A. Hudomal et al., Commun. Phys. **3**, 99 (2020).

DY 7.11 Wed 12:45 H6

Quantum local random networks and the statistical robustness of quantum scars — •Federica Maria Surace[1,2], Marcello Dalmonte[1,2], and Alessandro Silva[1] — [1]International School for Advanced Studies (SISSA), via Bonomea 265, 34136 Trieste, Italy — [2]The Abdus Salam International Centre for Theoretical Physics (ICTP), Strada Costiera 11, 34151 Trieste, Italy

We investigate the emergence of quantum scars in a general ensemble of random Hamiltonians (of which the PXP is a particular realization), that we refer to as quantum local random networks. We find two types of scars, that we call stochastic and statistical. We identify specific signatures of the localized nature of these eigenstates by analyzing a combination of indicators of quantum ergodicity and properties related to the network structure of the model. Within this parallelism, we associate the emergence of statistical scars to the presence of motifs in the network, that reflects how these are associated to links with anomalously small connectivity (as measured, e.g., by their betweenness). Most remarkably, statistical scars appear at well-defined values of energy, predicted solely on the basis of network theory. We study the scaling of the number of statistical scars with system size:

below a threshold connectivity, we find that the number of statistical scars increases with system size. This allows to define the concept of statistical stability of quantum scars.

DY 8: Quantum Computing (joint session TT/DY)

Time: Wednesday 11:15–13:00 Location: H7

DY 8.1 Wed 11:15 H7

Probing the critical current coupling of defects in Josephson junctions — •Alexander Konstantin Neumann[1], Benedikt Berlitz[1], Alexey V. Ustinov[1,2,3], and Jürgen Lisenfeld[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]National University of Science and Technology MISIS, Moscow 119049, Russia — [3]Russian Quantum Center, Skolkovo, Moscow 143025, Russia

Material defects form a major source of decoherence in state of the art superconducting quantum bits. It has been a long standing question whether defects residing in the tunnel barrier of Josephson junctions modify their critical current. We investigate this with spectroscopic measurements and QuTiP simulations on individual defects strongly coupled to a transmon qubit. By observing avoided level crossings at driving amplitudes allowing for multi-photon transitions, we quantify the strength of the critical current coupling. Moreover, we find an effective direct interaction between the defect and the qubit's readout resonator, providing an additional decoherence channel.

DY 8.2 Wed 11:30 H7

Cavity mediated quantum gate between distant charge qubits — •Florian Kayatz, Jonas Mielke, and Guido Burkard — Department of Phyiscs, University of Konstanz, Konstanz, Germany

Gate based quantum computers require high fidelity single-qubit and two-qubit gates to allow for arbitrary multi-qubit operations that are needed to perform a quantum algorithm. Ideally, one has "all-to-all" connectivity, i.e. an architecture with two-qubit gates between any desired pair of qubits. Notably, short-ranged interactions such as capacitive coupling and the exchange interaction cannot be harnessed to implement two-qubit gates between distant qubits. We investigate whether a high-fidelity iSWAP gate between distant charge qubits can be implemented by using a microwave resonator as an intermediate system mediating the interaction. In particular, we consider charge qubits formed by a single electron confined in a Si double quantum dot that are coupled to a microwave resonator via electric dipole coupling. We theoretically demonstrate that, in the dispersive regime, the photons can mediate an iSWAP gate. We then calculate the gate fidelity in the presence of the dominant noise sources, quasi-static charge noise, resonator damping and phonon induced charge relaxation, and find a very limited gate fidelity.

DY 8.3 Wed 11:45 H7

Crosstalk analysis for single-qubit and two-qubit gates in spin qubit arrays — •Irina Heinz and Guido Burkard — University of Konstanz, Konstanz, Germany

Scaling up spin qubit systems requires high-fidelity single-qubit and two-qubit gates. Gate fidelities exceeding 98% were already demonstrated in silicon based single and double quantum dots, whereas for the realization of larger qubit arrays crosstalk effects on neighboring qubits must be taken into account. We analyze qubit fidelities impacted by crosstalk when performing single-qubit and two-qubit operations on neighbor qubits with a simple Heisenberg model. Furthermore we propose conditions for driving fields to robustly synchronize Rabi oscillations and avoid crosstalk effects. In our analysis we also consider next to nearest neighbor crosstalk and show that double synchronization leads to a restricted choice for the driving field strength, exchange interaction, and thus gate time. Considering realistic experimental conditions we propose a set of parameter values to perform a nearly crosstalk-free CNOT gate and so open up the pathway to scalable quantum computing devices.

DY 8.4 Wed 12:00 H7

Spin shuttling in a silicon double quantum dot — •Florian Ginzel[1], Adam R. Mills[2], Jason R. Petta[2], and Guido Burkard[1] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Department of Physics, Princeton University, Princeton, New Jersey 08544, USA

The transport of quantum information between different nodes of the device is crucial for a quantum processor. In the context of spin qubits, this can be realized by coherent electron spin shuttling between quantum dots. Here we theoretically study a minimal version of spin shuttling between two quantum dots (QDs) occupied by one electron [1]. We analyze the possibilities and limitations of spin transport during a detuning sweep in a silicon double QD. This research is motivated by recent experimental progress [2,3]. Spin-orbit interaction and an inhomogeneous magnetic field play an important role for spin shuttling and are included in our model. Interactions that couple the position, spin and valley degrees of freedom open avoided crossings in the spectrum allowing for diabatic transitions and interfering paths. The outcomes of single and repeated spin shuttling protocols are explored by means of numerical simulations and an approximate analytic model based on the Landau-Zener model. We find that fast high-fidelity spin-shuttling is feasible for optimal choices of parameters or protected by constructive interference.

[1] Ginzel et al., Phys. Rev. B 102, 195418 (2020)
[2] T. Fujita et al., npj Quantum Information 3, 22 (2017)
[3] A. R. Mills et al., Nat. Comm. 10, 1063 (2019)

DY 8.5 Wed 12:15 H7

Simulating hydrodynamics on NISQ devices with random circuits — •Jonas Richter and Arijeet Pal — Department of Physics and Astronomy, University College London, UK

We show that pseudorandom circuits, recently implemented in Google's seminal "quantum supremacy" experiment, are not just abstract tools to outperform classical computers, but in fact form tailor-made building blocks to simulate certain aspects of quantum many-body systems on noisy intermediate-scale quantum computers. Specifically, we propose an algorithm consisting of a random circuit followed by a trotterized Hamiltonian time evolution to study transport properties in the linear response regime, which we numerically exemplify for one- and two-dimensional quantum spin systems. While the algorithm operates without an overhead of bath or ancilla qubits for initial-state preparation and measurement, our numerics further suggest that it is comparatively robust against systematic Trotter errors and noisy gates.

[1] J. Richter and A. Pal, Phys. Rev. Lett. 126, 230501 (2021)

DY 8.6 Wed 12:30 H7

Adaptive variational NISQ quantum algorithms for dynamics and excited states preparation — Yongxin Yao[1,2], Niladri Gomes[1,2], Feng Zhang[1,2], Cai-Zhuang Wang[1,2], Kai-Ming Ho[1,2], Thomas Iadecola[1,2], and •Peter P. Orth[1,2] — [1]Ames Laboratory, Ames, Iowa, USA — [2]Iowa State University, Ames, Iowa, USA

Simulating quantum dynamics of interacting many-body systems is one of the main potential applications of quantum computing, since the growth of entanglement makes such simulations exponentially hard on classical devices. The shallow circuit requirement of current QPUs limits algorithms based on Trotter product formulas to simulate early time dynamics. Here, we present an adaptive approach to construct a variational wave function ansatz for accurate quantum dynamics simulations based on McLachlan's variational principle [1]. The key idea is to dynamically expand the variational ansatz along the time-evolution path such that the McLachlan distance, which is a measure of the simulation accuracy, remains below a set threshold. We apply this adaptive variational quantum dynamics simulation approach (non)integrable quantum spin models and find the circuits to contain up to two orders of magnitude fewer CNOT gates than those obtained from first-order Trotter expansion. We also present results on development of an adaptive VQE-X algorithm for preparation of highly excited states in many-body models [2].

