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

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Overview of Invited Talks and Sessions

(Lecture Rooms H39, H44, H46, H47, and H48; Poster C)

Invited Talks

DY 4.1	Mon	15:00–15:30	H47	**Environmental Superstatistics** — •Christian Beck
DY 4.2	Mon	15:30–16:00	H47	**Statistical decomposition of atmospheric turbulence** — •Matthias Wächter, Allan Morales, Tanja Mücke, Nico Reinke, Joachim Peinke
DY 4.3	Mon	16:00–16:30	H47	**Quantitative approaches to the statistics of extreme events in atmospheric dynamics** — •Holger Kantz, Jochen Broecker, Leo Granger, Julia Gundermann
DY 4.4	Mon	16:30–17:00	H47	**Climate as a Problem of Non-equilibrum Statistical Mechanics** — •Valerio Lucarini
DY 14.1	Tue	15:00–15:30	H44	**When the beat goes off** — •Holger Hennig
DY 14.2	Tue	15:30–16:00	H44	**Chimera states and the transition from spatial coherence to incoherence** — •Philipp Hövel
DY 16.1	Wed	9:30–10:00	H46	**Dynamics of thin sheets: Crumpling, wrinkling and cracking** — •Pascal Damman
DY 18.10	Wed	12:00–12:30	H48	**The physics of information: from Maxwell's demon to Landauer** — •Eric Lutz
DY 20.1	Wed	15:00–15:30	H44	**Energiewende 2.0 * the transformation of energy systems in uncertain times** — •Jürgen-Fr. Hake, Wolfgang Fischer
DY 20.2	Wed	15:30–16:00	H44	**Basin Stability and its Consequences for Power Grids** — •Jürgen Kurths, Peter Menck, Peng Ji
DY 20.3	Wed	16:00–16:30	H44	**Requirements and Concepts for Self-Organized Agent-Based Control in Smart Distribution Grids** — •Astrid Niesse
DY 20.4	Wed	16:30–17:00	H44	**A 100% renewable power system in Europe** — •Martin Greiner, Sarah Becker, Rolando Rodriguez, Tue Jensen, Timo Zeyer, Anders Soendergaard, Gorm Andresen
DY 22.6	Wed	16:30–17:00	H48	**Entropy based approaches to transport** — •Thomas Christen
DY 26.1	Thu	9:30–10:00	H47	**Genuine quantum interference in interacting bosonic fields: The semiclassical propagator in Fock space** — •Juan Diego Urbina, Thomas Engl, Arturo Arguelles, Julien Dujardin, Peter Schlagheck, Klaus Richter
DY 29.1	Thu	15:00–15:30	H44	**Transitions in rotating Rayleigh-Benard convection at high Rayleigh numbers** — •Andreas Tilgner
DY 29.2	Thu	15:30–16:00	H44	**Connecting Statistics and Dynamics of Turbulent Rayleigh–Bénard Convection** — •Johannes Lülff, Michael Wilczek, Rudolf Friedrich, Richard Stevens, Detlef Lohse, Klaus Petschel, Ulrich Hansen
DY 29.3	Thu	16:00–16:30	H44	**Temperature statistics near the ultimate state of turbulent Rayleigh-Bénard convection** * — •Xiaozhou He, Dennis van Gils, Eberhard Bodenschatz, Guenter Ahlers
DY 29.4	Thu	16:30–17:00	H44	**Cloud formation studies in moist Rayleigh-Benard convection** — •Jörg Schumacher

Invited talks of the joint symposium SYSC

See SYSC for the full program of the symposium.

SYSC 1.1	Tue	9:30–10:00	H1	**Exploring the Physics of Superconducting Qubits Strongly Coupled to Microwave Frequency Photons** — •Andreas Wallraff
SYSC 1.2	Tue	10:00–10:30	H1	**Hybrid Quantum Circuit with a Superconducting Qubit Coupled to an Electron Spin Ensemble** — •Yuimaru Kubo, Cecile Grezes, Igor Diniz, Jun-ichi Isoya, Vincent Jacques, Anais Dreau, Jean-François Roch, Alexia Auffeves, Denis Vion, Daniel Esteve, Patrice Bertet
SYSC 1.3	Tue	10:30–11:00	H1	**Hybrid Quantum Systems with Rare-Earth Ion Spin Ensemble** — •Pavel Bushev
SYSC 1.4	Tue	11:00–11:30	H1	**Quantum Coherent Coupling between a Mechanical Oscillator and an Optical Mode** — Ewold Verhagen, Dalziel Wilson, Vivishek Sudhir, Nicolas Piro, Albert Schliesser, •Tobias Kippenberg
SYSC 1.5	Tue	11:30–12:00	H1	**Exploring Quantum Light-Matter Interactions of Quantum Dots in Photonic Crystal Nanostructures** — •Jonathan Finley, Arne Laucht, Michael Kaniber, Stefan Lichtmannecker, Thorsten Reichert, Guenther Reithmaier, Fabrice Laussy, Ulrich Hoheneester

Invited talks of the joint symposium SYMM

See SYMM for the full program of the symposium.

SYMM 1.1	Thu	9:30–10:00	H1	**Challenges for first-principles based computation of properties of oxide materials** — •Karsten Albe
SYMM 1.2	Thu	10:00–10:30	H1	**Deformation and Fracture of Solids: Tough Nuts at Atomic and Continuum Scales** — •Peter Gumbsch, Matous Mrovec, Kinshuk Srivastava, Daniel Weygand
SYMM 1.3	Thu	10:30–11:00	H1	**Crucial Issues and Future Directions of Through-Process Modeling** — •Guenter Gottstein
SYMM 1.4	Thu	11:00–11:30	H1	**Adaptive Resolution Simulations for Soft Matter: Applications and New Developments** — •Kurt Kremer
SYMM 1.5	Thu	11:30–12:00	H1	**Materials by design** — •Markus Buehler

Sessions

DY 1.1–1.10	Mon	9:30–12:15	H39	**Quantum Dynamics, Decoherence and Quantum Information I**
DY 2.1–2.8	Mon	9:30–11:30	H47	**Statistical Physics in Biological Systems I (joint with BP)**
DY 3.1–3.7	Mon	15:00–17:00	H39	**Quantum Dynamics, Decoherence and Quantum Information II**
DY 4.1–4.6	Mon	15:00–17:30	H47	**Focus Session: Atmospheric and Climate Complexity**
DY 5.1–5.5	Mon	15:00–16:15	H48	**Reaction-Diffusion Systems**
DY 6.1–6.9	Mon	15:00–17:30	H34	**Glasses and Glass Transition (joint session DY/CPP) I**
DY 7.1–7.25	Mon	17:30–19:30	Poster C	**Poster I**
DY 8.1–8.15	Mon	17:30–19:30	Poster C	**Poster I: Glasses and Glass Transition (joint session DY/DF/CPP)**
DY 9.1–9.24	Mon	17:30–19:30	Poster B2	**Poster I: Statistical Physics in Biological Systems (joint with BP)**
DY 10.1–10.11	Tue	9:30–12:30	H46	**Glasses (joint session DY/DF/CPP)**
DY 11.1–11.8	Tue	9:30–11:45	H47	**Statistics and Dynamics of/on Networks (joint session BP/DY/SOE)**
DY 12.1–12.12	Tue	9:30–12:45	H48	**Nonlinear Dynamics, Synchronization and Chaos I**
DY 13.1–13.5	Tue	9:30–12:00	H1	**Symposium: Strong Coupling in Solid State Quantum Systems (SYSC)**
DY 14.1–14.2	Tue	15:00–16:00	H44	**Nonlinear Dynamics, Synchronization and Chaos II**
DY 15.1–15.4	Tue	15:00–16:00	H37	**Evolutionary Game Theory (joint session BP/DY/SOE)**
DY 16.1–16.9	Wed	9:30–12:15	H46	**Pattern Formation**
DY 17.1–17.8	Wed	10:00–12:00	H47	**Soft matter**
DY 18.1–18.10	Wed	9:30–12:30	H48	**Statistical Physics Far from Thermal Equilibrium**

DY 19.1–19.9	Wed	9:30–12:30	H37	**Focus Session: Dynamics of Adaptive Networks (joint session BP/DY/SOE)**
DY 20.1–20.6	Wed	15:00–17:30	H44	**Focus Session: Modern Power Grid, Nonlinear Dynamics and Self-Organization (joint with SOE)**
DY 21.1–21.12	Wed	15:00–18:15	H47	**Granular Matter / Contact Dynamics**
DY 22.1–22.12	Wed	15:00–18:30	H48	**Statistical Physics (general)**
DY 23.1–23.9	Wed	15:00–17:30	H43	**Statistical Physics in Biological Systems II (joint with BP)**
DY 24.1–24.5	Wed	15:45–17:00	H37	**Networks, From Topology to Dynamics (joint session BP/DY/SOE)**
DY 25.1–25.12	Thu	9:30–12:45	H46	**Critical Phenomena and Phase Transitions**
DY 26.1–26.8	Thu	9:30–12:00	H47	**Quantum Chaos I**
DY 27.1–27.7	Thu	9:30–11:30	H48	**Fluid Dynamics and Turbulence**
DY 28.1–28.5	Thu	9:30–12:00	H1	**Symposium: Computational Challenges in Scale-Bridging Modeling of Materials (SYMM)**
DY 29.1–29.4	Thu	15:00–17:00	H44	**Focus Session: Rayleigh Benard System and Convective Turbulence**
DY 30.1–30.5	Thu	15:00–16:15	H47	**Quantum Chaos II**
DY 31.1–31.7	Thu	15:00–16:45	H48	**Anomalous Diffusion**
DY 32.1–32.10	Thu	15:00–17:30	H46	**Statistical Physics in Biological Systems III (joint with BP)**
DY 33.1–33.63	Thu	17:00–19:00	Poster C	**Poster II**
DY 34.1–34.1	Thu	19:00–20:00	H47	**Annual General Meeting of DY**
DY 35.1–35.8	Fri	9:30–11:30	H48	**Brownian Motion and Transport**
DY 36.1–36.12	Fri	9:30–12:45	H44	**Statistical Physics in Biological Systems IV (joint with BP)**

Annual General Meeting of the Dynamics and Statistical Physics Division

Donnerstag 19:00–20:00 H47

- Bericht
- Verschiedenes

DY 1: Quantum Dynamics, Decoherence and Quantum Information I

Time: Monday 9:30–12:15 Location: H39

DY 1.1 Mon 9:30 H39

Iterated Mori projector (IMoP) approach for driven dissipative quantum many body systems — •Peter Degenfeld-Schonburg and Michael J. Hartmann — Technische Universität München, Physik Department I, James Franck Str., 85748 Garching, Germany

We report on a pertubative method for driven dissipative quantum many body systems on a lattice that goes beyond Meanfield. Our approach is based on the Mori projection operator technique where we treat a single lattice site as the system of interest and trace out the dynamical many body environment comprised of all remaining lattice sites. The resulting on-site master equation describes the dynamics up to second order in the hopping. To account for a dynamical environment the master equation is solved iteratively. We apply our methods to arrays of coupled non-linear harmonic oscillators, i.e. to a Bose Hubbard model, in a driven and dissipative regime and numerically show the advantage of IMoP over Meanfield.

DY 1.2 Mon 9:45 H39

Counting statistics for Dicke-Superradiance — •Wassilij Kopylov, Clive Emary, and Tobias Brandes — TU Berlin, Institute of Theoretical Physics, Deutschland

We consider the Dicke-Hamiltonian valid in a rotating frame and couple it to a dissipative zero- temperature bath. We derive a cumulant generating function for emitted photons using the P - representation of the master equation with counting field for this model in the thermodynamic limit. The macroscopic occupation in the superradiant case is determined by the linear terms in the master equation.

DY 1.3 Mon 10:00 H39

Equation-of-motion method for full counting statistics: Steady-state superradiance — •Malte Vogl, Gernot Schaller, Eckehard Schöll, and Tobias Brandes — Institut für Theoretische Physik, TU Berlin, Berlin, Germany

For the multimode Dicke model in a transport setting that exhibits collective boson transmissions, we construct the equation of motion for the cumulant-generating function. Approximating the exact system of equations at the level of the cumulant-generating function and system operators at lowest order allows us to recover master equation results of the full counting statistics for certain parameter regimes at very low computational cost. The thermodynamic limit, which is not accessible with the master equation approach, can be derived analytically for different approximations.

Ref.: M.V., G. Schaller, E. Schöll, and T.Brandes, PRA **86**, 033820 (2012)

DY 1.4 Mon 10:15 H39

General Decoupling Procedure for Expectation Values of Four-Operator Products in Electron-Phonon Quantum Kinetics — •Nicolas Teeny and Manfred Fähnle — Max Planck Institute for Intelligent Systems, 70569 Stuttgart, Heisenbergstr.3,Germany

Electron-phonon quantum kinetic effects are important for studying the coherent ultrafast dynamics on time scales shorter than about a picosecond after exciting the electrons of a solid with a short laser pulse of duration smaller than 100 femtoseconds. An example is the femtosecond-demagnetization of a ferromagnetic film after exposure to a strong optical laser pulse. In the density-matrix formalism of electron phonon quantum kinetics the hierarchy of infinitely many coupled equations of motion for the expectation values of products of electron and phonon creation and annihilation operators of arbitrary order is usually terminated on the level of equations of motion for the expectation vales of three-operator products by using decoupling procedures for the four-operator products occurring in these equations. In the literature decoupling procedures are discussed for special types of electron and phonon states. In the talk generalized decoupling procedures are derived for arbitrary electron and phonon states.

DY 1.5 Mon 10:30 H39

The role of non-linear second-order coupling Hamiltonians in photoemission and Raman spectroscopy — Johannes Flick[1], Heiko Appel[1], and •Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

In this talk we employ an exact Fock space representation to study Holstein-Su-Schrieffer-Hamiltonian systems[1,2] coupled to quantized photon modes. In particular, we include non-linear electron-phonon couplings, which originate from an expansion to second order in the nuclear displacement[3]. We perform exact diagonalizations and real-time propagations for the model in Fock space and investigate the effect of the nonlinear couplings on photoemission (PE), inverse photoemission (IPE) and Raman spectra.

[1] W.P. Su, J.R. Schrieffer, A.J. Heeger Phys. Rev. Lett., **42** (1979), pp. 1698−1701
[2] T. Holstein, Ann. Phys. (N.Y.) **8**, 325 (1959)
[3] L. Cederbaum and W. Domcke, J. Chem. Phys. **60**, 7 (1974). **80**, 212303 (2009).

15 min. break.

DY 1.6 Mon 11:00 H39

Linear and non-linear responses in pump-probe spectroscopy — •Tanja Dimitrov[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

In this work, we investigate the time-dependent dipole response of molecular systems for pump probe laser experiments. We compare the response of widely used approximate adiabatic functionals in time-dependent density functional theory to the exact solution of the time-dependent Schrödinger equation for realistic model systems. In particular, we focus on the role of memory effects and the corresponding signature in the optical absorption spectra.

DY 1.7 Mon 11:15 H39

Efficiency scaling of non-coherent upconversion — •Jochen Zimmermann[1], Roberto Mulet[1,2], Thomas Wellens[1], Greg D. Scholes[1,3], and Andreas Buchleitner[1] — [1]Albert-Ludwigs-Universität Freiburg — [2]University of Havana, Cuba — [3]University of Toronto, Canada

A very promising approach to obtain efficient upconversion of light is the use of triplet-triplet annihilation of excitations in molecular systems. In real materials, besides upconversion, many other physical processes take place - fluorescence, non-radiative decay, annihilation, diffusion - and compete with upconversion. The main objective of the presented work [1] is to design a proof of principle model that can be used to shed light on the relevance of the interaction between the different physical processes that take part in these kinds of systems. Ultimately, we want to establish general principles that may guide experimentalists toward the design of materials with maximum efficiency. Here we show, in a 1D model system, that even in the presence of these processes upconversion can be optimized by varying the ratio between the two molecular species present in this kind of materials. We derive scaling laws for this ratio and for the maximum efficiency of upconversion, as a function of the diffusion rate J, as well as of the creation and of the decay rate of the excitations.

[1] J. Zimmermann, R. Mulet, T. Wellens, G.D. Scholes and A. Buchleitner. arXiv:1211.5004 [cond-mat.mtrl-sci]

DY 1.8 Mon 11:30 H39

Wave-packet revivals and decoherence in vibronically coupled systems — •Heiko Appel — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Electronic decoherence is central for our understanding of physical processes that are prevailing in a large variety of phenomena such as photosynthesis, vision or solar-cell applications. In this work, we investigate the coupled vibronic dynamics in short trans-polyacetylene oligomers which are described in terms of a Su-Schrieffer-Heeger (SSH) Hamiltonian. Using explicit matrix representations of Fock space operators, we illustrate how to construct a numerically exact solution for the coupled system of electrons, phonons and photons. From the exact solution of the model, we extract time scales for electronic decoherence and relate this to the decay of wave-packet revivals.

DY 1.9 Mon 11:45 H39

Influence of Vibrations on Energy Transfer and Optical Properties of Light-Harvesting Systems — •Gerhard Ritschel[1], Jan Roden[1,3], Walter T. Strunz[2], and Alexander Eisfeld[1,4] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Technische Universität Dresden, Germany — [3]University of California, Berkeley, USA — [4]Harvard University, Cambridge, USA

The transfer of electronic excitation energy as well as optical properties of complexes of interacting chromophores, e.g. the FMO complex or the LH2 antennae in biological photosynthetic systems, are strongly influenced by an environment. For a proper theoretical description it is essential to include non-Markovian effects resulting from an electron-environment coupling that is a rather structured function of energy leading to a complicated retroaction on the excitation dynamics. Based on the non-Markovian quantum state diffusion an approximate non-perturbative master equation can be derived that captures the whole range from coherent dynamics to incoherent diffusion. Especially situations where environment-assisted transfer occurs can be investigated. Using that approach we calculated energy transfer in one FMO subunit as well as in the full FMO trimer and calculated linear spectra at various temperatures employing the thermofield description.

DY 1.10 Mon 12:00 H39

Concersvative Brownian motion simulation of a hard-boson gas — •Wolfgang Paul — Institut für Physik, Martin Luther Universität, 06120 Halle (Saale)

We present a simulation study of the properties of the Tonks-Girardeau gas, a system of N hard-core bosons confined in a one-dimensional harmonic trap. For this system the ground-state wave function is exactly known based on a Bose-Fermi mapping theorem. We employ Nelsons* interpretation of quantum mechanics in which this N-body wave function gives rise to a set of stochastic differential equations for the positions of the N particles, which can be simulated by standard methods. Particularly, real space densities and momentum distributions can simply be determined by time averages along particle trajectories. Employing this approach we are able to significantly extend the range of particle numbers N treated numerically compared to earlier approaches, while reproducing all exactly known results for this model. We also show that for the bosons in a harmonic trap, contrary to what has been assumed so far, the momentum distribution reflects the system size scaling of the occupation numbers of the natural orbitals, i.e., it can be used to decide on the presence of a Bose-Einstein condensate.

DY 2: Statistical Physics in Biological Systems I (joint with BP)

Time: Monday 9:30–11:30 Location: H47

DY 2.1 Mon 9:30 H47

Cardiorespiratory data segmentation during sleep — •Sabrina Camargo[1], Maik Riedl[1], Celia Anteneodo[2], Thomas Penzel[3], and Niels Wessel[1] — [1]Department of Physics, Humboldt Universität zu Berlin, Berlin, Germany — [2]Department of Physics, PUC-Rio, Rio de Janeiro, Brazil — [3]Sleep Center, Charité University Hospital, Berlin, Germany

The variability in cardiorespiratory data is closely related to the regulation of sleep. When the brain is very active as in the REM sleep stage, heart rate as well as respiration have long-range correlations, while, in contrast, in deep sleep those correlations vanish after a few seconds, indicating that cardiovascular data can be useful to reflect sleep disturbances. But physiological data usually display a highly nonstationary behavior, caused by either environmental conditions or the inherent complexity of the underlying dynamics of the biological rhythms. Considering that the signal is composed of stationary segments, we apply a nonparametric segmentation approach in order to detect such locally stationary segments, where statistical measures of first and second order, for example, mean and variance, are more likely to remain constant. Thus, segmentation provides a picture of the nonstationarity of a time series, in particular, the intrinsic time scales. Moreover, by finding the stationary regimes, we are able to identify changes in time series, as those coming from the cyclic reduction of the airflow. We compare the segmentation outcomes in the presence and the absence of respiratory induced sleep disturbances and we verify an increased variability in blood pressure in patients suffering from this events.

DY 2.2 Mon 9:45 H47

Extended diffusion models for sleep stage switching — Anna Barkentien and •Jens Christian Claussen — INB, University of Lübeck, Germany

Short awakening periods especially occuring during the second half of the night follow a peculiar power law [1] for which biologically plausible models still are not available. A pure Markov analysis [2] assuming random switching however ignores any deterministic components in the dynamics which are manifest in time correlations. The phenomenological model proposed in [1] describes sleep depth by a one-dimensional diffusion process with a reflecting border for sleep and a restoring force for wake. In contrast to an Ornstein-Uhlenbeck process the restoring force is inversely proportional (or a power law with negative exponent) to the excursion distance from the sleep/wake border. We extend this model in [3] to account for the REM state and modify the restoring force law to account for deviations to the power law that are observed in data from some (but not all) labs and obtain a better fit to data [3].

[1] C.-C. Lo, L. A. Nunes Amaral, S. Havlin, P. Ch. Ivanov, T. Penzel, J.-H. Peter, and H. E. Stanley. Dynamics of sleep-wake transitions during sleep. Europhysics Letters, 57, 631, 2002.
[2] J. W. Kim, J. -S. Lee, P. A. Robinson, D. -U. Jeong, Markov Analysis of Sleep Dynamics. Phys. Rev. Lett. 102, 2009.
[3] A. Barkentien and J.C. Claussen (in preparation).

DY 2.3 Mon 10:00 H47

Caveats in Modelling Coarse-Grained Descriptions of a Bistable Frustrated Unit — •Darka Labavić[1], Hannes Nagel[2], Wolfhard Janke[2], and Hildegard Meyer-Ortmanns[1] — [1]School of Engineering and Science, Jacobs University Bremen — [2]Institut für Theoretische Physik, Universtät Leipzig

From a coarse-grained perspective the motif of a self-activating species, activating a second species which acts as its own repressor, is widely found in biological systems. In [1] we studied this model on the proteonic level in a fully stochastic version. In [2] we zoom into the level of genes which are described as directly producing proteins. We focus on the effect that inherent time scales of the underlying scale of this genetic circuit can have on the bifurcation patterns on the coarser scale of proteins. Depending on the ratio of binding and unbinding rates of the transcription factors to the decay times of the proteins, the appropriate averaging procedure for obtaining a coarse-grained description changes and leads to sets of deterministic equations, which considerably differ in their bifurcation structure. In particular, the desired intermediate range of regular limit cycles fades away when the binding rates of genes are not fast as compared to the decay time of the proteins. Our analysis illustrates that the common topology of the widely found motif alone does not imply universal features in the dynamics.

[1] Garai A, Waclaw B, Nagel H, and Meyer-Ortmanns H, J. Stat. Mech. (2012) P01009;
[2] Labavić D, Nagel H, Janke W, and Meyer-Ortmanns H, submitted

DY 2.4 Mon 10:15 H47

DNA denaturation in correlated environments — Viktoria Blavatska[1], •Christian von Ferber[2], and Yurij Holovatch[1] — [1]Institute for Condensed Matter Physics, NAS Ukraine, Lviv — [2]Applied Mathematics Research Centre, Coventry University, UK

We revisit the problem of DNA denaturation in the frames of the Poland-Scheraga model. This model predicts a first or second order transition depending on the value of the loop exponent.

Usually an unperturbed background is assumed within this model. However, in a biologically relevant environment correlated structures are prevalent and the transition may change due to the influence of this environment.

Applying renormalisation group methods we determine the loop exponent in higher orders up to the fourth order in the ϵ-expansion. In the absence of disorder this allows us to determine the numerical value of the exponent using resummation techniques.