[1] Yao et al., PRX Quantum 2, 030307 (2021)
[2] Zhang et al., arXiv:2104.12636 (2021)

DY 8.7 Wed 12:45 H7

Simulating a discrete time crystal over 57 qubits on a quantum computer — •Philipp Frey and Stephan Rachel — School of Physics, University of Melbourne, Parkville, VIC 3010, Australia

We simulate the dynamics of a spin-1/2 chain with nearest neighbor Ising interactions, quenched disorder and periodic driving over 57 qubits on a current quantum computer. Based on the dynamics of local spin depolarisation we observe discrete time crystalline (DTC) behaviour due to many body localisation (MBL). We probe random initial states along with fully polarised states and compare the cases of vanishing and finite disorder to distinguish MBL from pre-thermal dynamics. In order to extract the signal from the noisy data produced by current quantum computer devices, we develop a strategy for error mitigation and show that the results are robust under variations of the parameters introduced in this scheme. A transition between DTC and a thermal phase is observed via critical fluctuations in the sub-harmonic frequency response of the system, as well as a significant speed-up of spin depolarisation. Our findings are consistent with previous numerical simulations, but represent the realization of a DTC with largest system size to date.

DY 9: Many-Body Quantum Dynamics I (joint session DY/TT)

Time: Wednesday 13:30–14:45 Location: H6

Invited Talk DY 9.1 Wed 13:30 H6

Nanofriction in Ion Coulomb Systems — •Tanja Mehlstäubler — PTB, Bundesallee 100, 38116 Braunschweig

Single trapped and laser-cooled ions in Paul traps allow for a high degree of control of atomic quantum systems. They are the basis for modern atomic clocks, quantum computers and quantum simulators. Our research aims to use ion Coulomb crystals, i.e. many-body systems with complex dynamics, for precision spectroscopy. This paves the way to novel optical frequency standards for applications such as relativistic geodesy and quantum simulators in which complex dynamics becomes accessible with atomic resolution. The high-level of control of self-organized Coulomb crystals opens up a fascinating insight into the non-equilibrium dynamics of coupled many-body systems, displaying atomic friction and symmetry-breaking phase transitions. We discuss the creation of topological defects and Kibble-Zurek tests in 2D crystals and present recent results on the study of tribology and transport mediated by the topological defect.

DY 9.2 Wed 14:00 H6

Quantum many-body scars in tilted Fermi-Hubbard chains — •Jean-Yves Desaules[1], Ana Hudomal[1,2], Christopher Turner[1], and Zlatko Papić[1] — [1]School of Physics and Astronomy, University of Leeds, Leeds, United Kingdom — [2]Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia

Motivated by recent observations of ergodicity breaking due to Hilbert space fragmentation in 1D Fermi-Hubbard chains with a tilted potential [Scherg et al., arXiv:2010.12965], we show that the same system also hosts quantum many-body scars in a regime $U=\Delta>J$ at electronic filling factor $\nu=1$. We numerically demonstrate that the scarring phenomenology in this model is similar to other known realisations such as Rydberg atom chains, including persistent dynamical revivals and ergodicity-breaking many-body eigenstates. At the same time, we show that the mechanism of scarring in the Fermi-Hubbard model is different from other examples in the literature: the scars originate from a subgraph, representing a free spin-1 paramagnet, which is weakly connected to the rest of the Hamiltonian's adjacency graph. Our work demonstrates that correlated fermions in tilted optical lattices provide a platform for understanding the interplay of many-body scarring and other forms of ergodicity breaking, such as localisation and Hilbert space fragmentation.

DY 9.3 Wed 14:15 H6

(Classical) Prethermal phases of matter — •Andrea Pizzi[1], Andreas Nunnenkamp[2], and Johannes Knolle[3] — [1]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom — [2]School of Physics and Astronomy and Centre for the Mathematics and Theoretical Physics of Quantum Non-Equilibrium Systems, University of Nottingham, Nottingham, NG7 2RD, United Kingdom — [3]Department of Physics, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany

Systems subject to a high-frequency drive can spend an exponentially long time in a prethermal regime, in which novel phases of matter with no equilibrium counterpart can be realized. Due to the notorious computational challenges of quantum many-body systems, numerical investigations in this direction have remained limited to one spatial dimension, in which long-range interactions have been proven a necessity. Here, we show that prethermal non-equilibrium phases of matter are not restricted to the quantum domain. Studying the Hamiltonian dynamics of a large three-dimensional lattice of classical spins, we provide the first numerical proof of prethermal phases of matter in a system with short-range interactions. Concretely, we find higher-order as well as fractional discrete time crystals breaking the time-translational symmetry of the drive with unexpectedly large integer as well as fractional periods. Our work paves the way towards the exploration of novel prethermal phenomena by means of classical Hamiltonian dynamics with virtually no limitations on the system's geometry or size, and thus with direct implications for experiments.

DY 9.4 Wed 14:30 H6

Master equations for Wigner functions with spontaneous collapse and their relation to thermodynamic irreversibility* — •Michael te Vrugt[1,2], Gyula I. Tóth[3], and Raphael Wittkowski[1] — [1]Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany — [2]Philosophisches Seminar, Westfälische Wilhelms-Universität Münster, D-48143 Münster, Germany — [3]Interdisciplinary Centre for Mathematical Modelling and Department of Mathematical Sciences, Loughborough University, Loughborough, LE11 3TU, United Kingdom

Wigner functions allow for a reformulation of quantum mechanics in phase space. They are, as shown in our recent work [1], very useful for understanding effects of spontaneous collapses of the wavefunction as predicted by the Ghirardi-Rimini-Weber (GRW) theory. We derive the dynamic equations for the Wigner function in the GRW theory and its most important variants. The results are used to test, via computer simulations, David Albert's suggestion that the stochasticity induced by spontaneous collapses is responsible for the emergence of thermodynamic irreversibility. We do not observe the equilibration mechanism proposed by Albert, suggesting that GRW theory cannot explain the approach to thermal equilibrium.

[1] M. te Vrugt, G. I. Tóth, R. Wittkowski, arXiv:2106.00137 (2021)

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DY 10: Focus session: Nonlinear Dynamics of the Heart I (organized by Markus Bär, Stefan Luther and Ulrich Parlitz)

Time: Wednesday 15:00–16:30 Location: H6

Invited Talk DY 10.1 Wed 15:00 H6

Effect of fibrosis on propagation on non-linear waves and onset of arrhythmias in cardiac tissue — •Alexander Panfilov[1,2], Timur Nezlobinsky[1,2], and Farhad Pashakhanloo[3] — [1]Department of Physics and Astronomy, Ghent Unibversity, Belgium — [2]Ural Federal University, Ekaterinburg, Russia — [3]Cardiovascular Division, Beth Israel Deaconess Medical Center, Harvard Medical School, Boston, Massachusetts, 02115, USA

Cardiac fibrosis is a well-known arrhythmogenic condition which can lead to sudden cardiac death. Physically, fibrosis can be viewed as a large number of small obstacles in an excitable medium, which may create nonlinear wave turbulence or reentry. The relation between the specific texture of fibrosis and the onset of reentry is of great theoretical and practical importance. In my talk I present results of several recent studies which show how basic properties of wave propagation are affected by fibrosis. We also characterize properties of fibrotic texture which led to cardiac arrhythmias and propose a concept of minimal functional cluster which allows quantitatively predict the arrhythmia probability for different fibrosis densities and tissue excitabilities.

DY 10.2 Wed 15:30 H6

The mechanism of defibrillation of cardiac tissue by time-periodic low-energy shocks I: Refractory boundary length is key for prediction of success probabilities — •Markus Bär, Pavel Buran, and Thomas Niedermayer — Physikalisch-Technische Bundesanstalt, Abbestr. 2 - 12, 10587 Berlin

Rotating excitation waves and electrical turbulence in cardiac tissue are associated with arrhythmias such as life-threatening ventricular fibrillation. Experimental studies have shown that a periodic sequence of four or more electrical far-field pulses is able to terminate fibrillation with less energy than a single shock protocol. During this so-called periodic low-energy anti-fibrillatory pacing (LEAP), only tissue near sufficiently large conduction heterogeneities, such as large coronary arteries, is activated. By means of simulation of the impact of periodic pacing on fibrillation in a two-dimensional electrophysiological model exhibiting multiple stable spirals (vortices) with a representative array of heterogeneities, we show that the success probability for defibrillation depends exponentially on the length of the refractory boundary, i. e. the total length of the borders between refractory and excitable parts of the tissue. This exponential dependency is also derived analytically from simple arguments assuming that successful defibrillation by a low energy shock requires not only to annihilate all vortices, but also needs to prevent initiation of new vortices in the vulnerable excitable region near the refractory boundary.

DY 10.3 Wed 15:45 H6

The mechanism of defibrillation of cardiac tissue by time-periodic low-energy shocks II: Subsequent shortening of refractory boundary length enables low energy antifibrillatory pacing (LEAP) — •Pavel Buran, Thomas Niedermayer, and Markus Bär — Physikalisch-Technische Bundesanstalt, Abbestr. 2 - 12, 10587 Berlin

We present a generic mechanism for the success of LEAP protocols, which covers termination of multiple stable rotors as well as of states of spatiotemporal chaos. Previously, we found that knowledge of the refractory boundary length is sufficient to estimate the success probability of an individual LEAP pulse which is found to decay exponentially with this length in a medium with stable spirals. This result is also found in simulations of cardiac models exhibiting spatiotemporal chaos. Whereas single shock defibrillation requires instantaneous annihilation of all existing vortices, during LEAP the defibrillation process is more gradual and is based on a subsequent shortening of the total refractory boundary length. The average shortening factor, i. e. the ratio between the refractory boundary lengths just before subsequent pulses during periodic pacing can be determined numerically both for media with spatiotemporal chaos and multiple stable spirals and provides a good indicator for the efficiency of a given LEAP protocol.

Invited Talk DY 10.4 Wed 16:00 H6

Chaos and nonlinear dynamics in the heart: Experiments and simulations of arrhythmias and defibrillation — •Flavio Fenton — School of Physics, Georgia Institute of Technology, Atlanta, GA

In this talk we present experimental examples of chaotic dynamics including unstable periodic orbits (period 3 and higher orders) in the heart. As a nonlinear system we further demonstrate a universal mechanism for terminating spiral waves in generic excitable media using an established topological framework. Under this mechanism it is possible to explain when defibrillation shocks, by high- or low-energy methods, succeed or fail. Furthermore, it is also possible to design a single minimal stimulus capable to defibrillate, at any time, any turbulent state driven by multiple spiral waves. We demonstrate this in a variety of cardiac tissue models. The theory described here shows how this mechanism underlies all successful defibrillation and can be used to further develop existing and future low-energy defibrillation strategies.

DY 11: Many-Body Quantum Dynamics II (joint session DY/TT)

Time: Thursday 10:00–11:30 Location: H2

DY 11.1 Thu 10:00 H2

Anderson localization of composite particles — •Fumika Suzuki[1], Mikhail Lemeshko[2], Wojciech Zurek[3], and Roman Krems[4] — [1]IST Austria (Institute of Science and Technology Austria) — [2]IST Austria (Institute of Science and Technology Austria) — [3]Los Alamos National Laboratory — [4]University of British Columbia

We investigate the effect of coupling between translational and internal degrees of freedom of composite quantum particles on their localization in a random potential. We show that entanglement between the two degrees of freedom weakens localization due to the upper bound imposed on the inverse participation ratio by purity of a quantum state. We perform numerical calculations for a two-particle system bound by a harmonic force in a 1D disordered lattice and a rigid rotor in a 2D disordered lattice. We illustrate that the coupling has a dramatic effect on localization properties, even with a small number of internal states participating in quantum dynamics.

arXiv:2011.06279

DY 11.2 Thu 10:15 H2

An SYK-inspired model with density-density interactions — •Johannes Dieplinger[1], Soumya Bera[2], and Ferdinand Evers[1] — [1]Institute of Theoretical Physics, University of Regensburg, D-93040, Germany — [2]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India

Strong electron-electron interactions are challenging to capture theoretically. A rare example of an analytically tractable model is the Sachdev-Ye-Kitaev (SYK) model, which owes its tractability to the structureless and therefore artificial design: interactions are restricted to two body terms, whose matrix elements are randomly chosen and therefore do not commute with the local density, a fundamental symmetry of realistic electron-electron interactions. We here investigate a derivative of the SYK model, restoring this fundamental symmetry [1]. It features density-density-type interactions as well as a randomized single body term. We present numerical evidence that this model has a rich phase structure, featuring two integrable phases separated by several intermediate phases, including a chaotic one. The latter exhibits several key characterstics of the SYK model including the spectral and wave function statistics and therefore should be adiabatically connected to the non-Fermi liquid phase of the original SYK model. Thus, the presented model provides a further element for bridging the SYK-model and microscopic realism.

[1] J. Dieplinger, S. Bera, F. Evers, Annals of Physics, 168503 (2021)

DY 11.3 Thu 10:30 H2

Disorder-Free Localization in an Interacting 2D Lattice Gauge Theory — •Peter Karpov[1,2], Roberto Verdel[1], Yi-Ping Huang[3], Markus Schmitt[4], and Markus Heyl[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]National Univesity of Science and Technology "MISiS", Moscow, Russia — [3]National Tsing Hua University, Hsinchu, Taiwan — [4]University of Cologne, Cologne, Germany

Disorder-free localization has been recently introduced as a mechanism for ergodicity breaking in low-dimensional homogeneous lattice gauge theories caused by local constraints. We show that also genuinely interacting systems in two spatial dimensions can become nonergodic due to this mechanism. This is all the more surprising since the conventional many-body localization is conjectured to be unstable in two dimensions; hence the gauge constraints represent an alternative robust localization mechanism for interacting models in higher dimensions.

Specifically, we demonstrate nonergodic behavior in the quantum link model by obtaining a bound on the localization-delocalization transition through a unconventional percolation problem implying a fragmentation of Hilbert space. We study the quantum dynamics in this system by introducing the method of "variational classical networks", an efficient representation of the wave function in terms of a network of classical spins. We show that propagation of line defects has different light cone structures in the localized and ergodic phases.

[1] P. Karpov et al, Phys. Rev. Lett. **126**, 130401 (2021).
[2] R. Verdel et al, Phys. Rev. B **103**, 165103 (2021).

DY 11.4 Thu 10:45 H2

Superradiant many-qubit absorption refrigerator — Michal Kloc[1], Kurt Meier[1], Kimon Hadjikyriakos[2], and •Gernot Schaller[3] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [2]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328, Dresden, Germany

We show that the lower levels of a large-spin network with a collective anti-ferromagnetic interaction and collective couplings to three reservoirs may function as a quantum absorption refrigerator. In appropriate regimes, the steady-state cooling current of this refrigerator scales quadratically with the size of the working medium, i.e., the number of spins. The same scaling is observed for the noise and the entropy production rate.

[1] arXiv:2106.04164

DY 11.5 Thu 11:00 H2

Bose condensation of squeezed light — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics-UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

Light with an effective chemical potential and no mass is shown to possess a general phase-transition curve to Bose-Einstein condensation. This limiting density and temperature range is found by the diverging in-medium potential range of effective interaction. While usually the absorption and emission with Dye molecules is considered, here it is proposed that squeezing can create also such an effective chemical potential. The equivalence of squeezed light with a complex Bogoliubov transformation of interacting Bose system with finite lifetime is established with the help of which an effective gap is deduced. This gap phase creates a finite condensate in agreement with the general limiting density and temperature range. The phase diagram for condensation is presented due to squeezing and the appearance of two gaps is discussed. Phys. Rev. B 99 (2019) 205124

DY 11.6 Thu 11:15 H2

Interplay of thermal and plasmonic THz nonlinearities on graphene — Jeongwoo Han[1], Mattew L. Chin[2], •Stephan Winnerl[3], Thomas E. Murphy[2], and Martin Mittendorff[1] — [1]Department of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]University of Maryland, College Park, MD 20740, United States of America — [3]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Due to the linear dispersion, graphene has attracted much attention as a material platform of nonlinear optics, in particular in the infrared regime. While for higher photon energies the nonlinearities are mostly related to interband transitions and Pauli blocking, in the infrared regime intraband and thermal effects dominate. Here we present the experimental evidence of nonlinear THz absorption beyond thermal effects, i.e., plasmonic nonlinearity, by employing polarization-resolved terahertz pump-probe measurements on graphene disks. By varying the polarization between pump and probe beam, i.e., co- and cross-polarized configurations, we observe a significant polarization dependence of the pump-induced change in transmission. To quantitatively analyze this observation, we develop numerical simulation, allowing us to understand the interplay between thermal and plasmonic nonlinearities. While both contribute to the co-polarized configuration, thermal effects dominate the nonlinearity in the cross-polarized configuration.