Performing corresponding calculations for the situation of correlated

environments we find strong disorder effects.

DY 2.5 Mon 10:30 H47

Simulations of aggregation in homopolymer systems — •Johannes Zierenberg and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Germany

We investigate the aggregation transition of a coarse-grained many-polymer system. To this end we apply parallel multicanonical simulations for different system sizes and densities. Our data suggests that the aggregation process in the simple model is a first-order phase transition. We investigate the dependence of the transition temperature on the density and size of the system and look at generic properties.

DY 2.6 Mon 10:45 H47

Collective behaviour of competing, coupled particles on a 1d chain — •Ines Weber[1], Ludger Santen[1], and Martin Evans[2] — [1]Department of Theoretical Physics, Saarland University, 66041 Saarbrücken, Germany — [2]Department of Physics & Astronomy, University of Edinburgh, Edinburgh EH9 3JZ, UK

Biopolymers are dynamic filaments involved in a wide variety of biological processes such as intracellular transport. Experiments have shown them to exhibit non-equilibrium fluctuations and deformations induced by molecular motors. I will present a simple model of such processes, which comprises competing species of interacting particles on a lattice. They perform a 'tug-of-war' and induce deformation and drift on a 1d chain. Constraints given by hard core coupling to next-neighbour sites influence the system's dynamics and result in collective particle behaviour.

DY 2.7 Mon 11:00 H47

Coexistence and survival in conservative Lotka-Volterra networks — •Johannes Knebel[1], Torben Krüger[2], Markus Weber[1], and Erwin Frey[1] — [1]Arnold-Sommerfeld Center for Theoretical Physics and Center for NanoScience, Theresienstraße 37, 80333 München — [2]Department of Mathematics, Ludwig-Maximilians-Universität München, Theresienstraße 38, 80333 München

Conservative Lotka-Volterra (LV) models play a fundamental role in many fields of science such as population dynamics. New insights into the maintenance of biodiversity can be gained by understanding the long-term behavior of complex LV interaction networks and by revealing their coexistence and survival scenarios.

Here we present a classification scheme for coexistence scenarios in well-mixed, conservative LV networks. Our theoretical approach to study global stability properties builds on a deterministic analysis by using the Pfaffian of the interaction matrix, a simpler form of the determinant for skew-symmetric matrices. We find that the classification of conservative LV dynamics on the basis of their interaction topology is incomplete and that non-cyclic networks can also maintain coexistence of all species. The deterministic analysis also leads to a deeper understanding of the stability of ecological networks in finite populations as is reflected by a generalized scaling law for the extinction time in the vicinity of critical reaction rates. Our general results are illustrated for systems composed of four and five species.

DY 2.8 Mon 11:15 H47

Evolutionary game dynamics between random mutants — •Weini Huang[1], Bernhard Haubold[2], Christoph Hauert[3], and Arne Traulsen[1] — [1]Evolutionary Theory Group, Max Planck Insitute for Evolutionary Biology, August-Thienemann-Straße 2, 24306, Plön,Germany — [2]Bioinformatics Group,Max-Planck-Insitute for Evolutionary Biology, August-Thienemann-Straße 2, 24306, Plön,Germany — [3]Department of Mathematics, The University of British Columbia, 1984 Mathematics Road, Vancouver V6T1Z2, British Columbia, Canada

Polymorphism occurs when more than one genotype or phenotype exist in the same population. Although polymorphisms are often observed in populations, the emergence and maintenance of polymorphsims remain unclear.We investigate this question by introducing a new model, named as mutant games. In evolutionary game theory, the interactions of different types in a population are described by payoff matrices. However, the number of types is usually fixed and payoff matrices are typically predefined. This can be a limit to model a biological population with random mutations. In our mutant games, the interactions of mutants and resident types are represented by a dynamical payoff matrix. The resulting dynamics caused by random mutants under frequency dependent selection, leads to a remarkably higher diversity, compared to the mutants under constant selection. Interestingly, although arbitrary number of mutants are allowed in mutant games, an intermediate level of diversity is maintained.

DY 3: Quantum Dynamics, Decoherence and Quantum Information II

Time: Monday 15:00–17:00 Location: H39

DY 3.1 Mon 15:00 H39

Many-body localization and thermalization in the full probability distribution function of observables — •Elena Canovi[1], Davide Rossini[2], Rosario Fazio[2], Giuseppe Santoro[3,4,5], and Alessandro Silva[3,4] — [1]Institut für Theoretische Physik III, Universität Stuttgart — [2]NEST, Scuola Normale Superiore, and Istituto Nanoscienze-CNR, Piazza dei Cavalieri 7, I-56126 Pisa, Italy — [3]SISSA, Via Bonomea 265, I-34136 Trieste, Italy — [4]International Centre for Theoretical Physics (ICTP), PO Box 586, I-34014 Trieste, Italy — [5]CNR-IOM Demoscritos National Simulation Center, Via Bonomea 265, I-34136 Trieste, Italy

We investigate the relation between thermalization following a quantum quench and many-body localization in quasiparticle space in terms of the long-time full distribution function of observables. In particular we focus on the long-time behavior of an integrable XXZ chain subject to an integrability- breaking perturbation. We study the effect of integrability-breaking on the asymptotic state after a quench of the anisotropy parameter, looking at the behavior of the full probability distribution of the transverse and longitudinal magnetization of a subsystem. We compare the resulting distributions with those obtained in equilibrium at an effective temperature set by the initial energy. We find that, while the long time distribution functions appear to always agree qualitatively with the equilibrium ones, quantitative agreement is obtained only when integrability is fully broken and the relevant eigenstates are diffusive in quasi-particle space.

DY 3.2 Mon 15:15 H39

The Hows and Whys of Multidimensional Instantons: Tunnelling effects in gas- and condensed-phase systems — •Jeremy O. Richardson[1,2], Stuart C. Althorpe[1], and Michael Thoss[2] — [1]Department of Chemistry, University of Cambridge, UK — [2]Institut für Theoretische Physik und Interdisziplinäres Zentrum für Molekulare Materialien, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7/B2, D-91058 Erlangen

We describe a simple method for locating semiclassical instantons in multidimensional systems [1]. Using steepest-descent integration of a discretized form of Feynman's path integral, these instantons can be used to compute chemical reaction rates in the deep-tunnelling regime and the energy-level splitting pattern resulting from tunnelling between degenerate potential wells [2]. Applications are shown for systems in full dimensionality using *ab initio* potential-energy surfaces including proton-transfers and water cluster rearrangements [3].

The discretized instantons are closely related to the method of ring-polymer molecular dynamics [4], which explains why the latter is able to obtain reaction rates so reliably in the deep-tunnelling regime [1]. An extension to simulate nonadiabatic quantum dynamics using the mapping representation [5] in ring-polymer form is discussed.

[1] J. O. Richardson and S. C. Althorpe, *J. Chem. Phys.* **131**, 214106 (2009). [2] *ibid.* **134**, 054109 (2011). [3] J. O. Richardson, S. C. Althorpe and D. J. Wales **135**, 124109 (2011). [4] I. R. Craig and D. E. Manolopoulos, *J. Chem. Phys.* **123**, 034102 (2005). [5] G. Stock and M. Thoss, *Phys. Rev. Lett.* **78**, 578 (1997).

DY 3.3 Mon 15:30 H39

Creation and protection of entangled states through local operations and a non-Markovian environment — •Rebecca Schmidt, Jürgen T. Stockburger, and Joachim Ankerhold — Institut für Theoretische Physik, Universität Ulm, Albert Einstein-Allee 11, 89069 Ulm

Local operations alone cannot create entanglement. Dissipation normally has a destructive effect on entangled states. Suprisingly, the *combined* effect of local operations and dissipation can create and preserve entanglement for suitably chosen protocols. Building on recent techniques for the optimal control theory of open quantum systems [1], we show how to entangle two noninteracting harmonic oscillators under the influence of local operations and a 'mutual drag' induced by the environment. Even though the latter effect inevitably exposes the system to reservoir noise (mandated by the fluctuation-dissipation theorem), entanglement is created and maintained. Our use of stochastic Liouville-von Neumann equations [2] for the reduced system dynamics guarantees consistency with a physical reservoir model for arbitrarily strong/fast driving.

[1] R. Schmidt, A. Negretti, J. Ankerhold, T. Calarco and J.T. Stockburger, PhysRevLett **107**,130404(2011)
[2] J.T. Stockburger and H. Grabert, PhysRevLett **88**,170407(2002)

DY 3.4 Mon 15:45 H39

Genuine three-qubit entanglement from coupling to a heat bath — •Christopher Eltschka[1], Daniel Braun[2,3], and Jens Siewert[4,5] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Université de Toulouse, Laboratoire de Physique Théorique (IRSAMC), F-31062 Toulouse, France — [3]CNRS, LPT (IRSAMC), F-31062 Toulouse, France — [4]Departamento de Química Física, Universidad del País Vasco UPV/EHU, 48080 Bilbao, Spain — [5]Ikerbasque, Basque Foundation for Science, 48011 Bilbao, Spain

Initially unentangled qubits which do not interact which each other can become entangled by interacting with a common heat bath [1]. But with more than two qubits, there exist several inequivalent types of entanglement [2]. Therefore it is an important question which types of entanglement can be generated. While exactly determining and quantifying the entanglement for mixed states of more than two qubits is an unsolved problem, recent advancements [3] based on the Greenberger-Horne-Zeilinger symmetry [4] allow to determine a good lower bound for the entanglement. By using those methods we show that for three qubits coupled to the same heat bath indeed all types of entanglement can be generated for almost all separable initial states.

[1] D. Braun, Phys. Rev. Lett. **89**, 277901 (2002).
[2] W. Dür, G. Vidal, and J.I. Cirac, Phys. Rev. A **62**, 062314 (2000).
[3] C. Eltschka and J. Siewert, to be published in Scientific Reports.
[4] C. Eltschka and J. Siewert, Phys. Rev. Lett. **108**, 020502 (2012).

15 min. break.

DY 3.5 Mon 16:15 H39

Nonequilibrium Quantum Phase Transitions in the Ising Model — •Victor Manuel Bastidas Valencia, Clive Emary, Gernot Schaller, and Tobias Brandes — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We establish a set of nonequilibrium quantum phase transitions in the Ising model driven under monochromatic nonadiabatic modulation of the transverse field. We show that besides the Ising-like critical behavior, the system exhibits a novel anisotropic transition which is absent in equilibrium. The novel nonequilibrium quantum phases correspond to states which are synchronized with the external control in the long-time dynamics. A preprint including our results is available under the arXiv Reference: arXiv:1207.5242v1

DY 3.6 Mon 16:30 H39

Statistical mechanics for a periodically driven closed quantum system — •Achilleas Lazarides, Arnab Das, and Roderich Moessner — Max Planck Institute for the Physics of Complex Systems

We study closed quantum systems in the presence of periodic driving, that is, isolated systems not in contact with a bath. We find that the system reaches a periodic steady state which is well-described by an appropriate modification of standard statistical mechanical concepts.

DY 3.7 Mon 16:45 H39

The Casimir companion X — •Frank Boldt[1], James D. Nulton[2], Bjarne Andresen[3], Peter Salamon[2], and Karl Heinz Hoffmann[1] — [1]Institute of Physics, Chemnitz University of Technology - D-09107 Chemnitz, Germany — [2]Department of Mathematical Science, San Diego State University - San Diego, California, 92182, USA — [3]Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen , Denmark

In this talk a new invariant of motion for Hamiltonian systems is presented: the Casimir companion. For systems with simple dynamical algebras (e.g., coupled spins, harmonic oscillators) our new invariant is useful in problems that consider adiabatically varying the parameters in the Hamiltonian. In particular, it has proved useful in optimal control of changes in these parameters. The Casimir companion also allows simple calculation of the entropy of non-equilibrium ensembles.

DY 4: Focus Session: Atmospheric and Climate Complexity

This focus session is devoted to modern methods to analyze complex systems which are applied to climate and atmospheric physics. This is also in the context of the initiative "Mathematics of Planet Earth 2013", which is supported by many different science organisations. (Organizer Christian Beck)

Time: Monday 15:00–17:30 Location: H47

Invited Talk DY 4.1 Mon 15:00 H47

Environmental Superstatistics — •Christian Beck — School of Mathematical Sciences, Queen Mary, University of London, London E1 4NS, UK

Complex systems in driven nonequilibrium situations often consist of a superposition of various dynamics on well-separated time scales. Often one or several parameters (such as e.g. the local inverse temperature beta) fluctuate on a rather large time scale, much larger than the relaxation time of the local system, and one can then apply so-called superstatistical techniques. The basic idea is to have a superposition of two statistics, one given by ordinary statistical mechanics and the other one by that of the fluctuating parameter. The resulting marginal distributions typically have fat tails, which can be understood by methods borrowed from large deviation theory. The superstatistics concept has been recently applied to a variety of complex systems, in particular to the dynamics of tracer particles in turbulent flows, to traffic delay statistics, cancer survival statistics, and share price fluctuations. After a short review of the field I will describe some new results on environmentally relevant superstatistics, dealing with typical temperature distributions observed on Planet Earth, wind velocity fluctuations, as well as rainfall/flooding statistics.

Invited Talk DY 4.2 Mon 15:30 H47

Statistical decomposition of atmospheric turbulence — •Matthias Wächter, Allan Morales, Tanja Mücke, Nico Reinke, and Joachim Peinke — ForWind - Institut für Physik, Universität Oldenburg

Atmospheric turbulence shows pronounced intermittency in the probability density functions of wind velocity increments $u_r = u(t+\tau)-u(t)$, in the sense of very high probabilities of extreme events, over a wide range of scales τ. This intermittency is commonly observed to be significantly stronger and covering a wider range of scales than that found in homogeneous isotropic turbulence (HIT) in laboratory experiments.

We present a superposition approach which allows for a decomposition of atmospheric turbulence into subsets obeying statistics similar to HIT in the sense of Kolmogorov's theory of 1962. The practical relevance of atmospheric intermittency is demonstrated for the example of wind energy converters. Furthermore, we give an outlook to the application of our approach in wind tunnel experiments with the aim of generating wind tunnel flows similar to atmospheric turbulence.

Invited Talk DY 4.3 Mon 16:00 H47

Quantitative approaches to the statistics of extreme events in atmospheric dynamics — •Holger Kantz[1], Jochen Broecker[2], Leo Granger[1], and Julia Gundermann[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Dept.

Mathematics and Statistics, University of Reading, UK

We discuss various statistical aspects of extreme events based on empirical and theoretical grounds. We consider specifically extreme events caused by the dynamics of the atmosphere such as wind gusts, precipitation events and large temperature anomalies. Relevant quantities are the event rate/return time as a function of event magnitude for very rare events. Whereas data analysis shows that marginal distributions of most types of extremes do not have fat tails and hence extremes are not by orders of magnitudes larger than the standard deviation, correlations in the succession of extremes render large deviation results invalid. One potential theoretical approach to the estimation of the frequency of very rare events is offered by non-equilibrium fluctuation theorems, and we present preliminary results of a study of a two-dimensional hydrodynamical flow. Finally, we discuss predictability and performance of extreme event prediction and show that conclusions depend much stronger on the choice of the performance criterion than anticipated.

Invited Talk DY 4.4 Mon 16:30 H47

Climate as a Problem of Non-equilibrum Statistical Mechanics — •Valerio Lucarini — Klimacampus, Institute of Meteorology, University of Hamburg, Hamburg, Germany — Department of Mathematics and Statistics, University of Reading, Reading, UK

The investigation of the climate system is one of the grand challenges of contemporary science. Such a problem is gaining more and more relevance as exoplanets are being discovered at an accelerating rate and rather exotic atmospheric circulations are being conjectured, due to the vast variety of possible astronomical and astrophysical configurations. In this contribution we will discuss how non-equilibrium statistical mechanics (and, specifically the adoption of the mathematical framework provided by Axiom A dynamical systems) allows framing in a rigorous and efficient way classical problems of climate science such as the understanding of the climatic response to forcings of general nature and the parametrization of unresolved processes.

DY 4.5 Mon 17:00 H47

Rain in a test-tube! — •Martin Rohloff[1,2] and Jürgen Vollmer[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [2]Faculty of Physics, University of Göttingen, 37077 Göttingen, Germany

Demixing of multiphase fluids is important for precipitation in the atmosphere of the earth and other planets. The mechanisms of droplet growth that lead to precipitation are under vivid discussion.

We present a lab experiment in which repeated precipitation cycles can be observed. Binary mixtures of liquids are used as model systems. They undergo demixing when subjected to a shallow temperature ramp. We perform measurements of the droplet size distribution and turbidity measurements. Having access to the droplet size distribution for many oscillations and different types of binary mixtures, we identify the dependence on different material parameters like density, viscosity, surface tension, as well as the influence of heating rate and sample geometry.

DY 4.6 Mon 17:15 H47

Disentangling different types of El Niño episodes by evolving climate network analysis — Alexander Radebach[1,2,3], •Reik V. Donner[1], Jonathan F. Donges[1,2], Jakob G.B. Runge[1,2], and Jürgen Kurths[1,2] — [1]Potsdam Institute for Climate Impact Research, Germany — [2]Department of Physics, Humboldt University, Berlin, Germany — [3]Mercator Research Institute on Global Commons and Climate Change, Berlin, Germany

Complex network theory provides a powerful toolbox for studying the backbone of statistical interrelationships between multiple time series in various scientific disciplines. In this work, we apply the recently proposed climate network approach for characterizing the evolving correlation structure of the Earth's climate system based on reanalysis data of surface air temperatures. We provide a detailed study on the temporal variability of several global climate network characteristics, which allows deriving results that go significantly beyond recent findings. Based on a simple conceptual view on sparse climate networks, we are able to give a thorough interpretation of our evolving climate network characteristics, which allows a functional discrimination between recently recognized different types of El Niño episodes (so-called cold-tongue and warm pool events). In this respect, our analysis provides deep insights into the Earth's climate system, particularly its response to strong volcanic eruptions and large-scale impacts of different types of El Niño episodes, and thus contributes to the understanding of the global signatures of distinct phases of the El Niño Southern Oscillation (ENSO).

DY 5: Reaction-Diffusion Systems

Time: Monday 15:00–16:15 Location: H48

DY 5.1 Mon 15:00 H48

Boundary-mediated stabilization of a scroll ring in a tubular reactor — •Pavel Paulau, Harald Engel, and Jakob Löber — Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, Sekr EW 7-1, 10623 Berlin, Deutschland

It is known, that the scroll ring solutions to the Complex Ginzburg-Landau-equation have positive filament tension leading to the shrinking and disappearance of the ring. We utilize the fact, that the core of a two-dimensional spiral wave can be locked by the interaction with a Neumann boundary. It is shown, that a scroll ring in a tubular reactor can be stabilized due to interaction with the wall, preventing the shrinking of the scroll ring. The minimal radius of cylinder needed to get the robust stable scroll ring is defined.

DY 5.2 Mon 15:15 H48

Analytic solution for stabilized wave segments in an excitable medium — •Vladimir Zykov and Eberhard Bodenschatz — Max Planck Institute for Dynamics and Self-Organization, D-37077 Goettingen, Germany

The relationships between the medium excitability and the propagating velocity and the shape of a stabilized wave segment in excitable media are analytically derived for the wave with a trigger front and a phase wave at the wave back. Two universal limits restricting the region of existence of wave segments in the parameter space are demonstrated [1]. The predictions of the free-boundary approach are in good quantitative agreement with results from numerical reaction-diffusion simulations performed on the Kessler-Levine model.

[1] V.S. Zykov and E. Bodenschatz, Phys. Rev. Lett., submitted.

DY 5.3 Mon 15:30 H48

Efficient kinetic Monte Carlo method for reaction-diffusion problems with spatially varying annihilation rates — •Karsten Schwarz and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, Saarbrücken

We present an efficient Monte Carlo method to simulate reaction-diffusion processes with spatially varying particle annihilation or transformation rates as it occurs for instance in the context of motor-driven intracellular transport. Like Green's function reaction dynamics and first-passage time methods, our algorithm avoids small diffusive hops by propagating sufficiently distant particles in large hops to the boundaries of protective domains. Since for spatially varying annihilation or transformation rates the single particle diffusion propagator is not known analytically, we present an algorithm that generates efficiently either particle displacements or annihilations with the correct statistics, as we prove rigorously. The numerical efficiency of the algorithm is demonstrated with an illustrative example.

DY 5.4 Mon 15:45 H48

Experimental observation of solitons and backfiring during the electrochemical oxidation of carbon monoxide on Pt — •Philipp R. Bauer[1], Antoine Bonnefont[2], and Katharina Krischer[1] — [1]Physik-Department, TU München, Germany — [2]Institut de Chimie de Strasbourg, CNRS - Université de Strasbourg, France

Pattern formation during the electrooxidation of carbon monoxide is investigated with spatially resolved ATR-FTIR spectroscopy on thin platinum film electrodes. The use of a flow cell setup, in which the electrolyte passes the electrode from one side to the other, is effectively

isolating the surface dynamics in one spatial dimension. The dynamic properties of the system are enriched by adding small amounts of halide ions to the solution.

Tracking the adsorbed CO on the surface reveals solitary reaction waves, which move perpendicular to the flow of the electrolyte across the electrode. The waves may backfire, leading to the creation of another wave, which moves in the opposite direction. Furthermore, interpenetrating wave collisions are found, in which two colliding pulses endure the collision and move on. This soliton-like behavior during collisions is explained with a three variable model capturing the interplay of the chemical autocatalysis of the CO-subsystem and two inhibitory variables, namely the potential drop across the electrolyte and the blocking effect of the halide ions.

DY 5.5 Mon 16:00 H48

Controlling the position of fronts — •Jakob Löber, Eckehard Schöll, and Harald Engel — Institut für Theoretische Physik

We present a method to control the position as a function of time of a one-dimensional traveling front solution of a one-component reaction-diffusion system according to a specified protocol of movement. Given this protocol, the control function is found as the solution of a perturbatively derived integral equation. Two cases are considered. First, we derive an analytical expression for the space (x) and time (t) dependent control function $f(x,t)$ valid for arbitrary protocols and arbitrary bistable reaction kinetics. These results for the control agree well with results of an optimal control algorithm. Second, for stationary control the integral equation reduces to a Fredholm integral equation of the first kind. For the Schlögl model, we present an analytical solution of the problem to stop a front at a specified position. All analytical results are in good agreement with numerical simulations of the underlying reaction-diffusion equations. Extensions to two spatial dimensions and other equations supporting traveling wave solutions are considered.

DY 6: Glasses and Glass Transition (joint session DY/CPP) I

Time: Monday 15:00–17:30 Location: H34

Invited Talk DY 6.1 Mon 15:00 H34

Intra- and inter-molecular dynamics in glass-forming liquids — •Periklis Papadopoulos[1], Wilhelm Kossack[2], and Friedrich Kremer[2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Universität Leipzig, Germany

The intra- and inter-molecular interactions of salol and polystyrene, as low molecular weight and polymeric glass-forming model systems, are studied by Fourier-transform infrared (FTIR) spectroscopy and Broadband Dielectric Spectroscopy (BDS). By analysing the temperature dependencies of specific IR absorption bands it is demonstrated that each molecular moiety in the glass-formers has its own signature in the course of the dynamic glass transition: while some do not show any change at the calorimetric glass transition temperature, others exhibit a pronounced "kink". The effects cannot be attributed solely to microscopic thermal expansion, but instead indicate gradual conformational changes. The ease of application of this approach to a variety of systems in different geometries and external conditions can assist the modelling of glasses and the understanding of the coupling between the glass transition and molecular-level dynamics.

[1] P. Papadopoulos, W. Kossack, and F. Kremer, *Soft Matter*, 2013, **9**, 1600 - 1603

DY 6.2 Mon 15:30 H34

In-situ investigation of vapor-deposited thin films of toluene and ethylbenzene by AC chip-nanocalorimetry — •Mathias Ahrenberg[1], Katie R. Whitaker[2], Yeong-Zen Chua[1], Heiko Huth[1], Mark D. Ediger[2], and Christoph Schick[1] — [1]Institut für Physik, Universität Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — [2]Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA

Physical vapor deposition can be used to produce thin films with particular material properties. For example extraordinarily stable glasses can be obtained from organic molecules like toluene and ethylbenzene. We have investigated properties like packing efficiency and kinetic stability depending on substrate temperature and deposition rate by in-situ AC chip-nanocalorimetry. We have varied the substrate temperature covering the range from temperatures proven to yield high enthalpy glasses up to temperatures proven to yield low enthalpy glasses. This way the complete evolution of the mentioned stable glass properties is observed. Moreover AC calorimetry offers the possibility for isothermal measurements which enables to follow the transformation of the stable glass to the super-cooled liquid. Transformation experiments give suggestion of the transformation mechanism and its temperature dependence. The data are in agreement with a growth front for the transformation of the stable glass into the supercooled liquid.

DY 6.3 Mon 15:45 H34

Calorimetric glass transition of ultathin films of homopolymers and their blends — •Huajie Yin and Andreas Schönhals — BAM Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin, Germany

Glass transition behavior of different ultrathin polymer films (down to around 10 nm) was investigated by specific heat spectroscopy using differential AC calorimetry. For thin homopolymer films like polystyrene (PS) and poly(vinyl methyl ether) (PVME), no thickness dependence of dynamic glass transition temperature was observed down to 10 nm. Furthermore, the width of the glass transition is independent of the film thickness which indicates that the extent of the cooperativity is essentially smaller than 10 nm. For polymer blend thin films in the case of PS/PVME with the weight fraction of 50/50, the dynamic glass transition temperature was found to be decreasing with reducing the film thickness. This phenomenon is explained in terms of surface enrichment of PVME in the polymer blend system where PVME has a lower surface energy than PS. X-ray photoelectron spectroscopy (XPS) was used to probe the surface composition in order to confirm such surface enrichment phenomena.

DY 6.4 Mon 16:00 H34

Molecular dynamics of a discotic liquid crystal studied by Dielectric Relaxation and Specific Heat Spectroscopy — •Christina Krause[1], Huajie Yin[1], Andreas Wurm[2], Christoph Schick[2], and Andreas Schönhals[1] — [1]BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, D-12205 Berlin — [2]Institute of Physics, University of Rostock, Wismarsche Straße 43-45, D-18051 Rostock

The molecular dynamics of the discotic liquid crystal pyrene-1,3,6,8-tetracarboxylic tetra(2-ethylhexyl)ester is investigated by dielectric relaxation and specific heat spectroscopy. The data from dielectric spectroscopy shows 3 processes: a β-relaxation at low temperatures and an α-relaxation in the temperature range of the mesophases followed by conductivity. In both phases the dielectric α-relaxation is assigned to restricted glassy dynamics. Glassy dynamics is also detected in the plastic crystalline phase by means of specific heat spectroscopy but with a different temperature dependence of the relaxation rates. This is discussed considering the different molecular restrictions of the fluctuations: close to the columns (dielectric spectroscopy) and more in the intercolumnar space (specific heat spectroscopy). In the frame of the fluctuation approach a correlation length of glassy dynamics is calculated to 0.78 nm which correlates well to the core-core distance estimated by X-ray scattering.

DY 6.5 Mon 16:15 H34

Liquid to glass transition in a Wigner glass — •Fabian Westermeier, Michael Sprung, and Gerhard Grübel — HASYLAB, Deutsches Elektronen-Synchrotron, 22607 Hamburg, Germany

One of the interesting problems of disordered systems is the nature of the liquid to glass transition. While the glass transition in molecular glass formers can be typically achieved by cooling down the system, in colloidal systems the glassy state is experimentally accessible by changing the strength of the direct particle interactions.

Colloidal systems can be distinguished by their type of interaction. While so called hard sphere systems interact via a repulsive, short range interaction potential, electrostatically stabilized systems are interacting via a long-range, screened Coulomb potential which depends inter alia on the charge of the particles and the concentration of ad-

ditional ions in the solvent screening the direct particle interactions. As it is thus possible to tune the direct particle interaction strength of these systems, the glass transition can already occur at much lower volume fractions when compared to the hard sphere case.

We have used X-ray scattering techniques to investigate the glass transition of a charge stabilized system at a constant volume fraction, varying only the strength of the direct particle interactions. While the average structure of the colloidal suspensions shows only minor changes, the dynamics of the system vary strongly as a function of the direct particle interaction strength.

DY 6.6 Mon 16:30 H34

Temporal evolution of structural and dynamical heterogeneities in a metastable colloidal fluid — •Sebastian Golde[1,2], Markus Franke[2], and Hans Joachim Schöpe[2,3] — [1]Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [2]Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Germany — [3]MPI für Polymerforschung, Postfach 3148, 55021 Mainz, Germany

An interesting property of the metastable melt is that it exhibits spatial heterogeneous dynamics [1]. The dynamics can be understood as an accumulation of mobile and immobile particles. Recent work suggested that the local structure and dynamics of the metastable melt are correlated to each other [2]. In order to investigate these phenomena we used a hard sphere like colloidal model system. The local dynamics in the metastable colloidal melt were measured with our recently new designed multispeckle correlation spectroscopy setup which performs space- as well as time-resolved dynamic light scattering. The solidification kinetics was measured using an advanced time-resolved laser light Bragg scattering setup. The correlation between the particle dynamics and the solidification kinetics could be quantified by analyzing the temporal evolution of the local particle dynamics, the ensemble averaged dynamic structure factor and the solidification kinetics. Crossing the glass transition point we can show that there is fundamental link between crystallization and vitrification. [1] L. Berthier and G. Biroli, Rev. Modern Physics 83 (2011),[2] T. Kawasaki and H. Tanaka, JCPM 22 (2010)

DY 6.7 Mon 16:45 H34

Multiple reentrant glass transitions in confined hard-sphere glasses — •Suvendu Mandal[1,2], Simon Lang[3], Rolf Schilling[4], Vitalie Botan[4], Martin Oettel[4], Dierk Raabe[1], Thomas Franosch[3], and Fathollah Varnik[1,2] — [1]Max-Planck Institut fur Eisenforschung, Max-Planck Str. 1, 40237 Dusseldorf, Germany — [2]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universitat Bochum, Stiepeler Strasse 129, 44801 Bochum, Germany — [3]Institut fur Theoretische Physik, Friedrich-Alexander-Universitat Erlangen-Nurnberg, Staudtstraße 7, 91058, Erlangen, Germany — [4]Institut fur Physik, Johannes Gutenberg-Universitat Mainz, Staudinger Weg 7, 55099 Mainz, Germany

We perform molecular dynamics simulations for a polydisperse, densely packed hard-sphere fluid confined between two parallel walls [1]. The diffusion coefficient parallel to the walls is observed to vary by orders of magnitudes upon changing the wall separation while keeping the packing fraction fixed. A striking multiple reentrance scenario emerges for the transition from liquid to glass as the wall separation becomes comparable to the particle diameter. The non-monotonic behavior of the phase diagram is rationalized in terms of a numerical solution of a recently developed mode-coupling theory [1,2].

[1] S. Mandal, S. Lang, R. Schilling, V. Botan, M. Oettel, D. Raabe, T. Franosch, and F. Varnik submitted [2] S. Lang, V. Botan, M. Oettel, D. Hajnal, T. Franosch, R. Schilling PRL 105, 125701 (2010).

DY 6.8 Mon 17:00 H34

Shear banding in hard sphere glasses — Segun Ayodele[1], Dierk Raabe[1], Ingo Steinbach[2], and •Fathollah Varnik[1,2] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]ICAMS, Ruhr Universität Bochum, Germany

When an amorphous solid is exposed to a simple shear such as a planar Couette flow, the flow may become heterogeneous despite the fact that the macroscopic stress is constant across the system [1,2]. However, both in computer simulations [1,3] and experiments [2] the observed velocity profile is unsteady with significant spatio-temporal fluctuations. In this work, we address the question whether a steady shear banded solution may exist. For this purpose, we both perform an analysis of the underlying equations as well as lattice Boltzmann simulations, using as input the constitutive laws obtained from MD simulations [3].

[1] F. Varnik, L. Bocquet, J.-L. Barrat, L. Berthier, Phys. Rev. Lett. 90, 095702 (2003).

[2] R. Besseling, L. Isa, P. Ballesta, G. Petekidis, M.E. Cates, W.C.K. Poon, Phys. Rev. Lett. 105, 268301 (2010).

[3] S. Mandal, M. Gross, D. Raabe, F. Varnik, Phys. Rev. Lett. 108, 098301 (2012).

DY 6.9 Mon 17:15 H34

Re-establishment of the equipartition theorem for small systems in molecular dynamics ensemble — •Nima Hamidi Siboni[1,2], Dierk Raabe[2], and Fathollah Varnik[3] — [1]AICES, RWTH-Aachen, Germany — [2]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [3]ICAMS, Ruhr-Universität Bochum, Germany.

It has been reported recently that, in molecular dynamics (MD) simulations, periodic boundary condition leads to a violation of the equipartition theorem for systems containing particles with different masses [Shirts et al, J. Chem. Phys. **125** 164102 (2006)]. This effect is associated with the finite number of particles in MD simulations. Here, we propose a modification to MD simulation, which removes this problem. Our method is based on imposing Gaussian random fluctuations on the system's center of mass velocity. Using the analogy to a system exchanging momenta with impenetrable walls, we work out an analytical expression for the rate at which fluctuations are added to the system. The restoration of the equipartition is then demonstrated for small systems both at equilibrium as well as beyond equilibrium in the linear response regime.

DY 7: Poster I

This Poster Session has contributions from the Topics DY 1 and DY 3 Quantum dynamics; DY 2 Statistical physics in biological systems; DY 5 Reaction diffusion systems; DY 11 Statistics and dynamics of /on networks; DY 12 Nonlinear dynamics, synchronization and Chaos;

Time: Monday 17:30–19:30 Location: Poster C

DY 7.1 Mon 17:30 Poster C

Zeno effect for repeated projective and finite-time measurements — •Andreas Prinz-Zwick[1], Gert-Ludwig Ingold[1], Peter Talkner[1], and Juyeon Yi[2] — [1]Institut für Physik, Univ. Augsburg, Germany — [2]Dept. of Physics, Pusan National University, Korea

The decay of an unstable state can be slowed down by frequently repeated measurements and even be stopped completely under continuous observation. This so-called quantum Zeno effect has been studied for a single particle on a one-dimensional chain subject to repeated projective measurements on the first lattice site [1]. In contrast to previous work, we keep track of all possible measurement outcomes. While the Zeno effect is obtained for short times, asymptotically the system approaches a uniform state. As an extension, we have considered non-projective measurements where the system is coupled to a measurement apparatus as introduced in [2]. The Zeno effect is studied as a function of the duration of the measurement τ_m and the time between measurements τ_a. An optimal measurement is achieved by appropriately choosing the coupling strength as a function of τ_m. It is found that for not too large duration of the measurement, the Zeno effect becomes more pronounced when τ_m is increased [3].

[1] J. Yi, P. Talkner, G.-L. Ingold, Phys. Rev. A **84**, 032121 (2011)
[2] W. Zurek, Ann. Phys. (N.Y.) **9**, 855 (2000)
[3] A. Prinz-Zwick, Master thesis (Universität Augsburg, 2012)

DY 7.2 Mon 17:30 Poster C

Quantum-classical correspondence in the dynamics of the

Dicke model — •Lutz Bakemeier, Andreas Alvermann, and Holger Fehske — Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald, Deutschland

The Dicke model describes an ensemble of two-level systems coupled to a quantum oscillator. It shows several interesting properties in its classical limits. While the ground state features a quantum phase transition, the classical dynamics shows a transition from regular to chaotic motion.

We consider the question how the signatures of the classical model evolve in the quantum model when the classical limit is approached. Based on Chebyshev expansion and kernel polynomial numerical methods we give an overview of the quantum-classical correspondence observable in the dynamical spectral functions, the time evolution of individual states, and the global dynamics in phase space. We analyze the excitations in the dynamical spectral function which correspond to the collective modes of the classical model characterizing the quantum phase transition. For the global dynamics we discuss a quantum equivalent to the classical Poincaré surface of section on phase space. This quantity shows how the systems eigenstates localize on different parts of the energy shell and thus adequately describes the transition from regular to chaotic motion.

DY 7.3 Mon 17:30 Poster C

Strong driving in open quantum systems: Beyond Markovian dynamics — •Christine Brix and Jürgen T. Stockburger — Institut für Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

Strong driving of an open quantum system typically leads to a breakdown of the commonly used strategy of Born, Markov, and RWA approximations. Hence, the typical quantum optical master equation (Lindblad type) becomes unreliable. Here we present a non-RWA equation of motion which preserves the initially given separable structure of the interaction, keeping the dissipative terms "agnostic" of the system Hamiltonian which may contain driving of arbitrary strength and time dependence. In contrast to previous work the resulting stochastic equation of motion can now be cast in a form that does not involve a sign problem. This gain in efficiency allows new applications in both quantum information and chemical physics.

DY 7.4 Mon 17:30 Poster C

Controlled engineering of extended states in disordered systems — •Alberto Rodriguez[1], Arunava Chakrabarti[2], and Rudolf A Römer[3] — [1]Physikalisches Institut, Albert-Ludwigs Universität Freiburg, Hermann-Herder Strasse 3, D-79104, Freiburg, Germany — [2]Department of Physics, University of Kalyani, Kalyani, West Bengal-741 235, India — [3]Department of Physics and Centre for Scientific Computing, University of Warwick, Coventry, CV4 7AL, United Kingdom

We describe how to engineer wavefunction delocalization in disordered systems modelled by tight-binding Hamiltonians in $d > 1$ dimensions [1]. We show analytically that a simple product structure for the random onsite potential energies, together with suitably chosen hopping strengths, allows a resonant scattering process leading to ballistic transport along one direction, and a controlled coexistence of extended Bloch states and anisotropically localized states in the spectrum. We demonstrate that these features persist in the thermodynamic limit for a continuous range of the system parameters. Numerical results support these findings and highlight the robustness of the extended regime with respect to deviations from the exact resonance condition for finite systems. The localization and transport properties of the system can be engineered almost at will and independently in each direction. This study gives rise to the possibility of designing disordered potentials that work as switching devices and band-pass filters for quantum waves, such as matter waves in optical lattices.

[1] Phys. Rev. B 86, 085119-12 (2012)

DY 7.5 Mon 17:30 Poster C

Energy Transfer and Decoherence in Phase Space — •Per Liebermann[1,2] and Oliver Mülken[2] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Albert-Ludwigs-Universität Freiburg, Germany

Phase space methods can be used to describe both classical and quantum mechancal transport processes, such as, for instance, the energy transfer in photosynthetic light harvesting complexes. To gain a deeper insight into the phase space dynamics of the Continuous-Time Quantum Walk on a discrete network, a discrete Wigner function represents the quantum state of the system. Environmental effects such as decoherence are implemented in the framework of the Lindblad Master Equation. In this context, the Quantum Stochastic Walk contains the Random Walk and the Quantum Walk as special cases for both strong and weak coupling strengths. Furthermore a source and a drain are added to the trimer's network, leading to a simplified model for the excitation transport within the Fenna-Matthews-Olsen complex.

DY 7.6 Mon 17:30 Poster C

Simulation of a particle in a one-dimensional double-well potential using stochastic mechanics — •Jeanette Köppe and Wolfgang Paul — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Germany

It was shown that the well-known Schrödinger equation is equivalent to a conservative Brownian motion [1]. This concept enables to investigate the duration of quantum-mechanical processes, hence there is the opportunity to directly study particle dynamics.

Using Nelson's interpretation of quantum mechanics, we simulate the tunneling process of a particle in a one-dimensional double-well potential to demonstrate its predictive power. In particular, we determine the mean first passage time needed to cross the barrier, which is equal to the tunneling time in quantum mechanics, and study its dependence on the width and the height of the barrier. The respective results are compared to those calculated by "normal" quantum mechanics.

[1] E. Nelson, Phys. Rev. 150, 1079-1085 (1966)

DY 7.7 Mon 17:30 Poster C

Depletion of Superfluidity in a disordered non-equilibrium Quantum Condensate — •Alexander Janot[1], Timo Hyart[2], Bernd Rosenow[1], and Paul Eastham[3] — [1]Institut für Theoretische Physik, Universität Leipzig, 04009 Leipzig, Germany — [2]Institute of Physics, Leiden University, Niels Bohrweg 2, 2333 CA Leiden, Netherlands — [3]School of Physics, Trinity College, Dublin 2, Ireland

Observations of quantum coherence in driven systems, e.g. polariton condensates, have strongly stimulated experimental as well as theoretical efforts during the last decade. We analyze the superfluid stiffness of a non-equilibrium quantum-condensate in a disordered environment taking gain and loss of particles into account. To this end a modified effective Gross-Pitaevskii equation is employed. We find that the disorder-driven depletion of superfluidity is strongly enhanced due to the gain-loss mechanism. It turns out that the condensate remains stiff at finite length scales only.

DY 7.8 Mon 17:30 Poster C

Structure optimization for models of protein folding by means of "local heat pulse"-quench cycles — •Florian Günther[1], Arnulf Möbius[2], and Michael Schreiber[1] — [1]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Institute for Theoretical Solid State Physics, IFW, Dresden, Germany

Protein folding is a very challenging task because the energy landscape exhibits a huge number of local minima. For such simulations, efficient heuristic algorithms are of high value. We investigate, whether and how the "local heat pulse"-quench cycling (LHPQC) approach [1], which has proved to be highly efficient for traveling salesman and Coulomb glass problems, can be applied to protein folding tasks. For that, we consider the hydrophobic-polar lattice model [2] and the continuous "3-color, 46-bead" model [3]. In evaluating the efficiency of the LHPQC approach, we compare with standard procedures as simulated annealing.

[1] A. Möbius, A. Neklioudov, A. Diaz-Sanchez, K.H. Hoffmann, A. Fachat, and M. Schreiber, *Phys. Rev. Lett.* **79** (1997) 4297.
[2] K. F. Lau, and K. A. Dill, *Macromolecules* **22** (1989) 3986.
[3] J. D. Honeycutt, and D. Thirumalai, *Proc. Natl. Acad. Sci. USA* **87** (1990) 3526.

DY 7.9 Mon 17:30 Poster C

Improved modelling of forced Kramers escape — •Jakob Tómas Bullerjahn, Sebastian Sturm, and Klaus Kroy — Universität Leipzig, Faculty of Physics & Earth Sciences, Institute for Theoretical Physics, Brüderstr. 16, 04103 Leipzig, Germany

The forcible separation of non-covalent bonds, such as in protein unfolding and ligand dissociation, can be regarded as a transition between a bound and an unbound state [1]. This two-state system can be modelled by a test particle moving in an effective free energy landscape, trying to overcome an energy barrier separating the two states. Due

to external loading the unbound state is favoured, which makes the escape practically irreversible. However, established models of such forced rupture [1,2] are restricted to the adiabatic limit of small loading rates, thus making it impossible to apply them to all-atom simulations.

Starting from the test particle's equation of motion, we describe its irreversible escape from a potential well, driven by a time-dependent external force protocol. Our model is analytically tractable and yields an expression for the rupture force distribution measured in dynamic force spectroscopy experiments [3], which holds for small and large loading rates alike. It can be extended to non-Markovian processes with arbitrary memory kernels and reduces to the main result of [2] in the limit of small loading rates.

[1] E. Evans & K. Ritchie, Biophys.J. 72, 1541 (1997) [2] O. K. Dudko, G. Hummer & A. Szabo, Phys. Rev. Lett. 96, 108101 (2006) [3] M. Carrion-Vazquez, et al., Proc. Natl. Acad. Sci. 96, 3694 (1999)

DY 7.10 Mon 17:30 Poster C

Self-organized criticality in adaptive neural network models — •Matthias Rybarsch and Stefan Bornholdt — Institut für Theoretische Physik, Universität Bremen, Hochschulring 18, D-28359 Bremen

It has long been argued that neural networks have to establish and maintain a certain intermediate level of activity in order to keep away from the regimes of chaos and silence. Strong evidence for criticality has been observed in terms of spatio-temporal activity avalanches in cortical cultures first in ref. [1] and subsequently in many more experimental setups. These findings sparked intense research on theoretical models for criticality and avalanche dynamics in neural networks, where usually some dynamical order parameter is fed back onto the network topology by adapting the synaptic couplings. We here review and categorize two classes of models and also discuss a novel correlation-dependent mechanism for self-organized connectivity evolution, leading to a realistic distribution of avalanche sizes in agreement with the experimental findings [2].

[1] J.M. Beggs and D. Plenz: Neuronal Avalanches in Neocortical Circuits, J. Neurosci. 2003, 23(35):11167

[2] M. Rybarsch and S. Bornholdt: A minimal model for self-organization to criticality in binary neural networks, arXiv:1206.0166

DY 7.11 Mon 17:30 Poster C

Generative network models based on triadic substructures — •Marco Winkler and Jörg Reichardt — Institut für Theoretische Physik, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Often pairwise relationships between nodes are considered to be the fundamental building blocks of complex networks. However, over the last decade the overabundance of certain sub-network configurations, so called motifs, have attracted high attention. However, there is still a lack of generative models needed for testing the functional role of such subgraphs. Furthermore, supposed higher order link structures contribute to the probability of a link to emerge, models accounting for those should perform better in predicting hitherto unknown links. Motivated by these two aspects, we employ the framework of exponential random graph models (ERGMs) to define novel models based on triadic substructures. The fact that only a small portion of triads can actually be set freely poses a challenge for the formulation of such models. To overcome this obstacle we use decompositions of our networks into Steiner Triple Systems (STS). The latter are partitions of sets of nodes into pair-disjoint triads, which thus can be specified independently from each other. Combining the concepts of ERGMs and STS, we suggest novel generative network models. We present the benefits of our approach compared to models based on dyadic independence of links.

DY 7.12 Mon 17:30 Poster C

Boolean and continuous networks with checkpoint states — •Danijel Komljenović[1], Tiago Peixoto[2], Eva Ackermann[1], and Barbara Drossel[1] — [1]Institut für Festkörperphysik, TU Darmstadt — [2]Institut für theoretische Physik, Universität Bremen

Gene regulatory networks must function robustly in the presence of a stochastic environment and unreliable regulatory components. An observed mechanism employed by real organisms to fulfill this task is the enforcement of so-called "checkpoint states". This corresponds to a partial ordering of the dynamics where the trajectories cannot proceed from one checkpoint to the next until all requirements from the first checkpoint have been met. This guarantees a certain amount of predictability, while it leaves at the same time room for variation when the system moves between checkpoints. We show how such checkpoint dynamics can be explicitly constructed in a Boolean representation of gene regulatory dynamics. In this representation, a checkpoint is a state through which the dynamics must always go even when a fully stochastic update scheme is applied. Given a predefined set of checkpoints, we construct possible intermediary trajectories, and finally the ensemble of networks which fulfill it. We proceed by comparing the Boolean models with their continuous counterparts composed of differential equations describing in more detail the concentrations of proteins and mRNA. This allows us to identify the central criteria enabling the faithful reproduction of the Boolean dynamics in the continuous description, depending on the Hill coefficients of the continuous functions and the sequence of checkpoint states on the trajectory.

DY 7.13 Mon 17:30 Poster C

Inferring topology of biological networks from dynamics — •Haleh Ebadi and Konstantin Klemm — Bioinformatics Group, Institute or Computer Science, Leipzig University, Germany

An observation of a state transition provides partial information on the interactions constituting a high-dimensional deterministic system. Here we strive to quantify how the number of observed single state transitions and/or short trajectories reduces the number of interaction matrices consistent with the set of observations. As a test-bed, we use several established Boolean (threshold unit) models of cell cycle control in living organisms. The numerical study also uses ensembles of randomly reshuffled matrices as a null model. We find that the ability to reconstruct networks from measurements strongly depends on the types of threshold functions assumed by the underlying model.