DY 12: Active Matter (joint session DY/BP/CPP)

Time: Thursday 11:45–13:00 Location: H2

DY 12.1 Thu 11:45 H2

Orientation-dependent propulsion of active Brownian spheres: from advection to polygonal clusters* — •Jens Bickmann[1], Stephan Bröker[1], Michael E. Cates[2], and Raphael Wittkowski[1] — [1]Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany — [2]DAMTP, Centre for Mathematical Sciences, University of Cambridge, Cambridge CB3 0WA, United Kingdom

Controllability of the collective dynamics of active Brownian particles is much desired for numerous potential future applications. In addition to the regular way of achieving control via external interventions, e.g., by traps, internal interventions in the dynamics of active Brownian particles become increasingly popular. Most often, internal intervention is achieved by a propulsion of the particles that depends on space, time, or orientation. Using field-theoretical modeling and particle-based simulations, we investigate systems of interacting active Brownian spheres in two spatial dimensions with an orientation-dependent propulsion. We show that different forms of orientation-dependent propulsion can give rise to advection, anomalous diffusion, and even the emergence of polygon-shaped clusters. *Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1*

DY 12.2 Thu 12:00 H2

The Anomalous Transport of Tracers in Active Baths — •Omer Granek[1], Yariv Kafri[1], and Julien Tailleur[2] — [1]Department of Physics, Technion-Israel Institute of Technology, Haifa, 3200003, Israel — [2]Université de Paris, Laboratoire Matière et Systèmes Complexes (MSC), UMR 7057 CNRS, F-75205 Paris, France

We derive the exact long-time dynamics of a tracer immersed in a one-dimensional active bath. In contrast to previous studies, we find that the damping and noise correlations possess long-time tails with exponents that depend on the tracer symmetry. For an asymmetric tracer, the tails lead to superdiffusion and friction that grows with time when the tracer is dragged at a constant speed. For a symmetric tracer, we recover normal diffusion and finite friction. However, when the symmetric tracer is small compared to the active-particle persistence length, the noise becomes anticorrelated at late times and the active contribution to the friction becomes negative: active particles then enhance motion rather than opposing it.

DY 12.3 Thu 12:15 H2

Forces on objects immersed in active fluids — Thomas Speck and •Ashreya Jayaram — Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7-9, 55128 Mainz, Germany

Depending on their shape, objects immersed in active fluids may be subjected to a net force or net torque. We show that in a finite, periodic system, the force/torque on such an object is determined by the vorticity of the polarization of the surrounding active fluid which in turn is localized to regions close to the object where its curvature changes. We find that the system size L has a colossal influence on the magnitude of the force which grows as L^2 before saturating to a constant. We relate this force to the current away from the body

and substantiate our theoretical results with numerical simulations of active Brownian particles.

DY 12.4 Thu 12:30 H2

Active Cooling in Inertial Active Matter — •Lukas Hecht[1], Suvendu Mandal[2], Hartmut Löwen[2], and Benno Liebchen[1] — [1]Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany — [2]Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany

To cool down a target domain of an equilibrium system, the system must be coupled to an external bath to which heat can be transferred. However, active matter is intrinsically out of equilibrium and the active particles themselves do not obey the second law of thermodynamics. Therefore, we ask the question if we can actively cool down active particles in a target domain without transferring a significant amount of heat to particles in the environment.

In this work, we use the active Brownian particle (ABP) model with inertia to develop a route to cool down ABPs in a target domain without the need of an external bath. Such an active cooling requires two ingredients: First, we need the feature of inertial ABPs to undergo motility-induced phase separation into coexisting phases with different effective temperatures [1]. Second, a mechanism that localizes the phase-separated region in the target domain is required. We show several realizations of active cooling demonstrating how inertial effects in active matter can be utilized to actively cool down a target domain.

[1] S. Mandal, B. Liebchen, and H. Löwen, Phys. Rev. Lett. 123, 228001 (2019).

DY 12.5 Thu 12:45 H2

Arrested phase separation in nonreciprocally interacting colloids — •Sebastian Fehlinger and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

Non-reciprocal interactions are wide spread in nature and can lead to a huge variety of phenomenons in many physical systems. For the specific case of a binary mixture of passive particles, the breaking of the action reaction principle can lead to formation of self-propelled dimers and other active molecules. For a small system size, these active molecules have already been realized in experiments based on phoretically interacting binary colloidal mixtures [1].

This work focuses on the numerical simulation of the Langevin equations describing many noninteracting colloids which we complement with a continuum theory. We find that the nonreciprocal attractions destabilize the uniform disordered phase and lead to clusters which grow in the course of the time. Surprisingly, for a wide parameter range, the clusters only grow up to a certain size such that coarsening is arrested. We attribute this to the spatiotemporal organization of the composition of the binary mixture within the cluster which essentially screens the phoretic attractions.

[1] F. Schmidt, B. Liebchen, H. Löwen, G. Volpe, J. Chem. Phys. 150, 094905 (2019).

DY 13: Focus session: Nonlinear Dynamics of the Heart II (organized by Markus Bär, Stefan Luther and Ulrich Parlitz)

Time: Thursday 13:30–16:15 Location: H2

Invited Talk DY 13.1 Thu 13:30 H2

Multi-scale modeling of dyadic structure-function relation in ventricular cardiac myocytes — •Martin Falcke[1], Filippo G. Cosi[2], Wolfgang Giese[1], Wilhelm Neubert[1], Stefan Luther[2], Nagaiah Chmakuri[3], and Ulrich Parlitz[2] — [1]Max Delbrück Center for Molecular Medicine in the Helmholtz Association, Berlin, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [3]IISER Thiruvananthapuram, India

Cardiovascular disease is often related to defects of sub-cellular components in cardiac myocytes, specifically in the dyadic cleft, which include changes in cleft geometry and channel placement. Modeling of these pathological changes requires both spatially resolved cleft as well as whole cell level descriptions. We use a multi-scale model to create dyadic structure-function relationships to explore the impact of molecular changes on whole cell electrophysiology and calcium cycling. This multi-scale model incorporates stochastic simulation of individual L-type calcium channels (LCC) and ryanodine receptor channels (RyRs), spatially detailed concentration dynamics in dyadic clefts, rabbit membrane potential dynamics, and a system of partial differential equations for myoplasmic and lumenal free calcium and calcium-binding molecules in the cell bulk. We found action potential duration, systolic and diastolic calcium to respond most sensitive to changes in LCC current. The RyR cluster structure inside dyadic clefts was found to affect all biomarkers investigated. The shape of clusters observed in experiments by Jayasinghe et al. and channel density within the cluster showed the strongest correlation to the effects on biomarkers.

DY 13.2 Thu 14:00 H2

Optogenetics control of spiral waves dynamics in cardiac tissue — Sayedeh Hussaini[1], Aidai Mamyraiym kyzy[1], Laura N. Diaz-Maue[1], Johannes Schroeder-Schetelig[1], Vishallini Venkatesan[1], Raul A. Quiñonez Uribe[1], Claudia Richter[1], Vadim Biktashev[2], Rupamanjari Majumder[1], Valentin Krinski[1], and •Stefan Luther[1] — [1]Research Group Biomedical Physics, Max Planck Institute for Dynamics and Self-Organization, G\"ottingen, Germany — [2]Exeter University, Exeter, England, United Kingdom

The heart is an excitable medium. The formation of spiral waves in the heart is the main cause of life-threatening cardiac arrhythmias. Defibrillation is a method to control these abnormal waves. Due to the significant side effects of this method, the development of alternative methods is needed. To do this, we need to deepen our knowledge of the dynamics of spiral waves. For this, Optogenetics has shown its great potential. In this work, using optogenetics we control the dynamics of a spiral wave in a two-dimensional domain of the mouse heart. We apply global and structured illumination patterns at different light intensities. In the sub-threshold regime illumination, we observed the tendency of the spiral wave to drift along the LI gradient. This observation provides us with a new mechanistic insight into optogenetic defibrillation. Global epicardial illumination of the cardiac surface leads to an intramural exponential decay of illumination which may cause the drift of a spiral wave towards the epicardium, where the wave may be terminated with supra-threshold illumination.

DY 13.3 Thu 14:15 H2

Spatiotemporal correlation of cardiac tissue and its variation in response to temperature — •Alessandro Loppini[1], Alessio Gizzi[1], Christian Cherubini[1], Flavio Fenton[2], and Simonetta Filippi[1] — [1]Unit of Nonlinear Physics and Mathematical Modeling, Campus Bio-Medico University of Rome, 00128 Rome, Italy — [2]School of Physics, Georgia Institute of Technology, Atlanta, Georgia, USA

Complex emergent dynamics are at the basis of life-threatening cardiac arrhythmias, including tachycardia and fibrillation. In the past years, a large number of studies have shown that such irregular rhythms in myocardium electrical oscillations are anticipated by cardiac alternans, are supported by nonlinearities, tissue heterogeneity, and anisotropy, and are further shaped by the mechanical and thermal state of the tissue. In this context, a comprehensive understanding of the appearance and development of impaired rhythms, starting from the underlying spatiotemporal dynamics, is required to prevent cardiac failure. In this contribution, we discuss a novel correlation analysis of cardiac activation maps accounting for thermal feedback, showing its application on canine ventricular tissues monitored via optical mapping. Specifically, we define a characteristic length able to describe the emergent synchronization of the tissue and analyze its variations at alternans onset and during their development at different temperatures. Computed results show that the characteristic length is significantly lower in the alternans regime compared to physiological rhythms. Also, we further show that thermal-induced changes in the underlying dynamic result in corresponding variations of the characteristic length.