DY 7.14 Mon 17:30 Poster C

Hierarchy in directed networks — •Krzysztof Suchecki and Janusz Hołyst — Faculty of Physics, Center of Excellence for Complex Systems Research, Warsaw University of Technology, ul. Koszykowa 75, Warszawa, Poland

We introduce a definition of observable hierarchy in directed networks, related to the possible information or command flows in such networks and derived purely from the network topology. For trees, it is a simple average distance of leaf vertices from the root plus one. We generalize it for any directed network. In case of presence of directed loops, we assign all the vertices in a loop to the same hierarchy, which effectively means treating loops as single complex vertices. We analyze the average hierarchy value for different types of networks and in case of network models investigate its dependence on network parameters, as well as explain the obtained results. For directed Erdos-Renyi random graphs, we observe maximum hierarchy value depending on the graph density, that coincides with the percolation threshold.

DY 7.15 Mon 17:30 Poster C

Evolutionary optimisation of dynamical networks — •Steffen Karalus — Institut für Theoretische Physik, Universität zu Köln, Germany

A large class of empirical networks structurally evolve in the course of time adapting their topology to better fit the functional requirements. This functionality in most cases is associated with dynamical processes based on the network in the sense that the topology defines the local interaction pattern between the individual dynamical units. Thus, in the evolutionary process mutations act on the network topology whereas selection acts on a 'fitness' provided by dynamical properties. In many empirical situations the speed of the evolutionary dynamics is much slower than the process dynamics so that the two time scales can be considered as well separated. Exploiting these ideas it has been shown that network structures can be successfully evolved such that non-trivial dynamical behaviour emerges [1].

I will present further developments for improving the efficiency of the evolutionary dynamics as well as for providing deeper insight into the mechanisms of network evolution and the relation between network structure and dynamics in general. By this, not only more complicated dynamical problems and larger system sizes will become tractable but also a better understanding of the complexity of network evolution and how different evolutionary strategies perform can be achieved.

[1] S. Karalus and M. Porto, EPL 99, 38002 (2012).

DY 7.16 Mon 17:30 Poster C

Voter Model with Surface Tension — •Bruno Pace and Konstantin Klemm — Leipzig University

Spin systems are very central in the context of Statistical Physics for

their simplicity and generality. But also, any process out of the realm of physics that shares some intrinsic properties and symmetries with these models will inherit some of their characteristics like the phase transitions or scaling properties.

There is a well-known comparison between the Voter model and the Ising model at zero temperature. In the latter, however, curvature-driven surface tension orders the system. Here we propose a different microscopic mechanism inspired in the classic Voter dynamics for the emergence of a surface tension. It consists of making the agents actively persuasive: after choosing one node of the network, it will try to interact only with different state neighbours. Some characteristics of the out of equilibrium dynamics are explored.

DY 7.17 Mon 17:30 Poster C

A Parameter Estimation Method for Ordinary Differential Equations — •Oliver Strebel — Launitzstr. 21, 60594 Frankfurt

Estimating parameters for ordinary differential equations (ODE) is an active field of research. Prominent methods are least square and Kalman methods [1]. While the former suffer from various convergence problems [2], the latter face frequently the "loss of lock" problem of nonlinear filtering [3].

In this contribution a method is presented, which first determines the tangent slope and coordinate for given data of the solution of the ODE. With these values the ODE is transformed into a system of equations, which is linear for linear appearance of the parameters in the ODE. In this case no initial guess of the parameters is necessary. For nonlinear parameter dependence of the ODE nonlinear equations must be solved, using parameter guesses as initial values for the Newton iteration. In both cases the equations are solved repeatedly using randomly selected data points and the averaged results yield the estimates. For numerically generated data of the Lorenz attractor good estimates are obtained even at large noise levels.

[1] B. P. Bezruchko et al: Extracting knowledge from time series, Springer 2010.

[2] B. P. Bezruchko et al:, Chaos, Solitons & Fractals 29, p. 82, 2006.

[3] Z. Schuss: Nonlinear Filtering and Optimal Phase Tracking, Springer 2012.

DY 7.18 Mon 17:30 Poster C

Order by disorder in frustrated oscillators — •Florin Ionita[1], Darka Labavić[1], Michael Zaks[2], and Hildegard Meyer-Ortmanns[1] — [1]School of Engineering and Science, Jacobs University Bremen, PO Box 750561, D-28725 Bremen, Germany — [2]Institute of Mathematics, Humboldt-University at Berlin, Rudower Chaussee 25, 12489 Berlin, Germany

We study Kuramoto oscillators on regular and all-to-all topologies with geometric frustration due to repulsive couplings. As a result of this frustration we observe a proliferation of stationary states in the gradient dynamics, which differ by their patterns of phase-locked motion. As a special subset of these states we identify plane-wave solutions and prove their stability. When we turn on additive noise, we observe for an intermediate noise strength an order-by-disorder effect, similarly to the ordering effect that is induced by disorder in frustrated spin systems. Here it means that a disordered state with no synchronization turns into a state with partial synchronization, or a state with a low degeneracy turns into a state with a larger degeneracy of synchronized phases. Similar results are found for active rotators.

DY 7.19 Mon 17:30 Poster C

Entropic Stochastic Resonance of a Flexible Polymer Chain in Confined System — •Zhen Zhang[1,2], Hanshuang Chen[3], and Zhonghuai Hou[1,4] — [1]Institute of Theoretical Physics, Technical University Berlin, Hardenbergstrasse 36, 10623, Berlin, Germany — [2]Department of Chemical Physics, University of Science and Technology of China, Hefei, Anhui, 230026, China — [3]School of Physics and Material Science, Anhui University, Hefei, Anhui, 230039, China — [4]Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, Hefei, Anhui, 230026, China

We have investigated the dynamics of a flexible polymer chain in constrained dumb-bell-shape geometry subject to a periodic force and external noise along the longitudinal direction[1]. It is found that the system exhibits a feature of entropic stochastic resonance (ESR), i.e., the temporal coherence of the polymer motion can reach a maximum level for an optimal noise intensity. We demonstrate that the occurrence of ESR is robust to the change of chain length, while the bottleneck width should be properly chosen. A gravity force in the vertical direction is not necessary for the ESR here, however, the elastic coupling between polymer beads is crucial. Our study may shed new light on the understanding of polymer dynamics as well as its control in confined geometry, which is of great importance in biological systems.

[1] Zhen Zhang, Hanshuang Chen, and Zhonghuai Hou,Entropic stochastic resonance of a flexible polymer chain in a confined system, J. Chem. Phys. 137, 044904 (2012).

DY 7.20 Mon 17:30 Poster C

Dependence of irregular excitation patterns on bridge width during interaction of pacemaker — •Yvonne Richter[1], Claudia Lenk[2] und Philipp Maass[1] — [1]Fachbereich Physik, Universität Osnabrück, Germany — [2]Institut für Chemie und Biotechnik, Technische Universität Ilmenau, Germany

Irregular excitation patterns in reaction-diffusion systems are often associated with a reduced performance of the system or pathological states like, e.g. fibrillation of the heart. Understanding the generation of such states is important for the improvement or therapy of these systems. The interaction of two pacemaker located in distinct regions which are only connected by a small bridge can on the one hand generate irregular excitation patterns and on the other hand return the system into a more regular state dependent on the frequency ratio of the two pacemaker. This mechanism is investigated by calculations of the Bueno-Orovio equations. We present a performance comparison of two different calculation methods, finite element method and finite differences method. Additionally, the ability to reduce the calculation time by application of graphic card computation (CUDA) is tested. With the best performing program the dependence of the excitation patterns resulting from the interaction of the two pacemaker on the width of the bridge is studied. The strength of the irregularity, measured by entropy and phase coherence, and changes in the shape of the excitation patterns as well as differences in the frequency ratios, determining the three different irregularity regimes, will be analysed. The results will be compared with the FitzHugh-Nagumo model.

DY 7.21 Mon 17:30 Poster C

Experimental Chimera States in a Network of Mechanical Oscillators — Erik A. Martens[1,2], Shashi Thutupalli[1,3], •Antoine Fourrière[1], and Oskar Hallatschek[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Aqua, Technical University of Denmark, Lyngby, Denmark — [3]Dept. of Mechanical & Aerospace Engineering, Princeton University, Princeton, USA

Synchronization of oscillating units is at the heart of numerous natural phenomena. Over the last 10 years, theoretical studies have predicted the existence of counterintuitive 'chimera states', where a population of identical oscillators splits into a synchronous and asynchronous part. For a deep understanding of these collective states and their relevance, the physical mechanisms causing their emergence must be resolved. Here, we use a purely mechanical system of coupled metronomes to show that chimeras emerge naturally from a competition between two antagonistic synchronization patterns. We obtain a spectrum of complex states, encompassing and extending the set of previously described chimeras. Our mechanical model strongly suggests that such states are a ubiquitous feature in nature, manifesting themselves in technological settings ranging from power grids to optomechanical arrays.

DY 7.22 Mon 17:30 Poster C

Nonlocal control of pulse propagation in excitable media — •Clemens Bachmair and Eckehard Schöll — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

We discuss the effects of nonlocal control on propagating waves in excitable media. As a generic model we use a spatially extended FitzHugh-Nagumo system which locally couples with a diffusion term in the activator variable. The control is implemented in a non-invasive way by a convolution with different kernel. A particular focus is placed on the mexican hat function due to its significance in neuroscience. The control gives rise to different phenomena such as wave supression, multiple peak waves and more complex spatiotemporal patterns such as a spiking traveling wave.

DY 7.23 Mon 17:30 Poster C

Curvature dependent Feedback Control of two dimensional Excitation Waves — •Sonja Molnos, Jakob Löber, and Harald Engel — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

The propagating liquid-solid interface in an undercooled fluid can undergo a Mullins-Sekerka-instability, which for example leads to the formation of snowflakes [1]. We investigate a mechanism to create such instabilities in a reaction diffusion system. With the developed curvature-dependent feedback control it is possible to counteract the role of the eikonal equation and thereby destabilize the plane wave front. The appearance of the instability can be suppressed, choosing the the width of the active medium below a certain threshold. This can be explained using the Kuramoto-Sivashinsky equation.

[1] J. S. Langer, Rev. Mod. Phys. 52, 1 (1980)

DY 7.24 Mon 17:30 Poster C

Scroll ring dynamics under spatial Confinement — •Jan Frederik Totz[1], Oliver Steinbock[2], and Harald Engel[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL-32306-4390

Non-planar excitation waves are exhibited by a variety of dissipative non-equilibrium systems, including chemical waves, fuel combustion, catalytic oxidation of CO and electric activity in the heart muscle. Using the Ferroin-catalyzed Belousov-Zhabotinsky reaction, we investigate the dynamics of scroll rings in a chemical medium of adjustable height [1]. The close proximity to the boundaries leads to dramatic changes of the intrinsic dynamics, as the contraction can be reverted into an expansion of the organizing vortex ring. Results from chemical experiments are in good agreement with numerical simulations based on parameters derived from the used chemical concentrations and can be predicted qualitatively with a simple phenomenological model.

[1] Z. A. Jiménez, B. Marts, O. Steinbock, Phys. Rev. Lett. 102, 244101 (2009)

DY 7.25 Mon 17:30 Poster C

Patterns in anisotropic reaction diffusion systems — •Fabian Bergmann, Alexei Krekhov, and Walter Zimmermann — Universität Bayreuth, Theoretische Physik, 95440 Bayreuth, Germany

In 1952, Turing suggested a hypothetical reaction-diffusion model showing spatially periodic pattern. This class of models was recently identified as an important framework for understanding Biological Pattern Formation, such as the formation of pigment stripes in the skin of fishes [1]. Recently, anisotropic diffusion [2] and cross diffusion have been identified as two important extensions of Turing's model [3].

We investigate bifurcation scenarios in anisotropic reaction-diffusion systems including cross diffusion. We find for this class of systems a wide range of parameters, whereby two orthogonally oriented stripe patterns have the same threshold (codimension-two bifurcation). In this case, a nonlinear competition between both stripe orientations takes place beyond threshold. Near threshold this competition is analyzed in terms of amplitude equations, which are derived from the basic reaction-diffusion model. We find three different scenarios: (i) In a wide range of parameters either one or the other stripe pattern is stable, depending on the initial condition. (ii) In a second range the coexistence of both stripe patterns (rectangular patterns) is preferred. (iii) Both cases are separated by a parameter range, where surprisingly, only one of both stripe orientations is stable.

[1] S. Kondo and T. Miura, Reaction-Diffusion Model as Framework for Understanding Biological Pattern Formation, Science 329, 1616 (2010)

[2] H. Shoji, Y. Iwasa, A. Mochizuki and S. Kondo, Directionality of Stripes Formed by Anisotropic Reaction-Diffusion Models, J. Theor. Biol. 214, 349 (2002)

[3] N. Kumar and W. Horsthemke, Effects of cross diffusion on Turing bifurcations in two species reaction-transport systems, Phys. Rev. E 83, 036105 (2011)

DY 8: Poster I: Glasses and Glass Transition (joint session DY/DF/CPP)

Time: Monday 17:30–19:30 Location: Poster C

DY 8.1 Mon 17:30 Poster C

Room temperature ionic liquid's (RTILs) dynamic glass transition by calorimetric methods. — •Evgeni Shoifet[1,2], Heiko Huth[1], Sergey Verevkin[2], and Christoph Schick[1] — [1]Institute of Physics, Rostock University, Rostock, 18051, Germany — [2]Institute of Chemistry, University of Rostock, 18051 Rostock, Germany

Many of the ionic liquids are good glass formers. Nevertheless, only a few studies of the glass transition in ionic liquids are available so far. Particularly the frequency dependence of the dynamic glass transition (α-relaxation) is not known for most ionic liquids. The standard technique for such studies - dielectric spectroscopy - is not easily applicable to ionic liquids because of the high electrical conductivity. We try to use calorimetric techniques to obtain complex heat capacity and to investigate the dynamic glass transition of room temperature ionic liquids (RTILs) in a wide frequency range. This can give an insight in cooperative motions of ions and ion clusters in RTILs. The techniques that were used are DSC, TMDSC, and AC-chip calorimeter[5] covering a frequency range from 0.001 Hz to10000 Hz. Similar fragility was found not only in series of RTILs with different alkyl chain length in the cataion ([Cnmim]), but also for two different anions ([Co(NCS)2],[NTf2]). Also the decrease in thermal glass transition temperature (Tg) and add/even effect have been observed in cobalt RTIL, while the Tg in RTIL with sulfonic anion is increasing, with increase of alkyl chain length.

DY 8.2 Mon 17:30 Poster C

Nanoscale confinement of a low molecular weight liquid — •Anna Djemour, Jörg Baller, Carlo Di Giambattista, Marlena Filimon, Jens-Peter Bick, Andreas Michels, and Roland Sanctuary — Laboratory for the Physics of Advanced Materials, University of Luxembourg, 162A, Avenue de la Faiencerie, L-1511 Luxembourg

The enormous change of the molecular dynamics of glass formers when approaching the thermal glass transition temperature is usually attributed to the increase of the size of cooperative rearranging regions (CRR). Spatial confinement is known to take influence on the glass transition behaviour when the scale of confinement is in the same order as the size of the CRRs. In this work we present investigations of the glass transition of a low molecular weight epoxy resin (Diglycidil Ether of Bisphenol A, DGEBA) filled in different nanoporous silica glasses. The effect of confinement is studied by two different ways: i) properties of the glass former are investigated by modulated calorimetry, dielectric spectroscopy and X-ray scattering. ii) properties of the whole system, i.e. porous glasses filled with the glass former are investigated by thermo-mechanical analysis and dynamic mechanical analysis. Combining the results from both approaches contributes to the understanding of the glass former DGEBA under confinement.

DY 8.3 Mon 17:30 Poster C

Local Thermal Analysis as a Tool for Morphological Investigation of Polypropylene — Thomas Fischinger, •Lisa Maria Uiberlacker, and Sabine Hild — Institute for Polymer Science, Johannes Kepler University, Altenbergerstraße 69, 4040 Linz, Austria

A basic understanding of physical and chemical properties of polymers is of fundamental importance for the development of advanced polymers. Thermal analysis methods are generally used to provide important and reliable data. However, up to now mainly bulk properties of polymers have been detected. Conventional methods reach a limit for applications such as the investigation of crystal structures. Therefore, a method is proposed for nano-thermal characterization of polymers using scanning probe microscopy (SPM) in combination with heatable cantilever probes. This method is based on an appropriate temperature calibration, which provides a reliable correlation between applied voltage and the temperature at the tip. LTA measurements were applied to high moleculare isotactic polypropylene with varying lamellar thicknesses. Furthermore, the structure and morphology of randomly distributed isotactic propylene-1-hexene-copolymer (PHCP) were investigated with a focus on local thermal properties. In this study it will be shown that it is possible to investigate the differences in softening of α- and γ- structure of PHCP.

DY 8.4 Mon 17:30 Poster C

Bestimmung der molekularen Dynamik von Polyvinylpyrrolidon mittles NMR und DS — •Michael Lannert und Michael Vogel — Technische Universität Darmstadt, Institut für Festkörperphysik

Die molekulare Dynamik von Wasser in Polymer-Matrizen (D_2O-Polyvinylpyrrolidon-Mischung) wurde mittels Deuteronen NMR untersucht. Fragestellung ist, ob sich anhand der temperaturabhängigen Korrelationszeit der Rotation der C-D-Bindungen ein starkes oder fragiles Verhalten ausmachen lässt. Eine Theorie, welche die Existenz einer hochdichten (HDL) und niederdichten (LDL) Flüssigphase des Wassers im unterkühlten Regime voraussagt, legt einen "Fragil-Stark-Übergang"bei T $\approx$ 220K nahe. Zusätzlich zu den NMR-Messungen wurden Daten aus Dielektrischer Spektroskopie ausgewertet. Unter Annahme spezieller empirischer Modelle für die spektrale Dichte der unterliegenden Prozesse, namentlich einer Cole-Davidson Verteilung, kann so aus den DS Daten die mittlere Relaxationsrate der NMR-Experimente vorausgesagt und mit den tatsächlich erhaltenen Werten verglichen werden. Interpolationen der Temperaturabhängigkeit der Wasserdynamik mit eienm Arrheniusgesetz ergeben eine Aktivierungsenergie von $E_A = 0.5$eV, welche von der Wasserkonzentration unabhängig ist. Durch Kombination von NMR und DS sowie Abdeckung eines breiten Zeitfensters gelingt es somit, ein konsistentes Bild der Dynamik im untersuchten System zu zeichnen.

DY 8.5 Mon 17:30 Poster C

Thermomechanical Properties of Organic-Coatings: A scanning force microscopy study — •Bernhard Jachs[1], Bernhard Strauss[2], and Sabine Hild[1] — [1]Institute of Polymer Science, JKU Linz, Altenbergstraße 69, 4040 Linz, — [2]voestalpine Stahl Gmbh, 4020 Linz

Coil Coating is a continuous industrial process where one or more polymeric layers with thicknesses ranging from 5 up to 50 μm are applied on steel coils to protect them against environmental impacts. For further processing of the coated material, the knowledge of thermal and mechanical properties of the coating is crucial. Widely used analytical techniques (DSC, DMA) require special sample preparation where the coating has to be removed from the substrate or is prepared as a free standing coating film. In this work a SFM equipped with a heating stage was used to directly investigate mechanical properties of coatings as a function of temperature by performing nanoindentation measurements. Static measurements were carried out at different displacement rates and temperatures. By taking into account contact-mechanical models, which describe the tip-sample-interaction, the Elastic Modulus can be obtained as a function of temperature and displacement rate. Shifting the curves according to the Williams-Landel-Ferry equation yields a mastercurve which allows extrapolating mechanical properties beyond the measuring range. In addition, dynamic measurements have been carried out modulating the tip position at different frequencies and temperatures. Using proper viscoelastic models, Storage and Loss Moduli as well as loss tangent can be determined.

DY 8.6 Mon 17:30 Poster C

In-situ investigation of vapor-deposited thin films of toluene and ethylbenzene by AC chip-nanocalorimetry — •Mathias Ahrenberg[1], Katie R. Whitaker[2], Yeong-Zen Chua[1], Heiko Huth[1], Mark D. Ediger[2], and Christoph Schick[1] — [1]Institut für Physik, Universität Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — [2]Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA

Physical vapor deposition can be used to produce thin films with particular material properties. For example extraordinarily stable glasses can be obtained from organic molecules like toluene and ethylbenzene. We have investigated properties like packing efficiency and kinetic stability depending on substrate temperature and deposition rate by in-situ AC chip-nanocalorimetry. We have varied the substrate temperature covering the range from temperatures proven to yield high enthalpy glasses up to temperatures proven to yield low enthalpy glasses. This way the complete evolution of the mentioned stable glass properties is observed. Moreover AC calorimetry offers the possibility for isothermal measurements which enables to follow the transformation of the stable glass to the super-cooled liquid. Transformation experiments give suggestion of the transformation mechanism and its temperature dependence. The data are in agreement with a growth front for the transformation of the stable glass into the supercooled liquid.

DY 8.7 Mon 17:30 Poster C

Triplett-Solvatationsdynamik an unterkühlten Wassermischungen in hartem und weichem Confinement — •Vincenzo Talluto[1], Carl Böhmer[1], Thomas Walther[1] und Thomas Blochowicz[2] — [1]Institut für Angewandte Physik, Technische Universität Darmstadt, Schlossgartenstr. 7, 64289 Darmstadt — [2]Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstraße 8, 64289 Darmstadt

Die Triplett-Solvatationsdynamik ist eine Methode, mit der Relaxation in unterkühlten Flüssigkeiten nahe des Glasübergangs untersucht werden kann. Hierzu wird der Flüssigkeit ein Farbstoff beigemischt, welcher mittels eines UV-Laserpulses in einen langlebigen Triplettzustand angeregt wird. Über den zeitlichen Verlauf der Emissionswellenlänge des Farbstoffes kann die Relaxation der Solvatationshülle in einem Zeitbereich von 0.1 ms bis 1 s verfolgt werden. Je nach Farbstoff kann dabei eine dielektrische oder mechanische Response auf die Anregung des Farbstoffmoleküls beobachtet werden.

Der Vorteil dieser lokalen Methode liegt u.a. darin, dass z. B. Glasbildner in Confinement untersucht werden können. In gefüllten Porensystemen sind hier z. B. die Ergebnisse der herkömmlichen dielektrischen Spektroskopie nur schwer zu interpretieren. Wir präsentieren erste Messungen an Wasser-Alkohol-Mischungen als Bulk-Material, sowie im Confinement von Vycor-Poren und Mikroemulsionströpfchen mit dem Ziel, Oberflächen-, Dichte- und Finite-Size-Effekte voneinander zu trennen, deren Überlagerung eine eindeutige Interpretation dynamischer Daten bisher erschwert.

DY 8.8 Mon 17:30 Poster C

The interplay between inter- and intramolecular dynamics in a series of alkylcitrates — •Wycliffe Kipnusu[1], Wilhelm Kossack[1], Ciprian Iacob[1], Joshua Sangoro[2], and Friedrich Kremer[1] — [1]Institute of Experimental Physics I, University of Leipzig, Linnestr. 5, 04103 Leipzig, Germany — [2]Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830-6197, United States.

The inter- and intra-molecular dynamics in a series of glass-forming alkylcitrates is studied by a combination of Broadband Dielectric (BDS), Pulsed Field Gradient Nuclear Magnetic Resonance (PFG NMR), Dynamic Mechanical (DMS), and Fourier-Transform Infrared (FTIR) Spectroscopy. Analyzing the temperature dependencies of specific IR absorption bands in terms of their spectral position and the corresponding oscillator strengths enables one to unravel the intramolecular dynamics of specific molecular moieties and to compare it with the intermolecular dynamics. With decreasing temperature, the IR band positions of carbonyls and H-bonded moieties of citrates, show a red shift with a kink at Tg while other moieties whose dynamics are decoupled from those of the core units, exhibit a blue shift with nominal changes at Tg. The oscillator strength of the ester linkage and H-bonded units show a kink at a temperature where structural and faster secondary relaxations merge. By that, a wealth of novel information is obtained proving the fundamental importance of intramolecular mobility in the process of glass formation, beyond coarse-grained descriptions. Reference:Papadopoulos P. etal. Softmatter 2012 In press.