15 min. break.

Invited Talk DY 13.4 Thu 14:45 H2

Cardiac repolarization dynamics and arrhythmias in healthy and diseased hearts — •Esther Pueyo — University of Zaragoza, Zaragoza, Spain

The electrical activity of the heart is the result of a set of complex nonlinear biophysical and biochemical processes occurring at different scales within the cardiac tissue. The variability arising from these processes translates into variability at the cell, tissue, organ and whole-body levels. The importance of investigating variability in cardiac electrical activity, in general, and in cardiac repolarization (i.e. the return of cells to their resting state after electrical activation), in particular, has been well documented, having shown value for diagnosis, monitoring and treatment of cardiac diseases.

In this talk, I will present studies combining computational, experimental and clinical methods to investigate temporal and spatial variability in cardiac repolarization. I will show the role of stochasticity in contributing to this variability in health and diseased hearts. The link between enhanced repolarization variability and pro-arrhythmia will be described, with emphasis on the role of the autonomic nervous system as a modulator of this link.

DY 13.5 Thu 15:15 H2

Using small perturbations and machine learning for the control of spiral wave chaos — •Thomas Lilienkamp — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

The dynamics during life threatening cardiac arrhythmias like ventricular fibrillation is governed by chaotic spiral/scroll wave dynamics. In ex-vivo experiments and numerical simulations, a phenomenon called self-termination can be observed frequently, where the chaotic dynamics terminates by itself without any interaction. We demonstrate what implications this observation has on the structure of the state space, and how this structure can be exploited for an efficient control of the dynamics via small but finite perturbations (localized in space and time). We also discuss, how machine learning algorithms can be used for the control of such systems.

DY 13.6 Thu 15:30 H2

A simulation study of the effects of optogenetics on the human cardiac pacemaker: Prospects of Opto-ATP control. — Afnan Nabizath Mohamed Nazer[1], Sayedeh Hussaini[2,3], Raul A. Quinonez Uribe[2], Stefan Luther[2,3], and •Rupamanjari Majumder[1,2] — [1]University Medical Center Göttingen, 37075 Göttingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — [3]Institute for the Dynamics of Complex Systems, Goettingen University, Goettingen, Germany

High-frequency electric spiral and scroll waves often occur in the heart during lethal cardiac arrhythmias. Treatment of such arrhythmias necessitates removal of these waves. Currently, the most effective approach to eliminating these waves is defibrillation, which involves delivering high-voltage shocks to the heart. However, the technique is accompanied by numerous negative side effects that make it suboptimal.

Optimizing defibrillation primarily requires reducing defibrillation energy. To this end, the approach that works best for tachycardic arrhythmias is anti-tachycardia pacing (ATP). ATP relies on the external application of a series of low-energy, high-frequency electrical pulses that stimulate the heart faster than the arrhythmia. A biological evolution of this approach would be to replace the external energy source with the heart's own pacemaker. But such a step would require deeper understanding of pacemaker function. Recently, optogenetics has emerged as a powerful tool in cardiac research. Using optogenetic simulations, I explore the possibility to realise ATP in human hearts.

Invited Talk DY 13.7 Thu 15:45 H2

Dynamics of paroxysmal tachycardias — •Gil Bub — McGill University, Montreal, Canada

Reentrant cardiac arrhythmias can start and stop spontaneously, giving rise to paroxysmal bursting rhythms. Experiments and simulations suggest that the dynamics of these paroxysmal reentrant waves may be natural consequences of structural heterogeneity, action potential restitution, and tissue fatigue. Recent experimental studies show that reentrant wave termination is linked to alternans, the beat-to-beat variation in action potential duration and velocity. The impact of alternans on termination was also confirmed using simulations that include restitution curve dynamics. Initiation of these waves, however, is less well understood. Current challenges include the development of imaging technologies that can observe rare spontaneous initiation events in multiple samples to gain mechanistic insights.

DY 14: Mitgliederversammlung Fachverband DY

Tagesordnung:

Bericht DY-Aktivitäten und Entwicklung 2020 - 21

Planung Regensburg 2022

Verschiedenes

Time: Thursday 18:00–19:00 Location: MVDY

60 Minuten

DY 15: Condensed-Matter Simulations augmented by Advanced Statistical Methodologies (joint session DY/CPP)

Time: Friday 10:00–11:00 Location: H2

DY 15.1 Fri 10:00 H2

Simple model to describe stability of thin domains — •Ruben Khachaturyan[1], Arne J. Klomp[2], Karsten Albe[2], and Anna Anna Grünebohm[1] — [1]Interdisciplinary Center for Advanced Materials Simulation, Ruhr-University Bochum — [2]Department of Materials Science, Technical University of Darmstadt, Darmstadt, Germany

Ferro domains are important for contemporary electronics, particularly decreasing domain size allowing for denser information storage per unit area. Thermal fluctuations limit domain stability, which is the key property for ferroic data storage. Therefore the ability to estimate the expected lifetime of a domain is of crucial importance. In this work, we simulate 180° domains in BaTiO3 with different widths at various temperatures using ab initio based molecular dynamics simulation employing LAMMPS and feram codes. We then derived a model to analyze the lifetime of the domains depending on their width and temperature. The model treats domain walls as fluctuating strings. String stiffness reflects the information about energy for domain wall roughening and thermal fluctuations are considered as a field of random forces. Our findings allowed us to interpret the stochastic nature of thin domain collapses and identify associated energies. With further development of the model, we are planning to consider the behavior of ferroelastic and ferromagnetic domain walls.

DY 15.2 Fri 10:15 H2

Population Annealing Monte Carlo Using the Rejection-Free n-Fold Way Update Applied to a Frustrated Ising Model on the Honeycomb Lattice — •Denis Gessert[1,2] and Martin Weigel[1,3] — [1]Centre for Fluid and Complex Systems, Coventry University, Coventry, CV1 5FB, United Kingdom — [2]Institut für Theoretische Physik, Leipzig University, Postfach 100920, D-04009 Leipzig, Germany — [3]Institut für Physik, Technische Universität Chemnitz,

D-09107 Chemnitz, Germany

Population annealing (PA) is a MC method well suited for the study of systems with a rough free energy landscape, e.g. glassy systems. PA is similar to an equilibrium version of parallel simulated annealing runs with the addition of a resampling step at each temperature. While a large population may improve imperfect equilibration, it is evident PA will fail when almost no spins are flipped in the equilibration routine.

This is the case in systems with a low temperature phase transition where high Metropolis rejection rates make sampling phase space near infeasible. To overcome this slowdown we propose a combination of the PA framework with the rejection-free "n-fold way" update and achieve an exponential speed-up at low temperatures compared to Metropolis.

To test our method we study the Ising model with competing ferromagnetic nearest and antiferromagnetic next-to-nearest neighbor interactions of strengths $J_1 > 0$ and $J_2 < 0$, resp., on the honeycomb lattice. As T_c becomes arbitrarily small, when approaching the special point $J_2 = -J_1/4$ with $T_c = 0$, we consider this a good choice to test the efficacy of our method.

DY 15.3 Fri 10:30 H2

Noncontact friction: The role of viscous friction and its nonuniversality — •Miru Lee[1], Niklas Weber[2], Richard Vink[2], Cynthia Volkert[2], and Matthias Krüger[1] — [1]Institut für Theoretische Physik, Friedrich- Hund-Platz 1, 37077 Göttingen — [2]Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

Obtaining theoretical predictions for friction during sliding motion is challenging due to the complex nature of the problem. In the so-called noncontact regime, the friction tensor is given by the leading order of the pairwise interactions between the probe and the surface atoms [1]. In such a regime, one can thus find an analytic expression of the friction tensor [2]. Starting from a stochastic viscoelastic solid model, we identify the two paradigmatic dissipation mechanisms [3]: phonon radiation, prevailing even in a purely elastic solid, and phonon damping, e.g., caused by viscous motion of crystal atoms. At small probe-surface separations, phonon damping dominates over phonon radiation, and vice versa at large separations. Phonon radiation is furthermore universal; there exists a general one-to-one mapping between the mean probe-surface force and the resulting friction. In contrast, phonon damping is non-universal, and no such general relation exists; it is subject to the details of the underlying pairwise interaction, e.g., the interaction range. For certain cases, the friction can even *decrease* with increasing surface area the probe interacts with.

[1] M. Lee, R. Vink, M. Krüger, Phys. Rev. B **101**, 235426 (2020)
[2] A. I. Volokitin, et. al., Phys. Rev. B **73**, 165423 (2006)
[3] M. Lee, R. Vink, C. Volkert, M. Krüger, In preparation.