DY 8.9 Mon 17:30 Poster C

First Thermal Conductivity and Elastic Susceptibility measurements of Zr-based Bulk Metallic Glasses at Ultra Low Temperatures — •Marius Hempel, Daniel Rothfuss, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Heidelberg

The thermal conductivity and the elastic susceptibility of Zr-based superconducting bulk metallic glasses have been measured the first time in the temperature range down to 6 mK in order to study the interaction of atomic tunnelling systems with phonons and conducting electrons. Additional susceptibility measurements reveal a superconducting transition around 1 K.

Both, the elastic susceptibility and the thermal conductivity measurements use a novel SQUID-based contact free detection technique below 1 K which allows to dispense with a bias voltage in the case of the elastic measurements and reduces parasitic heat input during the thermal conductivity measurements.

The thermal conductivity of the bulk metallic glass $Zr_{52.5}Ti_5Cu_{17.9}Ni_{14.6}Al_{10}$ scales nearly quadratically with temperature as expected from the tunnelling model. The change of sound velocity of the of the bulk metallic glass $Zr_{55}Cu_{30}Al_{10}Ni_5$ shows a temperature dependence which is governed by resonant and relaxational processes. The latter are caused by the interaction with thermal phonons and quasi-particles in the vicinity of the superconducting transition.

DY 8.10 Mon 17:30 Poster C

Non-universal dielectric and elastic properties of glasses at very low temperatures — •Annina Luck, Marius Hempel, An-

dreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg

Based on many experimental observations the low temperature properties of glasses, governed by atomic tunneling systems, have long been viewed as being universal. In the last years, however, measurements of dielectric two-pulse polarization echoes have revealed that nuclear electric quadrupole moments involved in atomic tunneling systems can cause large material-dependent effects in magnetic fields.

To study the possible influence of nuclear electric quadrupoles in two level systems on the low frequency dielectric and elastic properties of glasses down to a temperature of 10 mK, we measured vitreous silica and the multicomponent glass N-KZFS11, which contains 25 mass percent of tantalum oxide. As ^{181}Ta carries a very large nuclear electric quadrupole moment, N-KZFS11 seems to be an ideal candidate to determine the influence of nuclear electric quadrupole moments on the physical properties of glasses at low temperatures.

Our measurements not only show a non-universal dieletric and elastic behaviour for these two glasses, but the results also differ significantly from various predictions of the standard tunneling model. We discuss these new findings and possible implications in terms of the tunneling model.

DY 8.11 Mon 17:30 Poster C

$1/f$ flux noise induced by spin glasses in superconducting qubits — •Juan Atalaya — Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie, Karlsruher, Deutschland.

Recently, it has been realized that the coherence time of flux qubits is limited by unknown sources of flux noise, which exhibits a $1/f$ spectrum at low frequencies $f \lesssim 10$kHz and at low temperatures $\lesssim 5$K. Experiments suggest that the main contribution to the flux noise may be produced by paramagnetic spins located on the surface of the superconducting loop. We consider a spin glass system of classical Heisenberg spins and investigate the low frequency dynamics of the total magnetization at temperatures near the spin glass freezing temperature. We discuss the role of anisotropy and temperature on the shape of the noise spectrum.

DY 8.12 Mon 17:30 Poster C

Glassy dynamics of orientation fluctuations in modulated phases — •Christian Riesch, Günter Radons, and Robert Magerle — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz

We report on glassy dynamics and aging behavior in a 2D stripe-forming system free of topological defects. Numerical simulations based on model B with Coulomb interactions were performed for a wide range of noise strengths. The autocorrelation function of the local stripe orientation obeys the scaling form $C_\theta(t, t_w) \sim t_w^{-b} \cdot f(t/t_w)$, typical for glassy dynamics, and we argue that the relaxation time of the orientation fluctuations diverges. Spatial correlations are anisotropic, exhibiting a fast decay parallel to the stripes and an emerging power-law behavior in the perpendicular direction. We also investigate aging effects in other modulated phases, such as a hexagonal system in 2D and a lamellae-forming system in 3D.

DY 8.13 Mon 17:30 Poster C

Theoretical methods to analyse scattering patterns in the systems of self-assembling anisotropic particles — •Sofia Kantorovich[1,2], Elena Pyanzina[1], Cristiano De Michele[2], and Francesco Sciortino[2] — [1]Ural Federal University, Lenin av. 51, 620000, Ekaterinburg, Russia — [2]Sapienza, University of Rome, Piazza A. Moro 5, 00185, Rome, Italy

Self-assembly is a phenomena which can be observed on the broad range of scales: starting from simple molecules to colloidal particles. This effect of spontaneous equilibrium formation of reversible aggregates might serve as a key to the synthesis of new smart materials, once self-assembly mechanisms are well understood. The aggregates formed in the systems might lead to significant changes in macroscopic responses of the systems, thus, becoming very important in soft matter and biophysics. One of the examples of self-assembling building blocks is short blunt-ended DNA duplexes which form chains. At low densities these chains form an isotropic phase, whereas, at high densities, these particular DNA solutions are known to order into the nematic liquid crystal phases. Here, we put forward a theoretical approach, which suggests how to predict the average chain length and the stacking free energy, based on the experimental scattering patterns. We show that the proposed method is rather general and might be used for any self-assembling anisotropic particles, as long as the chain-size distribution is exponential.

DY 8.14 Mon 17:30 Poster C

Dissociation behavior of pyridine coordination compounds in aqueous solutions — •Manuel Gensler[1], Christian Eidamshaus[2], Artur Galstyan[2], Ernst-Walter Knapp[2], Hans-Ulrich Reissig[2], and Jürgen P. Rabe[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]Institut für Chemie und Biochemie, Freie Universität Berlin

The pyridine core is ubiquitous in natural products and widely used for the construction of supramolecular structures [1]. We analyzed coordination compounds of mono- and bivalent pyridines with Cu(II) and Zn(II) by SFM based single molecule force spectroscopy (SMFS) in aqueous solutions. Using the Bell-Evans-Kramers model we determined surprisingly long rupture lengths from 0.25 nm for the monovalent pyridin with Cu(II) up to 0.52 nm for the bivalent pyridine with Cu(II). DFT calculations suggest a stepwise dissociation through an intermediate product in which a water ligand inserts in between the pyridine and metal ion. Such process is different to the known solvent-ligand-exchange mechanism of a pyridine-palladium complex in DMSO with a rupture length of only 0.17 - 0.19 nm [2]. Therefore additional water ligands may attribute to the mechanical properties of metallosupramolecular compounds and their corresponding natural systems.

[1] L.E. Kapinos and H. Sigel *Inorg. Chim. Acta* **2002**, *337*, 131-142. [2] F.R. Kersey et al. *J. Am. Chem. Soc.* **2006**, *128*, 3886-3887.

DY 8.15 Mon 17:30 Poster C

Probing the electronic structure of gas phase methanol by soft RIXS — •Andreas Benkert[1,2,3], Frank Meyer[1], Monika Blum[4], Regan G. Wilks[5], Marcus Bär[4,5], Wanli Yang[6], Friedrich Reinert[2,3], Clemens Heske[1,4,7], and Lothar Weinhardt[1,4,7] — [1]Inst. for Photon Science and Synchrotron Radiation, Karlsruhe Institute of Technology (KIT) — [2]Exp. Physik VII, Universität Würzburg — [3]Gemeinschaftslabor für Nanoanalytik, KIT — [4]Dept. of Chemistry, University of Nevada, Las Vegas — [5]Solar Energy Research, Helmholtz-Zentrum Berlin f. Mat. u. Energie — [6]Advanced Light Source, Lawrence Berkeley National Laboratory — [7]ANKA Synchrotron Radiation Facility Karlsruhe, KIT

We have investigated methanol in gas phase at atmospheric pressure using resonant inelastic soft x-ray scattering (RIXS). RIXS maps of both, the O K and C K edge, will be presented, and it will be shown that the observed emission lines can be attributed to different molecular orbitals in accordance to DFT-based calculations of isolated methanol molecules. This demonstrates the local character of the RIXS process.

In detail, we observe strong spectator shifts of up to 0.9 eV upon excitation into different absorption resonances at the O K edge. Furthermore, we find evidence for nuclear dynamics on the time scale of the x-ray emission process, leading to a dissociation of the hydrogen atom from the hydroxyl group. In addition, measurements of deuterated methanol allow us to separate the contributions of intact and dissociated methanol molecules in the emission spectra.

DY 9: Poster I: Statistical Physics in Biological Systems (joint with BP)

Time: Monday 17:30–19:30 Location: Poster B2

DY 9.1 Mon 17:30 Poster B2

Perturbed self-organized critical networks as a sleep model — li chen[1] and •christian meisel[1,2] — [1]Max-Planck-Institut for Physik komplexer Systeme, Noethnitzer Str. 38, 01187 Dresden, Germany — [2]Department of Neurology, University Clinic Carl Gustav Carus, Fetscherstr. 74, 01307 Dresden, Germany

Why do we need sleep is a long mystery for centuries. Here, we propose a perturbed self-organized critical binary networks as a possible model to mimic the whole processes for the brain during awake time and sleep. By systematically characterizing the network activity, our results shows that the input received in awake time always derivates our brains from critical state, with decreasing computational power, shorter effective response range, worse p-values etc. That is the reason why we need sleep to recover these brain functions by self-organizing back to critical networks by turning off all input from surroundings. An observation of the probability distribution of phase-lock interval from EEG data during growing sleep deprivation is given.

DY 9.2 Mon 17:30 Poster B2

Information filtering by synchronous spikes in a neural population — •Nahal Sharafi — Bunsenstrasse 10, 37073 Goettingen

Information about time-dependent sensory stimuli is encoded by the spike trains of neurons. Here we consider a population of uncoupled but noisy neurons (each subject to some intrinsic noise) that are driven by a common broadband signal. We ask specifically how much information is encoded in the synchronous activity of the population and how this information transfer is distributed with respect to frequency bands. In order to obtain some insight into the mechanism of information filtering espects found previously in the literature, we develop a mathematical framework to calculate the coherence of the synchronous output with the common stimulus for populations of simple neuron models. Within this frame, the synchronous activity is treated as the product of filtered versions of the spike trains of a subset of neurons. We compare our results for the simple cases of (1) a Poisson neuron with a rate modulation and (2) an LIF neuron with intrinsic white current noise and a current stimulus. For the Poisson neuron, formulas are particularly simple but show only a low-pass behavior of the coherence of synchronous activity. For the LIF model, in contrast, the coherence function of the synchronous activity shows a clear peak at high frequencies, comparable to recent experimental findings. We uncover the mechanism for this shift in the maximum of the coherence and discuss some biological implications of our findings.

DY 9.3 Mon 17:30 Poster B2

Modelling of rhythmic patterns in hippocampus — •Anastasia Lavrova[1], Michael Zaks[2], and Lutz Schimansky-Geier[2] — [1]Immanuel Kant Baltic Federal University, Kaliningrad, Russia — [2]Humboldt University at Berlin, Berlin, Germany

The hippocampal circuit can exhibit network oscillations in different frequency ranges (gamma - 30-80 Hz; theta - 4-12 Hz; as well as theta/gamma or a bursting regime) both in vivo and in vitro and switch between them.

Our goal is to investigate how coupling strength and delayed propagation influence synchronization and switching between different oscillatory states in minimal neuronal networks. To this end, we constructed a simple model of neurons comprising two fast-spiking and two slow-spiking cells, respectively. The network is described by coupled FitzHugh-Nagumo equations that well reproduce the dynamical behavior of different cells types: their periods, amplitudes, and phase shifts.

The model allows us to analyze the influence of synaptic strengths on the network synchronization and dynamical switching between theta, gamma, and bursting regimes. In particular, we perform a thorough bifurcation analysis and identify parameters of synaptic connections that can efficiently induce switches in the network activity.

DY 9.4 Mon 17:30 Poster B2

Interaction between Looped-Star Polymers — •Dieter Heermann and Benoit Knecht — Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 19, 69120 Heidelberg

We study the properties of looped star polymers, in which each arm is a ring that can be over- or underwound and compare them to the classic linear-arm star polymer. Looped star polymers are more compact and overwounding increases their density. The effective repulsion between looped stars is similar to that of linear star polymers with twice as many arms half the length, following a logarithmic–Gaussian potential. The force pushing the arms outwards is more than twice as strong for looped star polymers than it is for linear star polymers for a number of arms f>2.

DY 9.5 Mon 17:30 Poster B2

Collective behavior and structure formation of hydrodynamically interacting active particles — •Marc Hennes, Katrin Wolff, and Holger Stark — Institut für Theoretische Physik TU Berlin

Lattice Boltzmann simulations of active run-and-tumble particles (RTPs) subject to an external trapping force have shown the emergence of a self-assembled pump in the presence of hydrodynamic interactions[1]. Here, we extend these results to active Brownian particles (ABPs), simulated by means of Brownian Dynamics simulation including hydrodynamic interactions. ABPs, in contrast to RTPs, do not tumble but reorient smoothly due to thermal noise, external torques, and vorticity fields in the fluid. Here, we clarify that the pump is a dynamic cluster of ABPs which only forms above a threshold value for the swimming speed. We assign an effective dipole moment to the pump and show that in this non-equilibrium situation the orientations of the particles are Boltzmann-distributed around the pump direction. We also consider bottom-heavy particles in an external gravitational field. Without hydrodynamic interactions and at sufficiently large swimming speeds, these particles accumulate at the top of the simulation box. However, when they interact hydrodynamically, we find this steady state to be unstable and observe the emergence of spatially separated, dynamical toroidal structures, reminiscent of classical bioconvection.

[1] M.E.Cates et al., Phys.Rev.Lett. 104, 258101 (2010)

DY 9.6 Mon 17:30 Poster B2

Evolutionary food web model on a set of patches coupled by migration — •Eva Marie Weiel, Korinna T. Allhoff, and Barbara Drossel — Institut für Festkörperphysik, TU Darmstadt

Ecological food webs in a heterogeneous environment can be modelled by a complex network with two different types of connections. The local connections of these "networks on networks" represent the interaction through predation and competition of ecological populations in each habitat. The second type of connections represents migration between the habitats. Understanding how the spatial dimension affects the structure and stability of these complex networks is of large interest in ecological theory. We investigate the emergence, dynamics and interaction of food webs in a small set of patches. The dynamics in each patch is based on the often-cited evolutionary model introduced by Loeuille and Loreau in 2005. In addition to local evolution we include different types of migration between the patches and analyse their influence on the structure of the emerging food webs.

DY 9.7 Mon 17:30 Poster B2

Effects of a stage structure in a population dynamics model to explain cyclic dominance of pacific sockey salmon — •Fabian Fertig[1], Christoph Schmitt[1], Christian Guill[2], and Barbara Drossel[1] — [1]Institut für Festkörperphysik, TU Darmstadt — [2]Institut für Zoologie and Anthropologie, Georg-August-Universität Göttingen

The number of sockeye salmon that return from the ocean to their lakes of birth in the Fraser River basin in Canada shows a remarkably strong and regular four-year oscillation. This so-called cyclic dominance phenomenon is reproduced as a stable attractor by a recently introduced predator-prey model for salmon fry and their main predator in the rearing lakes, rainbow trout. However, rainbow trout is known to prey also strongly on kokanee salmon, which spend all their life in the lakes. Including kokanee in the model typically leads to a breakdown of cyclic dominance and often also to the extinction of one of the salmon species. This means either that the observed coexistence of the two species together with the occurence of cyclic dominance in the sockeye population is a transient phenomenon, or that the model is not detailed enough. In order to explore the conditions under which cyclic dominance could persist in the presence of both salmon species,

we investigate various models that take the stage structure of trout and the different preference of adult and juvenile trout for kokanee and sockeye salmon into account. We show that the parameter range for cyclic dominance can be increased in stage structured models.

DY 9.8 Mon 17:30 Poster B2

Simple models for generation cycles — •Torsten Pfaff[1], Barbara Drossel[1], and Christian Guill[2] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt — [2]Institut für Zoologie und Anthropologie, Georg-August-Universität Göttingen

Many biological species show population oscillations due to density dependent competition. The periods of the oscillations are related to the life cycle of the species, and they have been used to classify the oscillating systems.

We present three simple models consisting of a one dimensional time delay equation with only two parameters. These models show all essential properties of generation cycles. Due to their simplicity, they are helpful for obtaining a mechanistic understanding of the population oscillations, and they give new insights into the origin of the periods and into the size of the intervals that are covered by these periods. Based on the insights gained from our simple models, we also obtain a better understanding of the more complex models presented in the classical paper by Gurney & Nisbet 1985, and we can extend their results.

As an outlook, we argue that the simple models are useful for investigating generation effects in many species food webs.

DY 9.9 Mon 17:30 Poster B2

Nematic microstructure in biopolymer solutions — •Marc Lämmel and Klaus Kroy — Institut für Theoretische Physik, Leipzig, Germany

Domains of aligned filaments play an important role in solutions of semiflexible biopolymers. For instance, they occur as a consequence of shear induced ordering upon sample preparation or as a precursor of bundle formation. Here, we address the influence of such nematic order on the packing structure of semiflexible polymer networks, based on the wormlike chain model. The complicated many-body problem is approached utilizing the concept of the tube [1], which accounts for caging of a test filament by surrounding filaments. It is represented through a cylindrical confinement potential that is self-consistently determined. In particular, we analyze the effect of local nematic order on the micro-structure in terms of the tube radius distribution [2], which can experimentally be measured with high accuracy for F-actin solutions [3], allowing for a precise quantitative comparison of theory and experiment.

[1] Morse, D. C., Phys. Rev. E 63, 031502 (2001)

[2] Glaser, J. et al., Phys. Rev. E 84, 051801 (2011)

[3] Glaser, J. et al., Phys. Rev. Lett. 105, 037801 (2010)

DY 9.10 Mon 17:30 Poster B2

Stochastic tug-of-war model with symmetric motor properties does not provide processive cargo movement. — •Sarah Klein[1], Cecile Appert-Rolland[2], and Ludger Santen[1] — [1]Theoretische Physik, Universität des Saarlandes, 66123 Saarbrücken — [2]Laboratory of Theoretical Physics, Paris-Sud University, Orsay

Many different types of cellular cargos are transported bidirectionally along microtubules by teams of molecular motors. The motion of this object has been experimentally characterized *in vivo* as processive with rather persistent directionality. By means of an effective theoretical approach, introduced by Lipowsky *et al.* [1], it has been argued that the dynamics of these object are the result of a tug-of-war between different kinds of motors. This picture has been questioned in a recent article by Kunwar *et al.* [2], who considered the coupling between motor and cargo in more detail. In this contribution we discuss possible scenarios within this framework that eventually lead to the observed dynamic patterns of bidirectional cargo transport.

[1] M. J. I. Müller, S. Klumpp, R. Lipowsky, PNAS 105, 4609 - 4614 (2008)

[2] A. Kunwar, S. K. Tripathy, J. Xu, PNAS 108(47), 18960-18965 (2011)

DY 9.11 Mon 17:30 Poster B2

Modeling diversity of immune genes in host-parasite co-evolution — •Yixian Song and Arne Traulsen — Max Planck Institute for Evolutionary Biology Plön

We investigate an individual based stochastic model of host-parasite co-evolution. The model is made to simulate the origin and maintenance of the major histocompatibility complex (MHC) polymorphism, i.e., coexistence of diverse genetic variants in a population. In the genes of the MHC, the key component of adaptive immunity, very high levels of allelic diversity are observed. MHC molecules are essential in antigen presentation process by T-cells. The high polymorphism of MHC genes has drawn attention of evolutionary biologists and population geneticists. Our model is focused on one locus with two alleles. Thereby the dynamics of coexisting parasites and alleles are explored. The goal of this model is to develop a theoretical understanding of the dynamic equilibrium in which the MHC diversity in a population approximately remains from generation to generation, but changes in composition.

DY 9.12 Mon 17:30 Poster B2

Interaction Dynamics of Colloidal Particles in an Optical Light Tube — •Benjamin Tränkle and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, University of Freiburg, Germany

Specific reactions of Brownian particles are often affected by long and short ranging forces, such as hydrodynamic, entropic and steric forces. An example is the fusion of vesicles within a living cell. Colloidal particles can serve as a model system for the investigation of such interaction events. We trap two particles in a single potential, which is generated by an oscillating optical line trap. In this geometry, the reaction rate is increased due to the confined space, while rotational and translational degrees are preserved. An accousto-optic deflector (AOD) is used to steer the optical trap and therefore achieve kHz scanning rates. The spheres' positions are tracked simultaneously in 3 dimensions with back focal plane interferometry [1]. With this method we can measure the interaction dynamics of spheres diffusing in a single optical potential with a spatial precision in the nanometer range at kHz rates. Static and dynamic interaction information is gained by analyzing the particle trajectories. The AOD is also used to control the line potential, by steering the laser power during the scanning process. Thereby, we are able to change the reaction volume and investigate its effect on the reaction rate and interaction duration [2].

[1] Speidel et al., Interferometric 3D tracking of several particles in a scanning laser focus. Optics Express, 17(2):7-9, 2009.

[2]Tränkle et al., Interaction dynamics of two colloids in a single optical potential. Physical Review E, 86(2):1-5

DY 9.13 Mon 17:30 Poster B2

A simple polymer in a spherical cage — •Martin Marenz, Johannes Zierenberg, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100920, D-04009 Leipzig, Germany

We study the change of the pseudo phase transition of a simple homopolymer inside a spherical confinement. Of particular interest is the shift of the collapse and freezing transitions with shrinking radius of the sphere. The polymer is a simple bead-stick model, where the distance between neighboring monomers is fixed, between three monomers in a row acts a bending potential and all non neighboring monomers interact via a Lennard-Jones potential. We use modern Monte Carlo methods to investigate the phase space of this model. Most of the results are obtained by parallel tempering simulations followed by a multi-histogram reweighting method combining a direct and a recursive procedure. To crosscheck our results, especially near the pseudo phase transition, we used a parallelized kind of the multicanonical simulation.

To characterize the pseudo phase transition we analyse fluctuations of energetic and conformational observables. As zero order case the spherical cage is modeled only as a geometrical constraint without any interaction with the polymer. In further simulations we switched on a interaction between the polymer and the surface of the sphere and looked for effects induced by this interaction.

DY 9.14 Mon 17:30 Poster B2

Hybrid simulation model for spatiotemporal intracellular calcium signals — •Martin Rückl[1], Nagaiah Chamakuri[2], and Sten Rüdiger[1] — [1]Humboldt-Universität, Berlin — [2]RICAM, Linz, Austria

Calcium induced calcium release (CICR) from IP3R channels on the ER membrane and the interplay with calcium buffers can result in complex spatiotemporal calcium distributions in the cytosol which play an important role in intra- and extracellular signaling.

To model those patterns, we solve the coupled reaction diffusion and

master equations for both the DeYoung-Keizer [1] and the four state [2] stochastic IP3R gating models, using an interplay between a 3D finite element method and the Gillespie algorithm. We investigate the impact of the local calcium decay after a channel closing and the diffusive coupling of clustered channels on the collective stochastic behaviour of the channels. To obtain different calcium decays we performed simulations for different buffer configurations while the diffusive coupling is altered by means of a larger inter channel distance within a channel cluster. Our results can also be used to assess the reliability of different computationally cheaper approximations frequently used in other works.

[1] D.W. DeYoung and J. Keizer, Proc. Natl. Acad. Sci. U.S.A 89, 9895 (1992).

[2] G. Ullah, I. Parker, D.D. Mak, J.E. Pearson, Cell Calcium, 52(2):152-160, 2012

DY 9.15 Mon 17:30 Poster B2

Measuring structural changes in chromatin induced by ionizing radiation: an analysis of localization microscopy images — •Yang Zhang[1], Gabriell Máté[1], Sabina Hillebrandt[2], Patrick Müller[2], Michael G. Hausmann[2], and Dieter W. Heermann[1] — [1]Institute for Theoretical Physics, Heidelberg University, Germany — [2]Kirchhoff-Institute for Physics, Heidelberg University, Germany

The elaborate cell response to the arising of DNA double-strand breaks caused by ionizing radiation (IR) involves local remodeling and structural changes of the surrounding chromatin. In particular, experiments indicate different repair characteristics in heterochromatin (HC) and euchromatin (EC). However, there is still no detailed understanding of these changes of the genome organization. In this work we analyzed localization microscopy images by means of statistical physics and graph theory to provide a quantitative description of structural changes induced by IR. HeLa cells were exposed to different doses of IR. Positions of fluorescence stained nucleosomes were determined using localization microscopy. Simultaneously, markers of modified histones indicating HC or EC were localized. We then calculated the pair correlation functions as well as edge length distributions and mean coordination numbers for graphs obtained by triangulations of the marker positions. Our results show that HC regions undergo a relaxation immediately after exposure to ionizing radiation while EC regions show the opposite behavior. We further demonstrate that at later times after irradiation these alterations become less pronounced.

DY 9.16 Mon 17:30 Poster B2

Pulling experiments on biological molecules: model analysis and simulation — •Katharina Wenzel and Andreas Heuer — Westfälische Wilhelms Universität Münster

The implementation of AFM-pulling routines by Steered Molecular Dynamics (SMD) has created a powerful tool to provide information of the unfolding and refolding process of biological molecules. Here, a molecule is stretched under pulling with the help of an umbrella potential where the choice of pull speed and cantilever stiffness can play a critical role in the unfolding pathway. To investigate the influence of these parameters several pull experiments under the same circumstances are simulated with the Trp-cage Miniprotein TC5b in vacuo. It can be shown that simulations can lead to very unstable behaviour, especially for higher force speed and stiff cantilever.

To get a more general understanding a basic setup for pulling experiments with one particle under Brownian motion is implemented. Likewise the chosen pathway over the energy barrier as well as the degree of fluctuations strongly depend on the chosen speed and stiffness.

DY 9.17 Mon 17:30 Poster B2

Mutation and Migration in Structured Populations — •Matthias Lechner, Jonas Cremer, Anna Melbinger, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München

Despite the risk of exploitation, altruistic individuals are a common phenomenon in nature. The solution to this so called Dilemma of Cooperation is the purpose of many models in the field of evolutionary dynamics. A recent approach to explain this dilemma is to combine population dynamics with evolutionary game theory in a stochastic description, which shows a transient initial increase of cooperation [1]. This model was then extended by a group-structured population that is subject to repetitive regrouping events, giving rise to a long-term maintenance of cooperation under certain initial conditions [2].

Here, we study the consequences of introducing mutation and migration to this model. With the use of numerical simulations we show that both have similar effects on the system's dynamics. The evolution of purely cooperative groups turns out to be pivotal in the explanation of these changes. For mutation, we support this claim by an analytical approximation, which reproduces our numerical results. In summary, we find that although mutation and migration eventually inhibit cooperation in this model, cooperative behavior is still maintained for a wide range of parameters.

[1] A. Melbinger et al., PRL 105, 178101 (2010)

[2] J. Cremer et al., Scientific Reports, 2, 281 (2012)

DY 9.18 Mon 17:30 Poster B2

Swimming patterns of bacteria in confined microchannels with obstacles — •Michael Raatz, Matthias Theves, and Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Germany

Depending on environmental conditions, single bacteria can irreversibly attach to a solid-liquid or liquid-air interface and form the cores for surface associated growth into aggregates, where cells are embedded in a polymer matrix and become resistive to antibiotic treatment (biofilms). We use microfluidic channels and high-speed time lapse microscopy to investigate the movement of cells which are swimming in close proximity to the wall interface and interact with various arrangements of circular obstacles. Motility statistics show that in the presence of obstacles, the average run length of a bacterium and the probability distribution of turn angles changes when compared to an obstacle-free channel. At small collision angles with the obstacle, the cell trajectory is slightly deflected while large angle collisions can induce reversals in the direction of propagation of a cell. Furthermore, we observe cases where cells move around the obstacle in a circular path, maintaining a stable 'orbit' at a distance of one or two cell diameters from the obstacle surface.

DY 9.19 Mon 17:30 Poster B2

Evolution of increasingly complex filamentous molecules — •Philipp Zimmer[1], Emanuel Worst[2], Eva Wollrab[2], Albrecht Ott[2], and Karsten Kruse[1] — [1]Universität des Saarlandes, Theoretische Biologische Physik, Postfach 151150, 66041 Saarbrücken — [2]Universität des Saarlandes, Biologische Experimentalphysik, Postfach 151150, 66041 Saarbrücken

On the young earth, molecules with increasing complexity evolved under prebiotic conditions. How the interplay of different, competing molecular species and the spontaneous generation of new ones eventually led to the formation of cells remains poorly understood. Here we investigate a mechanism of "biased variation" and show that it provides a way to generate more complex structures. In this mechanism certain variations of existing molecular species are more likely to occur than others. Combined with an exponential amplification, this process can generate increasing complexity. We investigate this mechanism using a stochastic model for the evolution of linear molecules and we present a DNA-based experimental realization.

DY 9.20 Mon 17:30 Poster B2

In-phase and anti-phase synchronization in noisy Hodgkin-Huxley neurons — •Xue Ao, Peter Hänggi, and Gerhard Schmid — Institut für Physik, Universitätsstr. 1, 86159 Augsburg, Germany

We numerically investigate the influence of intrinsic channel noise on the dynamical response of delay-coupling in neuronal systems. The stochastic dynamics of the spiking is modeled within a stochastic modification of the standard Hodgkin-Huxley model wherein the delay-coupling accounts for the finite propagation time of an action potential along the neuronal axon. We quantify this delay-coupling of the Pyragas-type in terms of the difference between corresponding presynaptic and postsynaptic membrane potentials. For an elementary neuronal network consisting of two coupled neurons we detect characteristic stochastic synchronization patterns which exhibit multiple phase-flip bifurcations: The phase-flip bifurcations occur in form of alternate transitions from an in-phase spiking activity towards an anti-phase spiking activity. Interestingly, these phase-flips remain robust in strong channel noise and in turn cause a striking stabilization of the spiking frequency.

DY 9.21 Mon 17:30 Poster B2

Inverse statistical analysis in heart rate variability — •Haleh Ebadi — Bioinformatics Group, Department of Computer Science, University of Leipzig, Germany

This poster presents an investigation on heart cycle time series, using the inverse statistical analysis, a concept borrowed from turbulence. By inverse statistics, also sometimes called exit time statistics, we turn the variables around such that the fluctuating variable becomes the fixed variable, while the fixed variable becomes fluctuating. Using this approach, we studied the distribution of the exit time needed to achieve a predefined level of heart rate alteration. Such analysis uncovers the most likely waiting time needed to reach a certain change in the rate of heart beat. This analysis showed a significant difference between the raw data and shuffled data, when the heart rate accelerates or decelerates to a rare event. We also report that inverse statistical analysis can distinguish between the electrocardiograms taken from healthy volunteers and patients with heart failure.

DY 9.22 Mon 17:30 Poster B2

Bifurcation analysis of a thalamocortical mean field model — •Michael Schellenberger Costa, Thomas Martinetz, and Jens Christian Claussen — INB, University of Lübeck, Germany

Multiple studies have shown the importance of slow wave sleep for the development of memories. Furthermore slow oscillatory activity can be modulated by non-invasive stimulation, which leads to an enhancement of memory consolidation [1]. In order to optimize the experimental procedures and thereby further improve the memory consolidation, a detailed knowledge of the cortical response to the applied stimuli is essential. Mean field models of the cortex have been extensively studied [2], however the interplay between the thalamus and the cortex is know to be crucial for both slow wave sleep and the processing of sensory stimuli. Therefore we investigate the dynamic properties of an extended phenomenological mean field model of the thalamocortical system, that is able to resemble the EEG signal during slow wave sleep.

[1] L. Marshall et al, Nature 444, 610 (2006).
[2] M. Ursino, F. Cona and M. Zavaglia, Neuroimage 52, 1080 (2010).

DY 9.23 Mon 17:30 Poster B2

Limitations on entrainment frequency in cortical slow wave stimulation — •Arne Weigenand[1], Lisa Marshall[2], Thomas Martinetz[1], and Jens Christian Claussen[1] — [1]INB, University of Lübeck — [2]Neuroendocrinology, University of Lübeck, Germany

Stimulation of cortical slow waves during sleep has recently raised considerable attention due to enhancement of memory consolidation [1]. We consider the question how slow waves, comprised by bursty up and quiescent down states, can be entrained or strengthened by external stimulation. In a purely cortical model no limitation within the relevant frequency range occurs [2]. Stimulation by TMS or optogenetic methods [3,4] hint at an upper entrainment frequency of 4 Hz. In contrast, our optical stimulation experiments [5] revealed that entrainment is only possible up to 1 Hz. We account thalamic gating for this difference. Hence we consider the inclusion of thalamic feedback loops into generic cortical network models, for adaptation of parameters in a phenomenological mean-field model. We optimize pulse length and frequency to obtain an optimized stimulation protocol.

[1] L. Marshall et al, Nature 444, 610 (2006). [2] Weigenand, Martinetz, Claussen, Cogn. Neurodyn. 6, 367 (2012); Schütt, Claussen, Cogn. Neurodyn. 6, 343 (2012). [3] Massimini et al., PNAS 104, 8407 (2007). [4] Kuki et al, Frequency-dependent entrainment of neocortical slow oscillation to repeated optogenetic stimulation in the anesthetized rat, Neurosci. Res. (2012, in press). [5] Weigenand et al (in preparation).

DY 9.24 Mon 17:30 Poster B2

Approach for automated sleep stage classification from spectral data — •Stephan Volkland and Jens Christian Claussen — INB, University of Lübeck, Germany

Manual scoring of sleep stages according to the Rechtschaffen-Kales rule catalogue (or the only simplified AAMS rules) is done on 30s epochs and requires extensive manual labor. Further the inter-rater and intra-rater reliabilities are not fully satisfactory for subsequent quantitative analysis. Hence it would be desired to develop and use automatic methods: attempts in this direction have been tried numerously but not paved their way to clinical practice as the EEG signatures of the sleep stages differ between subjects even in a qualitative way. Furthermore it would be desired to detect and resolve sub-stages as well as acheive a higher time resolution; both is unfeasible for manual scoring which would then be slower than real time. Here we refer and compare to an approach by [1] where three quantitative indexes are derived from EEG and EMG and broken down to 8 possible states. Our approach also is based on EMG and EEG, whereby we also use EOG, and use full information from five physiological EEG bands as input for unsupervised clustering (k-means) of data where clusters then are assigned to sleep stages [2]. We observe that the known difficulties to reliably distinguish S1, REM and wake stages persist. For the range between stages S2 and S4, we however can obtain a reliable interpolation between the sleep stages even for 16s or shorter time intervals.

[1] B. Müller, W.D. Gäbelein, H. Schulz, Sleep 29, 967 (2006).
[2] Stephan Volkland, BA thesis, INB, Lübeck (2012).

DY 10: Glasses (joint session DY/DF/CPP)

Time: Tuesday 9:30–12:30 Location: H46

DY 10.1 Tue 9:30 H46

Towards reliable structural information of multicomponent glass systems — •Christoph Scherer[1,2], Friederike Schmid[1], and Martin Letz[2] — [1]Johannes Gutenberg-Universität, Mainz, Deutschland — [2]Schott AG, Mainz, Deutschland

Glasses have a huge range of applications, however, they are still theoretically not well understood. Also experimental access to the structure of glasses is limited. This motivates the study of glass systems by means of computer simulations.

In this work, a set of glass structures is generated on the computer by equilibrating a system of a few hundred atoms at high temperature, well above the glass transition temperature, with a classical molecular dynamics simulation (MD). Afterwards the system is cooled down to 0 K and structurally relaxed to the next (local) minimum by means of a quantum mechanical density functional (DFT) calculation. The glass properties before and after the structural relaxation are compared to experimental results. Especially, the phonon density of states is of interest, as it provides access to thermodynamical quantities.

This sets the basis for the next steps: The force fields for the MD simulation are generated by means of a structural fitting procedure. Here, the force field parameters are fitted in a way that the structure, namely the radial distribution function, of a short MD run at high temperature matches as closely as possible that one of a short DFT run at the same temperature. The dependence of the fitting accuracy of the classical force field on the final glass structure and glass properties is examined.

DY 10.2 Tue 9:45 H46

On the behavior of supercooled liquid water in Confinements formed by frozen water molecules: a molecular dynamics simulation study — •Felix Klameth and Michael Vogel — Institut für Festkörperphysik, TU Darmstadt, 64289 Darmstadt

Molecular dynamics simulations are performed to study the influence of an amorphous ice confinement on liquid water. Investigating water in confinement is believed to reveal information unaccessible for bulk water due to crystallization. Therefore, there are numerous studies on confined water, which claim, e.g., existence of a second critical point associated with a liquid-liquid phase transition in the supercooled regime [1]. However, transfer of information from confined water to bulk water is not straightforward because introducing walls changes the static properties of water due to specific interactions at the interfaces. To avoid this drawback, we use a neutral confinement comprised of immobilized water molecules. We compare static and dynamical properties found in pores with different radii to that of bulk water. The static characteristics, like the tetragonal order parameter, are not changed even near the pore wall. On the contrary, the dynamics inside the pore are dramatically influenced. We find a tremendous increase of the structural relaxation time of liquid water when approaching the pore wall. Thus, we observe a strong change of the local dynamics, which is neither accompanied by a variation of the local structure nor caused by specific wall-liquid interactions. Possible origins for this effect are discussed. [1] P. Kumar et al, PRL (2006), 97, 177802

DY 10.3 Tue 10:00 H46

Deuteron-NMR investigation on the dynamics of supercooled, confined water — •Matthias Sattig and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik

The dynamical behaviour of water in the regime of the supercooled liquid is a topic of large interest. In particular, the existence of a fragile-to-strong transition (FST) at T=225K related to the transition between two distinct phases of liquid water is controversially discussed [1]. Due to crystallization the temperature range proposed for the FST is hardly accessible in bulk water. Therefore, we confine heavy water to narrow pores in the mesoporous sillicate MCM-41. This suppresses the freezing of a substantial fraction of water, enabling direct investigation of the interesting temperatures. Deuteron-NMR methods are utilised to determain the rotational correlation times τ of water on time scales from ns up to s. The spin-lattice-relaxation time T_1 exhibits a typical minimum at about T=230K. Above this minimum the correlation times follow a Vogel-Fulcher-Tammann law. Below the minimum, two relaxation processes could be observed. The low-temperature processes show a different temperature dependence, where the curves τ(T) of all processes intersect at about T=230K. A comparison with literature data [2] from neutron scattering and dielectric spectroscopy gives rise to the idea that the observed crossover is due to this intersection of processes rather than to a FST. To test this idea studies on water confined to MCM-41 with different pore sizes and fillings are in progress.

[1] Mishima; Nature, Vol. 396, 329(1998) [2] Hedström; EPJST 141, 53(2007)

DY 10.4 Tue 10:15 H46

Modelling the relaxation of glass-forming systems at low temperatures: a potential energy approach — •Andreas Heuer and Christian Rehwald — Institute for Physical Chemistry, Corrensstr. 28/30, D-48149 Münster

Based on finite-size effects of a model glass-forming system we have introduced a model which allows one to express the dynamics of a macroscopic glass-former in terms of coupled subunits of temperature-independent size and temperature-dependent coupling constant [1]. The results are obtained from computer simulations on a binary mixture Lennard-Jones model, interpreted in terms of the underlying potential energy landscape. The model is denoted coupled landscape model (CLM).

After a short review of the CLM we present key predictions of this approach for temperatures far below the range accessible by computer simulations. In particular we present results for the violation of the Stokes-Einstein relation (connecting diffusivity and structural relaxation) and the validity of the time-temperature superposition. Finally, the CLM is compared with other models presently discussed for the explanation of the glass-transition phenomena.

[1] C. Rehwald, O. Rubner, A. Heuer, Phys. Rev. Lett. 105, 117801 (2010)

[2] C. Rehwald, A. Heuer, Phys. Rev. E 86, 051504 (2012)

DY 10.5 Tue 10:30 H46

Microrheology on supercooled liquids in terms of a Potential Energy Landscape approach — •Carsten Friedrich Erich Schroer and Andreas Heuer — Westfälische Wilhelms-Universität Münster, Münster, Germany

We perform MD simulations of a binary Lennard-Jones mixture where an external force is applied on a single tracer particle. The dynamics of the tracer particle includes several interesting features like non-linear mobilities and anomalous diffusion parallel to the force direction. Our main focus relies in the investigation of the underlying Potential Energy Landscape (PEL), especially in the energetic minima the system explores during its time evolution. Equally to equilibrium systems a coarse graining of these minima to mesoscopic regions allows the description of the system dynamics in terms of a continuous time random walk (CTRW). Extending the concept of the CTRW towards stationary non-equilibrium systems turns out to be an efficient tool for the understanding of non-equilibrium dynamics. First, the approach contains a decomposition between linear and non-linear effects, thus enables a detailed study of the transition between these dynamical regimes. Second, it allows the quantitative understanding of the anomalous diffusion of the tracer particle. Third, for the first time a connection between the non-Gaussian parameter α_2 in equilibrium and superdiffusivity in non-equilibrium can be established. With the help of the underlying PEL, important information can be gained about the dynamics, e.g. about the onset of non-linear effects. The non-linear regime can be discussed in terms of a rejuvenation scenario.

15 min. break.

DY 10.6 Tue 11:00 H46

Simulation of Aging in SiO2: Single Particle Jump Analysis — •Katharina Vollmayr-Lee[1], Robin Bjorkquist[2], and Landon Chambers[3] — [1]Bucknell University, USA — [2]Cornell University, USA — [3]Texas A&M, USA

Using molecular dynamics computer simulations, we study the aging dynamics of amorphous SiO2. Starting from fully equilibrated configurations at high temperatures the system is quenched to temperatures which are below Tc. We then observe the resulting microscopic dynamics as a function of the waiting time tw, the time elapsed since the temperature quench. We use single particle trajectories to identify "jumps" when the particle's average position changes over a short time interval significantly compared to its fluctuations. We find that the only tw-dependent microscopic quantity is the number of jumping particles per unit time. Similar to previous studies for fragile glass formers, we show here for the strong glass former SiO2 that neither the distribution of jump lengths nor the distribution of times spent in the cage are tw-dependent. We therefore find a surprising similarity of the jump dynamics of fragile and strong glass formers.

DY 10.7 Tue 11:15 H46

Excess free energy of supercooled liquids at disordered walls — •Ronald Benjamin and Jürgen Horbach — Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität Düsseldorf

We perform NVT molecular dynamics simulations of a supercooled liquid confined between identical walls of two types. In the first case flat structureless walls, represented by an external field are considered. In the second case we consider disordered walls consisting of the same supercooled liquid frozen into an amorphous configuration. Using a thermodynamic integration scheme [R.Benjamin and J. Horbach, J. Chem. Phys. **137**, 044707 (2012)] we are able to obtain the excess free energy of the supercooled liquid with respect to both kinds of walls. While a positive excess free energy (of the order of $10k_BT/\sigma^2$) is obtained with respect to a flat structureless wall, the excess free energy between the supercooled liquid and the frozen disordered walls turns out to be negative ($\approx -0.5k_BT/\sigma^2$) even though the potential energy of the supercooled liquid in presence of the disordered walls is the same as that of the bulk. This shows the purely entropic contribution to the excess free energy of the supercooled liquid in presence of the disordered walls. The existence of a negative excess free energy also shows that the thermodynamic properties of such a confined supercooled liquid is not identical to that of the bulk.

DY 10.8 Tue 11:30 H46

Multiple reentrant glass transitions of soft spheres at high densities — •Michael Schmiedeberg — Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40204 Düsseldorf, Germany

We study the dynamics of soft spheres by using Molecular Dynamics simulations. The relaxation time varies non-monotonically as a function of density at constant temperature (cf. [1,2]). We determine and study the jamming phase diagrams that indeed show multiple reentrant glass transitions if temperature and density are used as control parameters. However, if we switch to a new formulation of the jamming phase diagrams [3], where temperature over pressure and pressure are employed as control parameters, no non-monotonic behavior can be observed.

[1] L. Berthier, A.J. Moreno, and G. Szamel, Phys. Rev. E 82, 060501(R) (2010).

[2] M. Pica Ciamarra and P. Sollich, arXiv:1209.3334.

[3] T.K. Haxton, M. Schmiedeberg, and A.J. Liu, Phys. Rev. E 83, 031503 (2011).

DY 10.9 Tue 11:45 H46

Exact Nonlinear Response in the driven lattice Lorentz gas — •Sebastian Leitmann and Thomas Franosch — Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058, Erlangen, Germany

We determine the nonlinear time-dependent response of a tracer on a lattice with randomly distributed hard obstacles as a force is switched on. The calculation is exact to first order in the obstacle density and holds for arbitrarily large forces. In particular, we show that the nonlinear mobility in the stationary state becomes non-analytic in the driving force. Furthermore we demonstrate that the stationary veloc-

ity is approached exponentially fast for any finite values of the force, in striking contrast to the power-law relaxation predicted within linear response. We discuss the range of validity of our analytic results by comparison to Monte Carlo simulations.

DY 10.10 Tue 12:00 H46

From beta-relaxation to alpha-decay: Atomistic picture from molecular dynamics simulations for glass-forming Ni0.5Zr0.5 melt — •Helmar Teichler — Inst. Materialphysik, Univ Göttingen

In glass-forming melts the decay of structural fluctuation shows the well known transition from beta-relaxation (von-Schweidler law with exponent b) to alpha-decay (KWW law with exponent beta). Here we present results from molecular dynamics simulations for a metallic glass forming Ni0.5Zr0.5 model aimed at giving an understanding of this transition on the atomistic scale. At the considered temperature below mode coupling Tc, the dynamics of the system can be interpreted by residence of the particles in their neighbour cages and escape from the cages as rare processes. Our analysis yields that the fraction of residing particles is characterized by a hierarchical law in time, with von-Schweidler b explicitly related to the exponent of this law. In the alpha-decay regime the stretching exponent reflects, in addition, floating of the cages due to strain effects of escaped particles. Accordingly, the change from beta-relaxation to alpha-decay indicates the transition from low to large fraction of escaped particles.

DY 10.11 Tue 12:15 H46

Interaction between tunnelling systems in glasses — •Gudrun Fickenscher[1], Christian Schötz[1], Paul Fassl[1], Alexander Archer[1], Alexander Burin[2], Manfred von Schickfus[1], Andreas Fleischmann[1], and Christian Enss[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]Tulane University, New Orleans, USA

The low-temperature properties of glasses are governed by tunnelling systems as described in the well-established standard tunnelling model. Interactions between tunnelling systems and phonons lead to energy relaxation. In addition, the interaction between individual tunnelling systems, as predicted by spectral diffusion theory, causes phase decoherence phenomena. To study these interaction processes we have measured the decay of different types of polarization echoes in the standard glass BK7 with respect to the delay time at temperatures between 7.5mK and 70mK. The decay of 2- and 3-pulse echoes is strongly influenced by spectral diffusion. In the case of 3-pulse echoes we expect, in addition, a significant contribution to the decay by energy relaxation processes. On comparing the measured data to numerical calculations we find that the decay of the echo amplitude is slower than predicted by the standard theory at all temperatures. This leads us to the assumption, that there exists a small subspace of tunnelling systems which interact very little with phonons due to a very small coupling constant. Including this subspace in the calculations we can accurately fit the data for all echo types and temperatures with one consistent set of parameters.