DY 15.4 Fri 10:45 H2

Investigation of transferability in LDOS based DFT surrogate models for multiscale simulations — •Lenz Fiedler[1,2] and Attila Cangi[1,2] — [1]Center for Advanced Systems Understanding (CASUS) — [2]Helmholtz-Zentrum Dresden-Rossendorf

Density Functional Theory (DFT) is one of the most important computational tools for materials science, as it combines high accuracy with general computational feasibility. However, applications important to scientific progress can pose problems to even the most advanced and efficient DFT codes due to size and/or complexity of the underlying simulations. Namely the modeling of materials across multiple length and time scales at ambient or extreme conditions, necessary for the understanding of important physical phenomena such as radiation damages in fusion reactor walls, evade traditional ab-initio treatment. DFT surrogate models are a useful tool in achieving this goal by reproducing DFT results at drastically reduced computational cost by using machine learning methods. Yet, a lack of transferability of many approaches lead to repeated and costly training data generation procedures. Here, we present results of an investigation to transfer such machine learning DFT surrogate models between different simulation cell sizes, with the goal of reducing the overall amount of computational time for training data generation. The models are based upon the Materials Learning Algorithms (MALA) package [1] and the therein implemented LDOS based machine learning workflow [2].

[1]: https://github.com/mala-project
[2]: J. A. Ellis et al., Phys. Rev. B 104, 035120, 2021

DY 16: Machine Learning in Dynamical Systems and Statistical Physics (joint session DY/BP)

Time: Friday 11:15–12:30 Location: H2

DY 16.1 Fri 11:15 H2

Tayloring Reservoir Computing Performance via Delay Time Tuning — •Tobias Hülser, Felix Köster, and Kathy Lüdge — Institut für Theoretische Physik, TU Berlin

Reservoir Computing is a versatile, fast-trainable machine learning scheme that utilises the intrinsic information-processing capacities of dynamical systems. In recent years delay-based reservoir computing emerged as a promising, easy to implement alternative to classical reservoir computing. Previous work showed that a mismatch between input time and delay time enhances computational performance significantly[1]. For delays much higher than the input time, it was shown that certain inputs cannot be recalled by the network which lead to gaps in the memory capacity[2]. Via manipulating the delays in a system of ring-coupled Stuart-Landau oscillators, we show that some of the gaps can be closed. Moreover, we can tune the range of previous inputs the reservoir can memorise. Consequently, we find a significant increase in performance for nonlinear memory tasks and the NARMA10 task.

[1] S. Stelzer et al., Neural Networks 124, 158-169 (2020)
[2] F. Köster et al., Cogn. Comput. (2020)

DY 16.2 Fri 11:30 H2

Employing artificial neural networks to find reaction coordinates and pathways for self-assembly — •Jörn Appeldorn, Arash Nikoubashman, and Thomas Speck — Inst. für Physik, Universität Mainz, Germany

We study the spontaneous self-assembly of single-stranded DNA fragments using the coarse-grained oxDNA2 implementation [1]. A successful assembly is a rare event that requires crossing a free energy barrier. Advanced sampling methods like Markov state modeling allow to bridge these long time scales, but they require one or more collective variables (order parameters) that faithfully describe the transition towards the assembled state. Formulating an order parameter typically relies on physical insight, which is then verified, e.g., through a committor analysis. Here we explore the use of autoencoder neural networks to automatize this process and to find suitable collective variables based on structural information. For this step, one still needs to map configurations onto structural descriptors, which is a non-trivial task. Specifically, we investigate the latent space of EncoderMap [2] and how it changes with the amount of information contained in the descriptor. With this approach, we were able to determine the free energy landscape, the locations of the (meta)stable states, and the corresponding transition probabilities.

[1] - Snodin et al., J. Chem. Phys.(2015), 142, 234901 [2] - T. Lemke and and C. Peter,J.Chem.TheoryComput.(2019), 15, 1209-1215

DY 16.3 Fri 11:45 H2

Efficient Bayesian estimation of the generalized Langevin equation from data — •Clemens Willers and Kamps Oliver — Center for Nonlinear Science (CeNoS), Westfälische Wilhelms-Universität Münster, Corrensstr. 2, 48149 Münster, Germany

A recent topic of research attracting broad interest is the modeling of stochastic time series whose dynamics includes memory effects. To cover this non-Markovian case, the Langevin equation, which is frequently used in many fields of science, is extended by a memory kernel, yielding the generalized Langevin equation (GLE). Since a direct derivation of the GLE from basic mechanisms through the well known Mori-Zwanzig formalism is not accessible in many cases, it is a relevant question how to estimate the model solely based on measured data.

In our work we develop a realization of Bayesian estimation of the GLE. The Bayesian approach allows for the determination of both estimates and their credibility in a straightforward manner. To facilitate this method, we consider the GLE with white noise. Although this is an approximation, we still deal with a very general model class representing systems with memory.

Importantly for applications, we realize the method in a numeri-

cally efficient manner through a piecewise constant parameterization of the drift and diffusion functions of the model, a reformulation of the likelihood, and an effective initial guess for the estimate.

We illustrate our method by an example from turbulence. Here we are able to reproduce the autocorrelation function of the original data set, which is an essential characteristic of a turbulent flow.

DY 16.4 Fri 12:00 H2

Master memory function for delay-based reservoir computers — •Felix Köster[1], Serhiy Yanchuk[2], and Kathy Lüdge[1] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, 10623 Berlin — [2]Institut für Mathematik, TU Berlin, Str. des 17. Juni 136, 10587 Berlin

The reservoir computing scheme is a versatile machine learning mechanism, which shows promising results in time-dependent task predictions in comparable fast-training times. Delay-based reservoir computing is a modification in which a single dynamical node under the influence of feedback is used as a reservoir instead of a spatially extended system.

We show that many delay-based reservoir computers considered in the literature can be characterized by a universal master memory function (MMF). Once computed for two independent parameters, this function provides linear memory capacity for any delay-based single-variable reservoir with small inputs. Moreover, we propose an analytical description of the MMF that enables its efficient and fast computation. Our approach can be applied not only to the reservoirs governed by known dynamical rules such as Mackey-Glass or Ikeda-like systems but also to reservoirs whose dynamical model is not available.

DY 16.5 Fri 12:15 H2

Investigating the role of Chaos and characteristic time scales in Reservoir Computing — Marvin Schmidt[1,2], Yuriy Mokrousov[1,3], Stefan Blügel[1,3], Abigail Morrison[2,3,4], and •Daniele Pinna[1,3] — [1]Peter Grünberg Institute (PGI-1), Wilhelm-Johnen-Straße, 52428 Jülich, Germany — [2]Institute for Theoretical Neuroscience Institute of Neuroscience and Medicine (INM-6), Wilhelm-Johnen-Straße, 52428 Jülich, Germany — [3]Institute for Advanced Simulation (IAS-6), Wilhelm-Johnen-Straße, 52428 Jülich, Germany — [4]Computational and Systems Neuroscience & JARA-Institut Brain structure-function relationships (INM-10), Wilhelm-Johnen-Straße, 52428 Jülich, Germany

Reservoir Computing (RC) dynamical systems must retain information for long times and exhibit a rich representation of their driving. This talk highlights the importance of matching between input and dynamical timescales in RC systems close to chaos. We compare a chain of Fermi-Pasta-Ulam-Tsingou anharmonic oscillators and a sparsely connected network of spiking excitatory/inhibitory neurons. The first is toy model for magnetic spin-wave reservoirs while the latter that of a biological neural net. Both systems are shown to rely on a close matching of their relaxation timescales with the driving input signal's frequency in order to memorize and make precise use of the information injected. We acknowledge the HGF-RSF project TOPOMANN for funding.

DY 17: Theory and Simulation (joint session CPP/DY)

Time: Friday 13:30–15:00 Location: H3

Invited Talk DY 17.1 Fri 13:30 H3

Data-driven protein design and simulation — •Andrew Ferguson — University of Chicago, Chicago, IL, USA

Data-driven modeling and deep learning present powerful tools that are opening up new paradigms and opportunities in the understanding, discovery, and design of soft and biological materials. In this talk, I will first describe an approach integrating ideas from dynamical systems theory, nonlinear manifold learning, and deep learning to reconstruct protein folding funnels and molecular structures from one-dimensional time series in experimentally measurable observables obtainable by single molecule FRET. I will then describe our recent development and application of deep representational learning to expose the sequence-function relationship within homologous protein families and to use these principles for data-driven design of synthetic proteins with new and/or elevated function.

DY 17.2 Fri 14:00 H3

Are there knots in chromatin? — •Peter Virnau — Institut für Physik, Staudingerweg 9, Johannes Gutenberg-Universität Mainz, 55128 Mainz

The rise of HiC chromosome capture methods has recently enabled low-resolution structures of interphase chromatin [1]. In this presentation I will explain how structures based on single cell contact matrices are obtained from simulations of coarse-grained bead-spring polymer Go models [2]. The role of self-entanglements which naturally occur in this process [2,3] will be critically assessed in the light of theoretical arguments and recent experiments [4].