DY 11: Statistics and Dynamics of/on Networks (joint session BP/DY/SOE)

Time: Tuesday 9:30–11:45 Location: H47

DY 11.1 Tue 9:30 H47

Chimera states in neural systems — •Iryna Omelchenko[1,2], Oleh Omel'chenko[3], Philipp Hövel[1,2,4], and Eckehard Schöll[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin — [2]Bernstein Center for Computational Neuroscience, Humboldt-Universität zu Berlin — [3]Weierstrass Institute, Berlin — [4]Center for Complex Network Research, Northeastern University, Boston, USA

Chimera states are spatio-temporal patterns of synchrony and disorder observed in systems of nonlocally coupled identical elements. They are characterized by coexistence of spatial regions with regular synchronized and irregular incoherent motion. Initially discovered for phase oscillators, chimera states have been also found in systems of nonlocally coupled discrete maps [1], time-continuous chaotic systems [2], and have been recently realized in experiments [3].

We investigate the cooperative dynamics of nonlocally coupled neural populations modeled by FitzHugh-Nagumo systems, where each individual system displays oscillatory local dynamics, and demonstrate the existence of chimera states there. We analyse the stability of chimera states in the parameter space of the system and discuss mechanisms of transitions between different chimera types.

[1] I. Omelchenko, Yu. Maistrenko, P. Hövel, and E. Schöll, Phys. Rev. Lett. 106, 234102 (2011).

[2] I. Omelchenko, B. Riemenschneider, P. Hövel, Yu. Maistrenko, and E. Schöll. Phys. Rev. E 85, 026212 (2012).

[3] A.M. Hagerstrom, T.E. Murphy, R. Roy, P. Hövel, I. Omelchenko, and E. Schöll. Nature Physics 8, 658 (2012).

DY 11.2 Tue 9:45 H47

Scaling Laws in Critical Random Boolean Networks with General in- and out-Degree Distributions — •Marco Möller and Barbara Drossel — Institute for condensed matter physics, TU Darmstadt, Germany

We evaluate analytically and numerically the size of the frozen core and various scaling laws for critical Boolean networks that have a power-law in- and/or out-degree distribution. To this purpose, we generalize an efficient method that has previously been used for conventional random Boolean networks and for networks with power-law in-degree distributions. With this generalization, we can also deal with power-law out-degree distributions. When the power-law exponent is between 2 and 3, the second moment of a distribution changes, and the scaling exponent of the nonfrozen nodes depends on the degree distribution exponent.

Furthermore, the exponent depends also on the dependence of the cutoff of the degree distribution on the system size. Altogether, we obtain an impressive number of different scaling laws depending on the type of cutoff as well as on the exponents of the in- and out-degree distribution. We confirm our scaling arguments and analytical considerations by numerical investigations.

DY 11.3 Tue 10:00 H47

Small-World Network Spectra in Mean-Field Theory — •Carsten Grabow[1], Stefan Grosskinsky[2], and Marc Timme[3] — [1]Potsdam Institute for Climate Impact Research, Potsdam, Germany — [2]Mathematics Institute and Centre for Complexity Science, Warwick, UK — [3]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Collective dynamics on small-world networks emerge in a broad range of systems with their spectra characterizing fundamental asymptotic features. Here we derive analytic mean-field predictions for the spectra of small-world models that systematically interpolate between regular and random topologies by varying their randomness. These theoretical predictions agree well with the actual spectra (obtained by numerical diagonalization) for undirected and directed networks and from fully regular to strongly random topologies. These results may provide analytical insights to empirically found features of dynamics on small-world networks from various research fields, including biology, physics, engineering, and social science. (Based on Grabow, C., Grosskinsky, S. & Timme, M. Small-World Network Spectra in Mean-Field Theory. Phys. Rev. Lett 108, (2012).)

DY 11.4 Tue 10:15 H47

Robust large-scale properties in networks — •Tiago Peixoto and Stefan Bornholdt — Institut für Theoretische Physik, Universität Bremen, Hochschulring 18, D-28359 Bremen, Germany

Most network systems possess large- or mesoscale structures, which are not captured by local measures such as, e.g. degree and subgraph statistics. Many network models, as well as mean field analysis of dynamical processes on networks neglect such features. Here we include in a general fashion such large-scale properties in the the analysis of a paradigmatic percolation problem in networks with interdependence, as well as Boolean dynamics based on majority functions, meant to describe systems which are robust against noise, such as gene regulation.

A model for the evolution of such systems is proposed, where networks with more robust properties survive with greater probability. By mapping the evolutionary process into a statistical ensemble, the free energy of the system is minimized, and its equilibrium properties are obtained. The analysis reveals a topological phase transition at

a specific value of selective pressure, where a core-periphery topology emerges, characterized by the existence of a smaller subset of nodes which regulate the entire system; a feature which is also found in many real systems.

T. P. Peixoto, S. Bornholdt, Phys. Rev. Lett. 109, 118703 (2012); T. P. Peixoto, Phys. Rev. E 85, 041908 (2012); T. P. Peixoto, Phys. Rev. E 85, 056122 (2012)

15 min. break.

DY 11.5 Tue 10:45 H47

High performance simulation and visualization of epidemics on complex networks — •Peter A. Kolski[1,2], Thomas Selhorst[1], Martin Clauss[3], and Jörn Hoffmann[3] — [1]Friedrich-Loeffler-Institut, Wusterhausen, Germany — [2]University of Potsdam, Germany — [3]University of Leipzig, Germany

Dynamical processes on complex networks are a growing field of interest. Performing simulations on large system of this kind demand a high computational power. To handle dynamics on networks the NetEvo C++ library can assign dynamical systems to edges and nodes. Furthermore it solves these ODEs via the ODEint library and can perform heuristic optimization. We introduce an extension to NetEvo using OpenCL on GPUs. With this approach we achieve an increase of computational performance up to a factor of 100, compared to an optimized C++ code on a modern CPU. Additionally we developed a framework to visualize intermediate results and to perform instantaneous visual analytics. The software will be applied in epidemiology, simulating disease spread on trade networks by solving the SIR model*s ODEs. The modification of parameter in real-time and the immediate access to simulation results leads to intuitive insights into the behavior of epidemics on large complex networks.

DY 11.6 Tue 11:00 H47

Diffusion processes and entropy prodcution in weakly coupled complex networks — Grzegorz Siudem and •Janusz Hołyst — Faculty of Physics, Center of Excellence of Complex Systems Research, Warsaw University of Technology, Poland

We consider diffusion phenomena on a pair of weakly coupled complex networks. Assuming that a density of internetwork connections is much lower than a density of intranetwork links we could make use of a time separation for processes taking place in and between the networks. As result we truncated the system dynamics to a simple Markov Chain and we received an equation corresponding to the Fick's First Law. We got an analytical form for internetwork diffusion coupling and estimated entropy production during the equilibration process.

DY 11.7 Tue 11:15 H47

A Network Generation Process for Temporal Graphs — •Peter A. Kolski[1,2], Thomas Selhorst[1], Markus Abel[2], and Arkady Pikovsky[2] — [1]Friedrich-Loeffler-Institut, Wusterhausen, Germany — [2]University of Potsdam, Germany

In this work we show a mechanism for creating Temporal Graphs inspired by real world trade transportation. In the last years complex networks have been in the focus of theoretical and applied research. Although networks like the power grid or water assets have continuos flow on the edges, trade networks are intrinsically discrete. We present a generic model for the generation and evolution of these Temporal Graphs: A continuous state is assigned to each node, described by a dynamical process. In our case we use an integrate-and-fire model. Once a threshold is exceeded, a node becomes "active" and, according to a cost function, selects another active node. This way an edge is temporarily established. Through these edges, nodes interact by resetting their states to zero. In addition, the cost function is modified in a way that the probability to reuse the edge is increased. We present first results on the analysis of this model by i) the degree distribution of the graph formed of the aggregated edges and ii) the degree distribution at a single time. In addition, we study the differences between a two-dimensional and a full graph. In particular we discuss details in the temporal evolution of the degree distribution, as one of the most important characteristics.

DY 11.8 Tue 11:30 H47

Transmission grid extensions during the build-up of a fully renewable European electricity supply — •Sarah Becker[1], Rolando A. Rodriguez[2], Gorm B. Andresen[2], Stefan Schramm[1], and Martin Greiner[2] — [1]Frankfurt Institute for Advanced Studies, Goethe-Universität Frankfurt — [2]Aarhus Department of Engineering and Department of Mathematics, Aarhus University, Denmark

Spatio-temporal generation patterns for wind and solar photovoltaic power in Europe are used to investigate the effect of an increasing penetration of these variable renewable energy sources (VRES) on the European electricity system, in particular on the required link capacities of the transmission grid. VRES growth predictions according to the official National Renewable Energy Action Plans of the EU countries are used and extrapolated logistically up to a fully VRES-supplied power system. It is examined how the need for transmission rises in the future. We find that quadrupling today's international net transfer capacities over the next forty years reduces the final need for backup energy by more than one third. The remaining backup energy is due to correlations in the generation patterns, and can thus not be reduced by transmission. Additionally, our results show how the optimal mix between wind and solar energy shifts from about 70% to 80% wind share as the transmission grid is enhanced. Finally, we exemplify how reinforced transmission affects the import and export opportunities of single countries during the VRES ramp-up and the coupled transmission grid extension.

DY 12: Nonlinear Dynamics, Synchronization and Chaos I

Time: Tuesday 9:30–12:45 Location: H48

DY 12.1 Tue 9:30 H48

Monte Carlo Sampling in Open Dynamical Systems — •Jorge C. Leitão[1], Eduardo G. Altmann[1], and João Viana Lopes[2] — [1]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]CEsA - Centre for Wind Energy and Atmospheric Flows, Faculdade de Engenharia da Universidade do Porto, 4200-465 Porto, Portugal

In this presentation I will show how Monte Carlo methods can be used to efficiently perform averages on chaotic open dynamical systems. I will introduce a new algorithm, based on the well known Wang-Landau algorithm, to compute both the escape time distribution and the maximum Lyapunov exponent of the system in polynomial time, much faster than the exponential scaling of the standard uniform sampling. From the algorithmic point of view, this problem corresponds to sample a landscape with fractaly-distributed minima (singularities).

DY 12.2 Tue 9:45 H48

Chaotic systems with absorption — •Eduardo G. Altmann[1], Jefferson S. E. Portela[2], and Tamas Tel[3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, Germany — [3]nstitute for Theoretical Physics - HAS Research Group, Eotvos University, Budapest, Hungary

In this talk we will introduce a dynamical-systems operator formalism to describe absorption. In opposite to scattering or open systems, in which trajectories escape, in systems with absorption (e.g., in acoustics and optics) it is the intensity associated to the trajectory (ray) which decays in time. Applying our formalism to fully chaotic systems we obtain new expressions for the escape rate and an increased multifractality of the invariant sets when compared to the spectrum of dimensions obtained without taking absorption and return times into account. Results are illustrated by analytical calculations in simple maps and simulations in the cardioid billiard.

DY 12.3 Tue 10:00 H48

Estimating forces by observing a noise-driven mechanical system — •Andreas Ruttor, Philipp Batz, and Manfred Opper — Technische Universität Berlin

Predicting the dynamics of a mechanical system is easy as long as its properties, e.g. moments of inertia and friction coefficients, are ex-

actly known. But for real devices, e.g. robots, this is usually not the case. Applying a noisy control force leads in combination with friction to a stationary stochastic dynamics. We show that one can estimate the forces in the system as a function of its state by observing these movements. While it is possible to measure accelerations directly, this approach requires very dense and evenly spaced observations. In contrast, our method estimates the probability distribution in phase space, which works with larger time intervals between data points, too. It is even possible to choose the position of the observations randomly. Prior knowledge about the system can be included in a parametric model of the potential energy. But we also have a non-parametric approach based on Gaussian process regression, which works without that information.

DY 12.4 Tue 10:15 H48

Noise-induced oscillations in network motifs of non-linear oscillators with delay — •Andrea Vüllings[1], Valentin Flunkert[2,1], and Eckehard Schöll[1] — [1]Technische Universität Berlin, Germany — [2]IFISC, Palma de Mallorca, Spain

We investigate noise-induced oscillations of network motifs composed of non-linear oscillators (super- or subcritical Hopf-normal forms), which are paradigmatic for neural networks and coupled semiconductor lasers. Fluctuations are modeled by Gaussian white noise, and finite signal propagation velocities are accounted for by a time-delayed coupling. Using a self-consistent mean-field approach, we study stochastic synchronization and compare our results with numerical simulations. We find that the delay can enhance or destroy the collective oscillations in a network motif depending upon the delay time. For the supercritical case with nonzero amplitude-phase coupling (corresponds to the linewidth enhancement factor in semiconductor-laser physics) a noise-induced frequency shift of the oscillations is observed. In the case of noisy subcritical Hopf-normal forms we observe coherence resonance. We study numerically the effect of the time delay on the optimal noise strength in the coupled system.

DY 12.5 Tue 10:30 H48

Phase retrapping in a φ Josephson junction — the butterfly effect — •Edward Goldobin[1], Dieter Koelle[1], Reinhold Kleiner[1], and Roman G. Mints[2] — [1]Universität Tübingen, 72076 Tübingen, Germany — [2]Tel Aviv University, Tel Aviv 69978, Israel

We consider retrapping of the phase in a point-like φ Josephson junction[1,2] upon switching from a finite voltage state back to a zero-voltage state, i.e. retrapping of a particle moving viscously in a tilted periodic double-well potential when the tilt is adiabatically reduced. We find the dependence of the retrapping current (tilt) γ_R on the damping parameter α and analyze in which well of the double-well potential the phase is trapped for given α. In the limit of low damping α (low temperature) the system exhibits a butterfly effect — extreme sensitivity of the destination well on the damping α and even on temperature $T \propto \ln(\alpha)$, which leads to an impossibility to forecast the destination well where the phase will be retrapped.

[1] E. Goldobin et al., Phys. Rev. Lett. **107**, 227001 (2011).
[2] H. Sickinger et al., Phys. Rev. Lett. **109**, 107002 (2012).

DY 12.6 Tue 10:45 H48

The relevance of Arnold tongues for systems with time-varying delay — •Andreas Otto, David Müller, and Günter Radons — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

Is it possible to convert a dynamical system with variable time delay into a system with constant delay? In this talk nonlinear time scale transformations of time delay systems are investigated, which are connected with a topological conjugation of the retarded arguments of the delay differential equations.

A necessary and sufficient condition for the existence and a method for the transformation of systems with time-varying delay to systems with constant delay are presented. For instance, in case of a time-varying delay similar to a circle map the existence of a transformation to constant delay depends on whether the parameters of the variable delay are located in an Arnold tongue or not.

The results can be helpful for the numerical solution and the characterization of the dynamical behavior of non-autonomous delay differential equations.

15 min. break.

DY 12.7 Tue 11:15 H48

Spontaneous formation of chimera states under strong global coupling: theory — •Lennart Schmidt[1,2], Konrad Schönleber[1], Katharina Krischer[1], and Vladimir García-Morales[1,2] — [1]Physik Department, Nonequilibrium Chemical Physics, Technische Universität München, Garching, Germany — [2]Institute for Advanced Study - Technische Universität München, Garching, Germany

Chimera states are spatiotemporal patterns in coupled oscillatory media, where synchronized and incoherent domains coexist. A nonlocal coupling is believed to be indispensable for the formation of such states. By means of a modified complex Ginzburg-Landau equation (MCGLE) we demonstrate, however, that chimera states arise spontaneously through a bifurcation from cluster states when just a strong global coupling is present. This prediction was validated experimentally with the oscillatory electrooxidation of silicon in fluoride containing electrolytes, for which the MCGLE was originally derived. The results confirm that the proposed new route to chimeras is robust. Furthermore, as a global coupling is much more frequently encountered than a nonlocal coupling, the occurrence of chimeras is considerably more likely than previously anticipated.

DY 12.8 Tue 11:30 H48

Spontaneous formation of chimera states and other cluster patterns under strong global coupling: experiment — •Konrad Schönleber, Andreas Heinrich, Carla Zensen, Lennart Schmidt, Vladimir Garcia-Morales, and Katharina Krischer — Technische Universität München, Garching, Deutschland

We investigate the spatial thickness distribution of oxide layers formed at illuminated n-type silicon samples during the anodic electrodissolution in fluoride containing electrolytes by means of spatially resolved ellipsometric imaging. Spontaneous pattern formation in the oxide thickness can be observed for intermediate illumination strengths while the total current and spatially averaged oxide thickness oscillate simply periodic. The patterns are typically cluster patterns where the electrode splits into several domains showing different oscillatory behavior for example subharmonic clusters or chimera states. These patterns are well captured by a modified Ginzburg-Landau equation with nonlinear global coupling. In addition, a novel type of spatial organization involving periodically growing and collapsing oscillating domains with peculiar front dynamics are discussed.

DY 12.9 Tue 11:45 H48

Geometric signature of complex synchronisation scenarios — Jan H. Feldhoff[1,2], •Reik V. Donner[1], Jonathan F. Donges[1,2], Norbert Marwan[1], and Jürgen Kurths[1,2] — [1]Potsdam Institute for Climate Impact Research, Germany — [2]Department of Physics, Humboldt University, Berlin, Germany

Synchronisation between coupled oscillatory systems is a common phenomenon in many natural as well as technical systems. Varying the strength of coupling often leads to qualitative changes in the complex dynamics of the mutually coupled systems including different types of synchronisation such as phase, lag, generalised, or even complete synchronisation. Here, we study the geometric signatures of coupling along with the onset of generalised synchronisation between two coupled chaotic oscillators by mapping the systems' individual as well as joint recurrences in phase space to a complex network. For a paradigmatic continuous-time model system, the transitivity properties of the resulting joint recurrence networks display distinct variations associated with changes in the structural similarity between different parts of the considered trajectories. They therefore provide a useful indicator for the emergence of generalised synchronisation.

DY 12.10 Tue 12:00 H48

Testing time series reversibility using complex network methods — Jonathan F. Donges[1,2], •Reik V. Donner[1], and Jürgen Kurths[1,2] — [1]Potsdam Institute for Climate Impact Research, Germany — [2]Department of Physics, Humboldt University, Berlin, Germany

The absence of time-reversal symmetry is a fundamental property of many nonlinear time series. Here, we propose a set of novel statistical tests for time series reversibility based on standard and horizontal visibility graphs. Specifically, we statistically compare the distributions of time-directed variants of the common graph-theoretical measures degree and local clustering coefficient. Unlike other tests for reversibility, our approach does not require constructing surrogate data and can

be applied to relatively short time series. We demonstrate its performance for realisations of paradigmatic model systems with known time-reversal properties as well as picking up signatures of nonlinearity in some well-studied real-world neuro-physiological time series.

DY 12.11 Tue 12:15 H48

Statistics, Predictability and Dynamics of Critical Transitions — •Xiaozhu Zhang[1], Christian Kühn[2], and Sarah Hallerberg[1] — [1]Network Dynamics Group, Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany — [2]Vienna University of Technology, Institute for Analysis and Scientific Computing, 1040 Vienna, Austria

Critical transitions in multistable systems have been discussed as models for a variety of phenomena ranging from the extinctions of species to socio-economic changes and climate transitions between ice-ages and warm-ages. From Bifurcation theory we can expect a critical transition to be announced by a decreased recovery from external perturbations. The consequences of this critical slowing down have been observed as an increase in variance and correlation before to the transition happens. However, it is not clear, whether these changes in observation variables are statistically relevant such that they could be used as predictors for critical transitions. In this contribution we investigate the predictability of critical transitions in the Van der Pol Oscillator under the influence of external noise. We focus especially on the statical analysis of the success of predictions and the overall predictability of the system.

DY 12.12 Tue 12:30 H48

A comparison of different measures of predictability — •Stefan Siegert and Holger Kantz — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We consider the event that the temperature anomaly in a certain location exceeds a fixed threshold. For this event probabilistic forecasts are issued one day into the future based on a) an auto-regressive model and b) a global circulation model (GCM) of atmospheric dynamics. The quality of these forecasts is then evaluated by comparison to the actual realizations of the exceedance events. It was observed previously that, under certain circumstances, the autoregressive forecast can outperform the GCM forecast. This was shown by analyzing the predictions using different measures of predictive skill, namely the Brier Skill Score (BSS) and the Area Under the Curve (AUC).

In this contribution, differences between these two predictability measures are illustrated, using the example of temperature anomalies. It is shown that the ranking of the two models depends crucially on the predictability measure used; one model can be better than the other in terms of BSS, but worse in terms of AUC, and vice versa. Causes and consequences of these differences are elaborated and discussed.

DY 13: Symposium: Strong Coupling in Solid State Quantum Systems (SYSC)

Time: Tuesday 9:30–12:00 Location: H1

Invited Talk DY 13.1 Tue 9:30 H1

Exploring the Physics of Superconducting Qubits Strongly Coupled to Microwave Frequency Photons — •Andreas Wallraff — ETH Zurich, Switzerland

Using modern micro and nano-fabrication techniques combined with superconducting materials we realize electronic circuits the properties of which are governed by the laws of quantum mechanics. In such circuits the strong interaction of photons with superconducting quantum two-level systems allows us to probe fundamental quantum properties of light and to develop components for applications in quantum information technology. Here, I will present experiments in which we have created and probed entanglement between stationary qubits and microwave photons freely propagating down a transmission line [1,2]. In these experiments we use superconducting parametric amplifiers realized in our lab [3] to detect both qubit and photon states efficiently. Using similar techniques we aim at demonstrating a deterministic scheme for teleportation of quantum states in a macroscopic system based on superconducting circuits.

[1] C. Eichler et al., Phys. Rev. A **86**, 032106 (2012)
[2] C. Eichler et al., Phys. Rev. Lett., in print (2012) [arXiv:1209.0441]
[3] C. Eichler et al., Phys. Rev. Lett. **107**, 113601 (2011)

Invited Talk DY 13.2 Tue 10:00 H1

Hybrid Quantum Circuit with a Superconducting Qubit Coupled to an Electron Spin Ensemble — •Yuimaru Kubo[1], Cecile Grezes[1], Igor Diniz[2], Jun-ichi Isoya[3], Vincent Jacques[4], Anais Dreau[4], Jean-François Roch[4], Alexia Auffeves[2], Denis Vion[1], Daniel Esteve[1], and Patrice Bertet[1] — [1]Quantronics Group, SPEC (CNRS URA 2464), CEA-Saclay, 91191 Gif-sur-Yvette, France — [2]Institut Néel, CNRS, BP 166, 38042 Grenoble, France — [3]Research Center for Knowledge Communities, University of Tsukuba, 305-8550 Tsukuba, Japan — [4]LPQM (CNRS, UMR 8537), Ecole Normale Supérieure de Cachan, 94235 Cachan, France

We report the experimental realization of a hybrid quantum circuit combining a superconducting qubit and an ensemble of electronic spins. The qubit, of the transmon type, is coherently coupled to the spin ensemble consisting of nitrogen-vacancy (NV) centers in a diamond crystal via a frequency-tunable superconducting resonator acting as a quantum bus [1,2]. Using this circuit, we prepare arbitrary superpositions of the qubit states that we store into collective excitations of the spin ensemble and retrieve back into the qubit[3]. We also report a new method for detecting the magnetic resonance of electronic spins at low temperature with a qubit using the hybrid quantum circuit [4], as well as our recent progress on spin echo experiments.

[1] Y. Kubo et al., Phys. Rev. Lett. **105**, 140502 (2010)
[2] Y. Kubo et al., Phys. Rev. A **85**, 012333 (2012)
[3] Y. Kubo et al., Phys. Rev. Lett. **107**, 220501 (2011)
[4] Y. Kubo et al., Phys. Rev. B **86**, 064514 (2012)

Invited Talk DY 13.3 Tue 10:30 H1

Hybrid Quantum Systems with Rare-Earth Ion Spin Ensemble — •Pavel Bushev — Physikalisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

Interfacing photonic and solid-state qubits within a hybrid quantum architecture offers a promising route towards large scale distributed quantum computing. Ideal candidates for such coherent interface are optically active spin ensembles coupled to a superconducting resonators. Laser crystals doped with rare-earth ions present an excellent material with active spins, transitions in optical frequency range and hyperfine structure. The magnetic anisotropy of these materials makes their application in hybrid quantum systems quite challenging.