[1] T.J. Stevens et al, Nature 544, 59-64 (2017). [2] S. Wettermann et al, Comp. Mat. Sci 173, 109178 (2020). [3] J.T. Siebert et al, Polymers 9, 317 (2017). [4] D. Goundaroulis, Biophys. J. 118, 2268-2279 (2020).

DY 17.3 Fri 14:15 H3

Surface Segregation in Athermal Polymer Blends due to Conformational Asymmetry — •Russell Spencer[1] and Mark Matsen[2] — [1]Georg-August Universität Göttingen, Institute for Theoretical Physics, 37077 Göttingen, Germany — [2]University of Waterloo, Waterloo, Ontario, Canada

Monte Carlo simulations are used to investigate the surfaces of athermal blends of stiff and flexible polymers. We vary the bending modulus of the stiff polymers, κ, from zero to the point where the bulk undergoes an isotropic-to-nematic transition. For hard walls characteristic of polymer/solid surfaces, the flexible polymers generally segregate to the surface. However, prior to the bulk transition, there is a surface ordering transition, where a thin nematic layer rich in stiff polymers forms at the surface. On increasing κ further, the thickness of the nematic layer rapidly increases as the bulk isotropic-to-nematic transition is approached. For soft boundaries representative of polymer/air surfaces, a thin layer rich in stiff polymers but without nematic order forms on the outer edge of the surface with a more significant layer rich in the flexible chains beneath. In this case, the nematic layer never appears, and the surface profile evolves continuously with increasing κ.

DY 17.4 Fri 14:30 H3

Ultra-coarse-graining of homopolymers in inhomogeneous systems — •Fabian Berressem[1], Christoph Scherer[2], Denis Andrienko[2], and Arash Nikoubashman[1] — [1]Johannes Gutenberg University, Mainz — [2]Max Planck Institute for Polymer Research, Mainz

We develop coarse-grained (CG) models for simulating homopolymers in inhomogeneous systems, focusing on polymer films and droplets. If the CG polymers interact solely through two-body potentials, then the films and droplets either dissolve or collapse into small aggregates, depending on whether the effective polymer-polymer interactions have been determined from reference simulations in the bulk or at infinite dilution. To address this shortcoming, we include higher order interactions either through an additional three-body potential or a local density-dependent potential (LDP). We parameterize the two- and three-body potentials via force matching, and the LDP through relative entropy minimization. While the CG models with three-body interactions fail at reproducing stable polymer films and droplets, CG simulations with an LDP are able to do so. Minor quantitative differences between the reference and the CG simulations, namely a slight broadening of interfaces accompanied by a smaller surface tension in the CG simulations, can be attributed to the deformation of polymers near the interfaces, which cannot be resolved in the CG representation, where the polymers are mapped to spherical beads.

DY 17.5 Fri 14:45 H3

How to accurately estimate the specific heat of liquid polymers? — •Debashish Mukherji[1], Hongyu Gao[2], Tobias P. W. Menzel[2], and Martin H. Mueser[2] — [1]Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada — [2]Department of Materials Science and Engineering, Saar-

land University, 66123 Saarbruecken, Germany

The field of atomistic simulations of polymers is in a mature stage, yet predictions of specific heat from molecular simulations and successful comparisons with experimental data are scarce if existing at all. One reason for this may be that the internal energy and thus the specific heat cannot be coarse-grained so that they defy their rigorous computation with united-atom models. Moreover, many modes in a polymer barely contribute to the specific heat because of their quantum mechanical nature. Here, we adopt an existing method [1], which defines a specific heat for a harmonic reference, to estimate the specific heat difference between classical and quantum-mechanical systems and use this as a correction factor. Thereby, we predominantly correct the stiff, high-frequency harmonic modes, while leaving the specific-heat contributions of the slow (anharmonic) modes intact [2]. We show how to construct corrections for both all-atom and united-atom descriptions of chain molecules. Corrections computed for a set of hydrocarbon oligomers and commodity polymers deviate by less than kB/10 per particle. The results compare well with experimental data.

[1] Horbach, Kob, and Binder, JPCB 103, 4104 (1999). [2] Gao, Menzel, Mueser, and Mukherji, PRM 5, 065605 (2021).

DY 18: Symposium: Synchronization Patterns in Complex Dynamical Networks (organized by Jakub Sawicki, Sabine Klapp, Markus Bär and Jens Christian Claussen) (joint session DY/SOE)

The program of this session is embedded in a symposium supported by DPG section DY and SOE as well as TU Berlin, SFB 910 and the BCSCCS e.V in Honor of Professor Eckehard Schöll's 70th Birthday. Eckehard Schöll has been the local organizer of the DPG-SKM conferences in Berlin for many years and was awarded the DPG badge of honour (Ehrennadel) for his service to the community.

Time: Friday 13:30–16:00 Location: ESS

Invited Talk DY 18.1 Fri 13:30 ESS

Network-Induced Multistability Through Lossy Coupling — •Jürgen Kurths — PIK, Potsdam, Germany — HU Berlin, Germany

The stability of synchronized networked systems is a multi-faceted challenge for many natural and technological fields, from cardiac and neuronal tissue pacemakers to power grids. For these, the ongoing transition to distributed renewable energy sources leads to a proliferation of dynamical actors. The de-synchronization of a few or even one of those would likely result in a substantial blackout. Thus, the dynamical stability of the synchronous state has become a leading topic in power grid research. Here we uncover that, when taking into account physical losses in the network, the back-reaction of the network induces new exotic solitary states in the individual actors and the stability characteristics of the synchronous state are dramatically altered. These effects will have to be explicitly taken into account in the design of future power grids. We expect the results presented here to transfer to other systems of coupled heterogeneous Newtonian oscillators.

Invited Talk DY 18.2 Fri 14:00 ESS

Control of synchronization in two-layer power grids — •Simona Olmi[1], Carl Totz[2], and Eckehard Schöll[2] — [1]Istituto dei Sistemi Complessi - CNR - Firenze, Italy — [2]Technische Universität Berlin - Germany

In this talk we suggest to model the dynamics of power grids in terms of a two-layer network, and use the Italian high voltage power grid as a proof-of-principle example. The first layer in our model represents the power grid consisting of generators and consumers, while the second layer represents a dynamic communication network that serves as a controller of the first layer. In particular, the dynamics of the power grid is modelled by the Kuramoto model with inertia, while the communication layer provides a control signal P_i^c for each generator to improve frequency synchronization within the power grid. We propose different realizations of the communication layer topology and different ways to calculate the control signal. Then we conduct a systematic survey of the two-layer system against a multitude of different realistic perturbation scenarios, such as disconnecting generators, increasing demand of consumers, or generators with stochastic power output. When using a control topology that allows all generators to exchange information, we find that a control scheme aimed to minimize the frequency difference between adjacent nodes operates very efficiently even against the worst scenarios with the strongest perturbations.

30 min. break.

Invited Talk DY 18.3 Fri 15:00 ESS

Relay and complete synchronization of chimeras and solitary states in heterogeneous networks of chaotic maps — Elena Rybalova[1], Eckehard Schöll[2], and •Galina Strelkova[1] — [1]Institute of Physics, Saratov State University, Astrakhanskaya str. 83, Saratov 410012, Russia — [2]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

In this talk we discuss the phenomena of relay and complete synchronization in a heterogeneous three-layer network of chaotic maps. In the considered network two remote layers are not directly coupled but interact via a relay layer with which they are pairwise and symmetrically coupled. All the three layers represent rings of nonlocally coupled discrete-time oscillators but the relay layer is completely different in its spatiotemporal dynamics from that of the outer layers. We consider the cases when the individual elements of the relay layer and of the outer layers are described by Lozi maps and Henon maps, respectively, and vice versa. We establish and explore relay and complete synchronization of chimera structures and solitary state modes in a heterogeneous multiplex network and analyze the role of the relay layer structure in the resulted synchronous patterns. The results are illustrated by diagrams of desynchronized and synchronous regimes in the "inter-layer coupling - intra-layer coupling of the relay layer" parameter planes.

Invited Talk DY 18.4 Fri 15:30 ESS

A bridge between the fractal geometry of the Mandelbrot set and partially synchronized dynamics of chimera states. — •Ralph G Andrejzak — Universitat Pompeu Fabra, Barcelona, Catalonia, Spain

A simple quadratic map with a complex-valued parameter c allows one to generate enormously rich dynamics and patterns. Fractal Julia sets and the Mandelbrot set divide the complex plane into stable and divergent regions of the map's initial conditions and parameters c. What happens if one couples several quadratic maps? We address this question using a minimal two-population network of two pairs of two quadratic maps. In dependence on c, the network enters into qualitatively different dynamical states. The network iterates can diverge to infinity or remain bounded. Bounded solutions can get fully synchronized, fully desynchronized, or enter into different partially synchronized states, including a symmetry-broken chimera state. We will at first inspect examples for these different dynamical states in the domain of the complex-valued iterates of the network. We then illustrate that the boundaries between different dynamical states form intriguing fractal patterns in the domain of the complex-valued c.

DY 19: Transport (joint session TT/DY)

Time: Friday 13:30–15:00 Location: H6

DY 19.1 Fri 13:30 H6

Spin-relaxation in superconducting graphene systems — •Michael Barth, Jacob Fuchs, Andreas Costa, Klaus Richter, Jaroslav Fabian, and Denis Kochan — Universität Regensburg

The spin-relaxation time τ_s is a fundamental quantity as it determines how long spins can propagate before they relax. For quasi-particles in s-wave superconductors that scatter off magnetic impurities this quantity is expected to decrease by lowering the temperature, known as the Hebel-Slichter-effect [1]. We have shown that this decrease of the spin-relaxation time does not happen generally in all superconductors [2]. A completely opposite behavior can be observed, if Yu-Shiba-Rusinov (YSR) states develop deeply inside the superconducting gap, since then the magnetic moments energetically decouple from the coherence peaks what in turn weakens an exchange interaction with quasi-particles. By employing analytical and numerical methods we have shown that such deep lying in-gap YSR states are formed if a system with magnetic impurities is doped to resonances. As an explicit example we will present results for graphene and bilayer graphene decorated with light magnetic impurities as hydrogen and fluorine.

[1] L. C. Hebel and C. P. Slichter, Phys. Rev. 113, 1504 (1959)
[2] D. Kochan, M. Barth, A. Costa, K. Richter, J. Fabian, Phys. Rev. Lett. 125, 087001 (2020)

DY 19.2 Fri 13:45 H6

Aharonov-Bohm Oscillations in Minimally Twisted Bilayer Graphene — Christophe De Beule[1], Fernando Dominguez[2], and •Patrik Recher[2,3] — [1]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg — [2]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — [3]Laboratory for Emerging Nanometrology, 38106 Braunschweig, Germany

We investigate transport in the network of valley Hall states that emerges in minimally twisted bilayer graphene under interlayer bias. To this aim, we construct a scattering theory that captures the network physics. In the absence of forward scattering, symmetries constrain the network model to a single parameter that interpolates between one-dimensional chiral zigzag modes and pseudo-Landau levels. Moreover, we show how the coupling of zigzag modes affects magnetotransport. In particular, we find that scattering between parallel zigzag channels gives rise to Aharonov-Bohm oscillations that are robust against temperature, while coupling between zigzag modes propagating in different directions leads to Shubnikov-de Haas oscillations that are smeared out at finite temperature.

DY 19.3 Fri 14:00 H6

Spin interference effects in quantum rings in the presence of SU(2) fields — Alberto Hijano[1,2,3], Tineke van den Berg[3], Diego Frustaglia[4], and •Dario Bercioux[3,5] — [1]University of the Basque Country, UPV/EHU, Bilbao, Spain — [2]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, E-20018 Donostia-San Sebastián, Spain — [3]Donostia International Physics Center, Paseo Manuel de Lardizbal 4, E-20018 San Sebastián, Spain — [4]Departamento de Física Aplicada II, Universidad de Sevilla, E-41012 Sevilla, Spain — [5]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Spain

We present a theory of conducting quantum networks that accounts for Abelian and non-Abelian fields acting on spin carriers [1]. We apply this approach to model the conductance of mesoscopic spin interferometers of different geometry (such as squares and rings), reproducing recent experimental findings in nanostructured InAsGa quantum wells subject to Rashba spin-orbit and Zeeman fields [2,3] (as, e.g., the manipulation of Aharonov-Casher interference patterns by geometric means). Moreover, by introducing an additional field-texture engineering, we manage to single out a previously unnoticed spin-phase suppression mechanism. Our approach can also be used for the study of complex networks and the spectral properties of closed systems.

[1] Hijano *et al.*, Phys. Rev. B **103**, 155419 (2021)
[2] Nagasawa, *et al.*, Nat. Commun. **4**, 2526 (2013)
[3] Wang *et al.*, Phys. Rev. Lett. **123**, 266804 (2019)

DY 19.4 Fri 14:15 H6

Length dependent symmetry in narrow chevron-like graphene nanoribbons — •Koen Houtsma[1], Mihaela Enache[1], Remco Havenith[1,2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, 9747AG Groningen, the Netherlands — [2]Stratingh Institute for Chemistry, University of Groningen, 9747AG Groningen, the Netherlands

Graphene nanoribbons (GNRs) are an exciting material due to their excellent and tunable electronic properties. For instance, GNRs with armchair edges possess a width-dependent band gap, whereas zigzag GNRs are expected to host spin-polarized edge states and be semimetallic [1]. Previously, narrow chevron-like GNRs, which host a combination of zigzag and armchair edge terminations, were fabricated on a Au(111) substrate from the prochiral precursor 6,12-dibromochrysene through a combination of Ullmann-type coupling and cyclodehydrogenation [2]. Depending on the number of monomer units the ribbons are made of, an even and an odd number lead to a mirror and a point symmetric ribbon, respectively. Using scanning tunneling spectroscopy we investigated the potential effect of this length dependent symmetry on the electronic properties. In addition, bends are formed in these ribbons through a common coupling defect. We characterized these bends using a combination of high-resolution scanning tunneling microscopy and spectroscopy. The bends are based on the formation of both a five- and six-membered ring and their electronic properties are altered.

[1] K. Nakada et al., Phys. Rev. B 54, 17954 (1996)
[2] T.A. Pham et al., Small 13, 1603675 (2017)

DY 19.5 Fri 14:30 H6

Thermal fluctuations of two-dimensional crystalline membranes: a scale-invariant but nonconformal field theory — •Achille Mauri and Mikhail I. Katsnelson — Radboud University, Institute for Molecules and Materials, Nijmegen, The Netherlands

Statistical fluctuations of two-dimensional membranes have been the subject of extensive investigations, from string theories to biological and condensed matter systems such as graphene and other atomically-thin 2D materials. In the case of solid layers subject to vanishing external tension, the interplay of thermal fluctuations and anharmonic phonon-phonon interactions gives rise to a crucial renormalization of the elastic constants: as a result, the long-wavelength behavior of phonon fluctuations is scale-invariant and it is controlled by an interacting fixed point of the renormalization group (RG). In this contribution, we argue that, in contrast with several other field-theories, the emergent dilatation symmetry is not enhanced to the full conformal invariance. We analyze in particular, the structure of the energy-momentum tensor $T_{\mu\nu}$ within an ϵ-expansion, after extension of the problem from the physical dimension $D = 2$ to a non-integer dimensionality $D = 4 - \epsilon$. The trace $T_{\mu\mu}$ reduces, at the fixed point, to the total divergence of a non-trivial virial current, implying the absence conformal invariance.

DY 19.6 Fri 14:45 H6

Viscous, elastic and ballistic shear response of electron fluids probed through optical spectroscopy — •Davide Valentinis[1,2], Jan Zaanen[3], Dirk van der Marel[4], and Joerg Schmalian[1,2] — [1]Institut für Quantenmaterialien und Technologien, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstra{\ss}e 1, D-70569 Stuttgart (DE) — [3]Department of Quantum Matter Physics, University of Geneva, 24 Quai Ernest-Ansermet, 1211 Geneva 4, Switzerland — [4]Institute-Lorentz for Theoretical Physics, Leiden University, PO Box 9506, NL-2300 RA Leiden, The Netherlands

Can optical spectroscopy provide complementary and unambiguous fingerprints of spatial nonlocality in bulk and layered materials, and under which conditions? To answer these questions, we investigate the nonlocal current response of 3D charged Fermi liquids, and 2D isotropic and anisotropic metals, taking into account momentum-conserving collisions and momentum-relaxing scattering in kinetic-theory approaches. In strongly interacting Fermi liquids, a propagating shear mode of Fermi-surface deformation, analogous to transverse sound in liquid helium, determines characteristic oscillating patterns of the thin-film transmission as a function of radiation frequency. We develop a kinetic theory for the distribution function of 2D Fermi gases with arbitrary electronic dispersion relation, using a collision operator

formalism. The skin depth and surface impedance are shown to qualitatively depend on the shape and orientation of the polygonal Fermi surface.