I will present our study of Er:YSO crystal coupled to superconducting resonator. The comparions of erbium to other rare-earth ions will also be given.

Invited Talk DY 13.4 Tue 11:00 H1

Quantum Coherent Coupling between a Mechanical Oscillator and an Optical Mode — Ewold Verhagen, Dalziel Wilson, Vivishek Sudhir, Nicolas Piro, Albert Schliesser, and •Tobias Kippenberg — EPFL, Institute for Condensed Matter Physics, CH-1015, Switzerland

Cavity quantum optomechanics is a rapidly developing field which concerns the radiation pressure coupling of optical and mechanical degrees of freedom [1]. Using on-chip micro-cavities that combine both optical and mechanical degrees of freedom in one and the same device [2], radiation pressure back-action of photons is shown to lead to effective cooling [3] of the mechanical oscillator mode predicted by Braginsky [4]. In our research this is reached using cryogenic He-3 buffer gas precooling to ca. 700 mK in conjunction with laser cooling, allowing cooling of micro-mechanical oscillator to only 1.7 quanta, implying the oscillator resides more than 1/3 of its time in ground state. Moreover it is possible in this regime to observe quantum coherent coupling in which the mechanical and optical mode hybridize and the coupling rate exceeds the mechanical and optical decoherence rate [5]. This accomplishment enables a range of quantum optical experiments, including state transfer from light to mechanics using the phenomenon of optomechanically induced transparency [6].

[1] T. J. Kippenberg and K. J. Vahala, Science (2008)
[2] T. J. Kippenberg et al., Phys. Rev. Lett. (2005)
[3] V. B. Braginsky et al., Phys. Lett. A (2002)

[4] A. Schliesser et al., Nat. Phys. (2008)
[5] E. Verhagen et al., Nature (2012)
[6] S. Weis et al., Science (2010)

Invited Talk DY 13.5 Tue 11:30 H1

Exploring Quantum Light-Matter Interactions of Quantum Dots in Photonic Crystal Nanostructures — •Jonathan Finley[1], Arne Laucht[1,2], Michael Kaniber[1], Stefan Lichtmannecker[1], Thorsten Reichert[1], Guenther Reithmaier[1], Fabrice Laussy[1,3], and Ulrich Hoheneester[4] — [1]Walter Schottky Institut, Am Coulombwall 4a, 85748 Garching, Germany — [2]University of New South Wales, Sydney, Australia — [3]Facultad de Ciencias, C-V 509, Universidad Autónoma de Madrid C, Fco. Tomás y Valiente 7, 28049 Madrid, Spain — [4]Universität Graz, Austria

This talk will provide an overview of recent experimental and theoretical studies of electrically tunable few quantum dot (QD) photonic crystal nanostructures. Cavity-QED experiments performed in the strong coupling regime provide new information the temperature and excitation induced dephasing, allowing us to probe its influence on the emission spectrum [1-3]. Furthermore, we observe cavity mediated coherent coupling of two different quantum dots via a common optical mode [4], efficient guiding of single photons into the slow light modes of a linear waveguide [5] and demonstrate on-chip single photo detection using integrated superconducting single photon detectors [6].

[1] A. Laucht et al., New J. Phys. **11**, 023034 (2009)
[2] A. Laucht et al., Phys. Rev. Lett. **103**, 087405 (2009)
[3] A. Laucht et al. Phys. Rev. B **81**, 241302 (2010)
[4] A. Laucht et al., Phys. Rev. B **82**, 075305 (2010)
[5] A. Laucht et al., Phys. Rev. X **2**, 011014 (2012)
[6] G. Reithmaier et al., preprint (2012)

DY 14: Nonlinear Dynamics, Synchronization and Chaos II

Time: Tuesday 15:00–16:00 Location: H44

Invited Talk DY 14.1 Tue 15:00 H44

When the beat goes off — •Holger Hennig — Dept. of Physics, Harvard University, Cambridge, MA, USA

Although human musical performances represent one of the most valuable achievements of mankind, the best musicians perform imperfectly. Musical rhythms are not entirely accurate and thus inevitably deviate from the ideal beat pattern. Nevertheless, computer generated perfect beat patterns are frequently devalued by listeners due to a perceived lack of human touch. Professional audio editing software therefore offers a humanizing feature which artificially generates rhythmic fluctuations. However, the built-in humanizing units are essentially random number generators producing only simple uncorrelated fluctuations. In the first part of this talk, it will be shown that long-range fluctuations as an inevitable natural companion of both simple and complex human rhythmic performances [1]. Moreover, listeners strongly prefer long-range correlated fluctuations in musical rhythms [2]. Thus, the favorable fluctuation type for humanizing interbeat intervals coincides with the one generically inherent in human musical performances. In the second part of the talk I will present new developments and ongoing work in this field. Funding through DFG grant no. HE 6312/1-2 is acknowledged.

[1] HH, R. Fleischmann, A. Fredebohm, Y. Hagmayer, A. Witt, J. Nagler, F. Theis and T. Geisel, PLoS ONE, 6, e26457 (2011)
[2] HH, R. Fleischmann, and T. Geisel, Physics Today 65, 64-65 (2012)

Invited Talk DY 14.2 Tue 15:30 H44

Chimera states and the transition from spatial coherence to incoherence — •Philipp Hövel — Institut für Theoretische Physik, Technische Universität Berlin — Bernstein Center for Computational Neuroscience Berlin — Center for Complex Network Research, Northeastern University, Boston

Chimera states exhibit surprising dynamics in nonlocally coupled systems of identical oscillators. These hybrid states consist of both spatially coherent and synchronized as well as incoherent parts. Initially discovered for phase oscillators, they have been recently found in a large variety of different models and have also been realized in experiments [1]. In my presentation, I will give an overview of the wide spectrum of possible local dynamics and demonstrate that the habitat of chimeras ranges from time-discrete maps via chaotic models to neural oscillators [2]. Furthermore, I will address analytical results on the symmetry and stability of these peculiar states [3].

[1] A. M. Hagerstrom, T. E. Murphy, R. Roy, P. Hövel, I. Omelchenko, and E. Schöll. Nature Physics **8**, 658 (2012).
[2] I. Omelchenko, Yu. Maistrenko, P. Hövel, and E. Schöll, Phys. Rev. Lett. **106**, 234102 (2011).
[3] I. Omelchenko, B. Riemenschneider, P. Hövel, Yu. Maistrenko, and E. Schöll. Phys. Rev. E **85**, 026212 (2012).

DY 15: Evolutionary Game Theory (joint session BP/DY/SOE)

Time: Tuesday 15:00–16:00 Location: H37

DY 15.1 Tue 15:00 H37

How selection pressure changes the nature of social dilemmas in structured populations — •Flavio Pinheiro[1,2], Francisco Santos[1,3], and Jorge Pacheco[1,4] — [1]ATP-Group CMAF at Universidade de Lisboa, Lisbon, Portugal — [2]Centro de Física at Universidade do Minho, Braga, Portugal — [3]Departamento de Engenharia Informática & INESC-ID, IST-UTL, Lisboa Portugal — [4]Departamento de Matemática e Aplicações at Universidade do Minho, Braga, Portugal

When members of a population engage in dyadic interactions reflecting a prisoner's dilemma game, the evolutionary dynamics depends crucially on the population structure, described by means of graphs and networks. Here, we investigate how selection pressure contributes to change the fate of the population. We find that homogeneous networks, in which individuals share a similar number of neighbors, are very sensitive to selection pressure, whereas strongly heterogeneous networks are more resilient to natural selection, dictating an overall robust evolutionary dynamics of coordination. Between these extremes, a whole plethora of behaviors is predicted, showing how selection pressure can change the nature of dilemmas populations effectively face. We further show how the present results for homogeneous networks bridge the existing gap between analytic predictions obtained in the framework of the pair-approximation from very weak selection and simulation results obtained from strong selection.

DY 15.2 Tue 15:15 H37

How 'first carrot, then stick' incentives promote cooperation — •Tatsuya Sasaki[1,2], Xiaojie Chen[1], Åke Brännström[3,1], and Ulf Dieckmann[1] — [1]International Institute for Applied Systems Analysis, Laxenburg, Austria — [2]University of Vienna, Vienna, Austria — [3]University of Umeå, Umeå, Sweden

Social institutions often use rewards and penalties to promote cooperation. As providing such incentives tends to be costly, it is important to find efficient strategies for gauging positive and negative incentives as a situation demands. Most game-theoretical studies of cooperation have, however, modeled rewarding and punishing in isolation and by focusing on peer sanctioning, through which each player separately decides whether or not to sanction a co-player.

Here, we study how a sanctioning policy we call 'first carrot, then stick' affects the evolution of cooperation in public good games. Assuming the existence of institutions that can provide incentives on a limited budget, we examine an adaptive sanctioning policy that switches the incentive from rewarding to punishing when defectors decrease below a certain frequency. We find that in well-mixed popula-

tions this policy is more efficient in promoting and maintaining full cooperation than either rewards or penalties alone. We also demonstrate that this finding extends to spatially structured populations. Such an institutional hybrid incentive with adaptive feedback is a simple yet unifying solution for encouraging cooperative behaviors.

DY 15.3 Tue 15:30 H37

Learning, Evolution and Population Dynamics — Juergen Jost and •Wei Li — MPI for Math. in the Sci.

We study an iterated game, in which players from opposite populations are randomly paired, for the investigation of the interplay between individual optimization and population effects and for the comparison of different strategies and learning schemes. Players can rely on the information from previous encounters. A population adapts by selection, and/or the members of the population could learn individually, e.g., by reinforcement learning, or socially, via imitation.

The situation each player faces is changing, as coevolution exerts a high pressure on any learning strategy. Thus, the game between the populations is about quickly finding and converging to a favorable equilibrium. Within the population, the contest is about getting higher pay-offs.

The first aspect favors simple evolutionary schemes or learning strategies over more complex ones. The second aspect relates to the most effective use of the information from previous rounds or available within some social network inside the population.

We find an improved reinforcement learning that outperforms most evolutionary strategies, as well as the standard reinforcement learning with optimal parameters. The best imitating strategy here is payoff-biased. Imitating behavior can spread within a mixed population who can defeat a pure population with solely individual learners, independently of the precise learning scheme employed.

DY 15.4 Tue 15:45 H37

Banish or vanish? The evolution of cooperation by social exclusion — •Tatsuya Sasaki[1,2] and Satoshi Uchida[3] — [1]International Institute for Applied Systems Analysis, Laxenburg, Austria — [2]University of Vienna, Vienna, Austria — [3]Rinri Institute, Tokyo, Japan

Fines and exclusion are ubiquitous, yet very different ways of punishing freeriders. In the former, punishers are allowed to fine freeriders at a cost to themselves. It is clearly difficult for only fines to promote cooperation due to this punisher's cost. Less clear is the latter, in which punishers are allowed to exclude freeriders from the common good at a cost to themselves. When does exclusion solve the commons dilemma?

We investigate the replicator dynamics in standard public good games with costly exclusion. Costly exclusion reduces the group size, but not necessarily the group benefit, and thus, the punisher's net payoff may increase through excluding freeriders. We demonstrate how exclusion of freeriders can establish a coercion-based regime. Our results do not require a genetic relationship, repeated interaction, reputation, or group selection. Instead, only a limited number of freeriders are required to prevent the second-order freeriders from eroding the social immune system.

DY 16: Pattern Formation

Time: Wednesday 9:30–12:15 Location: H46

Invited Talk DY 16.1 Wed 9:30 H46

Dynamics of thin sheets: Crumpling, wrinkling and cracking — •Pascal Damman — Universite de Mons, Mons, Belgium

Thin elastic sheets are mechanically unstable to boundary or substrate-induced compressive loads. Moderate compression results in regular wrinkling while further confinement can lead to crumpling/folding or blistering. Close inspection of a simple candy wrap reveals that these patterns are universal and often coexist in the same object. These regions of stress focusing are often considered as a hindrance for technological applications, acting as nucleation points for mechanical failure. Conversely, they can be exploited constructively to build tailored 3D thin structures and to understand how the mechanical forces shape living systems, i.e., the morphogenesis.

This talk will be focused on the emergence of complex patterns for confined thin sheets. Two physical models will be described: the curtain model (i.e., a sheet confined at one edge) and the Euler buckling of a sheet resting on a soft foundation.

DY 16.2 Wed 10:00 H46

Patterned ground in permafrost: an experimental study — •Antoine Fourrière and Lucas Goehring — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Deutschland

Permafrost experiences annual freezing and thawing cycles. Differential frost heave results in the slow and natural emergence of periodic patterns at the surface of these soils. Due to the very long timescales involved, i.e. 1 to several thousand of years, field measurements can hardly provide the data needed to distinguish between the different theoretical ideas that could explain this pattern formation process. In particular, the physical mechanisms that link small-scale dynamics, such as cryosuction of water through a porous medium or the expansion of a frozen fringe, to meter-scale patterned ground are still an issue and have to be adressed. Here we present experimental work that mimics the initial stages of patterned ground formation in permafrost. We observe the evolution of surface topography for a granulate volume of $20 \times 20 \times 10\,\mathrm{cm}$ during several freeze-thaw cycles. The particle size distribution and the water fraction are varied. Surface modulation is observed for particular composition of the soil. The temperature evolution $T(z,t)$ inside the sample is modelled in the framework of the Stefan problem. By comparing the model results with the measured temperature profile, simple ideas like the evolution of the freezing front and the presence of a frozen fringe can be tested.

DY 16.3 Wed 10:15 H46

Selection theory of free crystal growth in convective systems — •Martin von Kurnatowski and Klaus Kassner — Otto-von-Guericke-University Magdeburg, Department of Theoretical Physics, Universitätsplatz 2, 39106 Magdeburg

The liquid-solid-interface of a crystal growing freely in its undercooled melt forms dendritic patterns. Understanding these patterns is crucial for controlling the material properties of solid substances such as metals. In the simplest models, the growth is governed by heat transport. Neglecting surface tension, one obtains a so-called Stefan problem having a parabolic solution. This zeroth-order problem does not lead to the selection of values for important system parameters that are experimentally fully determined. Capillary effects at the two-phase boundary constitute a singular perturbation selecting the length scale of the pattern.

Solution methods are usually based on the use of Green's functions [1]. However, with convection this method is normally not applicable due to the nonlinearity of the field equations. Density changes at the phase transition are a possible cause for convection. A potential flow and a Stokes flow are two simple approximations for the flow velocity field. This contribution focuses on the latter but more extended results have also been obtained. To approach the nonlinearities analytically, we use asymptotic decomposition as a powerful extension to the standard method. It yields an eigenvalue equation to be solved numerically.

[1] E. A. Brener and V. I. Melnikov, Adv. Phys. 40, p. 53-97 (1991)

DY 16.4 Wed 10:30 H46

Crystal Growth in a Channel: From Merry-Go-Round Fingers to Seesaw Dynamics — •Klaus Kassner[1], Jean-Marc Debierre[2], and Rahma Guerin[2] — [1]Otto-von-Guericke-Universität, Magdeburg — [2]Institut Matériaux Microélectronique Nanosciences de Provence, Marseille

We study three-dimensional solidification in capillaries of various cross sections (triangular, square, hexagonal, circular) by numerical simulation, using Karma's phase-field model. Besides symmetric and asymmetric steady states expected from acquaintance with the 2D case, we find a number of hitherto unknown dynamical states, some of which were quite unexpected. In particular, there is chiral symmetry breaking leading to rotation of a growing nanocrystal in a hexagonal or circular channel. This seems to be the simplest system so far in which spontaneous breaking of chiral symmetry has been observed. A general characterization of oscillatory states (including movies) and bifurcation

diagrams in terms of the undercooling and system size will be given. Some chaotic states have also been observed.

15 min. break

DY 16.5 Wed 11:00 H46

Orientational selection in pattern formation — •Vanessa Weith, Alexei Krekhov, and Walter Zimmermann — Universität Bayreuth, Theoretische Physik I, 95440 Bayreuth, Germany

Spatially periodic patterns in two-dimensional isotropic systems are on large length scales orientationally disordered. Examples are lamellae in diblock copolymers with the lamellae perpendicular to substrates or stripe patterns occurring in experiments on gas convection in large aspect ratio systems.

The orientational selection of the wave vector **q** of lamellae in diblock copolymers or stripe patterns in model systems can be induced by appropriate surface preparations of confining substrates. In addition we show, that the orientation of **q** of lamellae and stripe patterns can be controlled by traveling, spatially periodic modulations of the control parameter. Assuming a parallel orientation of the wave vector **k** and the velocity **v** of the modulation, we find in the case of a small velocity that the wave vector of patterns, **q**, orients perpendicular to **v** and parallel to **v** in the case of larges values of $|\mathbf{v}|$.

DY 16.6 Wed 11:15 H46

Pattern formation in Cahn-Hilliard models for Langmuir-Blodgett transfer — •Markus Wilczek, Svetlana V. Gurevich, and Rudolf Friedrich — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Deutschland

Langmuir-Blodgett transfer is an established method for covering substrates with monolayer films. During the transfer, partial condensation of the monolayer can lead to the formation of patterns in different phases of the transferred monolayer. Experimental parameters like the transfer velocity influence the properties of the patterns, like the orientation and wavelength of stripes.

In this work, we investigate the pattern formation process in the framework of spinodal decomposition by means of Cahn-Hilliard models. Besides the transfer onto homogeneous substrates, the influence of prestructured substrates is studied. In particular, the occurrence of synchronization phenomena is described.

In addition, the transition between different orientations of stripe patterns is investigated, revealing the occurrence of secondary instabilities leading to certain patterns.

DY 16.7 Wed 11:30 H46

Looking beneath the surface: A study of desiccation cracks over patterned substrates — •Pawan nandakishore and Lucas Goehring — Max Planck Insititute for Dynamics and Self Organization, Goettingen, Germany

From cracks on planetary surfaces to cracks in dried paint, to cracks in microscopic thin films, contraction cracks occur at many length scales and, following linear elasticity theory these patterns should scale across these length scales. We investigate the crack patterns formed due to the presence of sinusoidal substrates and substrates with a single peak or trough. To this effect, we look at desiccated mud cracks by drying a bentonite slurry over the different substrates. The relevant parameters in this problem are the layer height, wavelength and amplitude of the substrate. We characterize the topology of the pattern, and show that an order parameter, characterized by the orientation of the cracks, behaves non monotonically. At low layer heights the crack pattern is disordered and contains wavy cracks. As the layer height is increased, a highly anisotropic crack pattern is formed when the wavelength matches the natural crack spacing of the film, or close to the layer thickness. This pattern is characterized by cracks that run parallel and perpendicular to the substrate. When the layer height is further increased the pattern becomes disordered however there are no wavy cracks present. Combining these observations from the sinusoidal substrates and the observations from the single peaks and troughs we attempt to acquire a means to decipher what lies beneath the crack pattern.

DY 16.8 Wed 11:45 H46

Revisiting the Scaling Analysis of Irreversible Aggregation Dynamics — •Jürgen Vollmer — Max Planck Insitute for Dynamics and Self-Organization, 37077 Göttingen, Germany

The analysis of the size distribution of droplets condensing on a substrate is a test ground for scaling theories. Surprisingly, a faithful description of its evolution must explicitly address microscopic nucleation and growth mechanisms of the droplets [1]. In view of this we discuss how this breaking of universality relates to other systems with vastly polydisperse droplet size distributions, like the growth of droplets in clouds.

[1] J Blaschke, T Lapp, B Hof, and J Vollmer, PRL 109, 068701 (2012).

DY 16.9 Wed 12:00 H46

Origin of Complexity in Cellular Automata — •Vladimir Garcia-Morales — Technische Universität München - Institute for Advanced Study, Lichtenbergstr. 2a, D-85748 Garching, Germany

Cellular automata (CA) constitute paradigmatic models of complexity in nature, from snowflakes, patterns in mollusc seashells and spiral waves in the Belousov- Zhabotinsky reaction to neural networks and the fundamental physical reality. A universal map encompassing all 1D deterministic first-order in time CA has been very recently derived [1]. This map is to be considered as the discrete counterpart of partial differential equations in continuum systems. The map does not depend on freely adjustable parameters and is valid for any neighborhood and alphabet size. It can be easily extended to an arbitrary number of dimensions and topologies and higher orders in time. Symmetry arguments applied to the map allow to classify all dynamical CA rules into equivalence classes and a theorem can be proved which establishes how a CA rule is constructed in terms of rules of lower range [2]. The crucial result is that the most complex CA rules can be found with a simple prescription, starting from rules possessing the symmetry upon addition modulo an integer number p, and weakly breaking this symmetry through an additional degree of freedom. It is illustrated how this mechanism is the origin of complexity in 1D CA.

[1] V. Garcia-Morales, Phys. Lett. A 376 (2012) 2645.
[2] V. Garcia-Morales, Phys. Lett. A (2012, in press), http://dx.doi.org/10.1016/j.physleta.2012.11.052

DY 17: Soft matter

Time: Wednesday 10:00–12:00 Location: H47

DY 17.1 Wed 10:00 H47

Particle tracking in drying colloidal films — Jan S. Vesaratchanon and •Lucas Goehring — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Colloidal dispersions, such as paints, coatings, inks, drops of wine or coffee, usually dry into either a uniformly flat surface or a dispersed phase that is deposited mostly at the edges forming a ring. This ring formation can be similarly observed elsewhere in the so called "coffee-ring effect". However, the conditions which select for these two extreme cases, or an intermediate deposit, are not known. Furthermore, understanding the basic transport and flow properties during the drying process can be useful in many industrial applications. We use a particle tracking microscopy technique in order to investigate the motion of particles during drying. By adding fluorescent particles as tracers into drying colloids of relatively similar particle size, we are able to extract the trajectories of individual fluorescent particles along with their coordinates and time. Our experimental setup allows us to measure drift velocity of individual particles approaching a solidification front, along with drying front velocity (i.e., how fast colloids dry), particle density and self-diffusion parameters. Variation of particle size and drying rate during experiments allows us to understand the scaling of key parameters relevant to the drying of colloidal films.

DY 17.2 Wed 10:15 H47

Model System for the Random Organization and Jamming Transition — •Lars Milz[1,2] and Michael Schmiedeberg[2] — [1]Universität Regensburg, 93053 Regensburg, Germany — [2]Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40204 Düsseldorf, Germany

Random organization is a non-equilibrium phase transition between a steady state and an absorbing state. This transition was observed in a system with periodically sheared non-Brownian particles where at low densities or low shear amplitudes the particle organize such that collisions are avoided while at large densities or large shear amplitudes collisions still occur [1,2]. We consider a simplified model system without shear where in each step particles are displaced if they overlap. For displacements in random directions we observe the random organization transition and explain how the shear amplitude and density in [1,2] can be mapped onto the packing fraction, which is our only control parameter. Interestingly, for deterministic displacements we find crystallization in 2D and the jamming transition in 3D. Therefore, our model system provides a simple method to study the random organization transition and a link between this non-equilibrium transition and the jamming transition.

[1] D.J. Pine et al., Nature 438, 997(2005).
[2] L. Corté et al., Nature Physics 4, 420 (2008).

DY 17.3 Wed 10:30 H47

A phase field model for platelet-polymer nanocomposit melts — •Thomas Gruhn and Heike Emmerich — MPS, Universität Bayreuth

Nanocomposites of clay nanoplatelets in a polymer matrix combine a high mechanical strength with a low gas permeability so that they can be used, for example, as high quality fire protection materials. The orientational and spatial distributions of the platelets are very important for the materials properties and depend sensitively on the production process. We have developed a novel simulation method for studying the alignment and the density distribution of platelets in the polymer melt. The method combines phase field and liquid crystal theory and allows us to study the dynamics of a system with coexisting domains of high and low platelet concentrations as well as isotropic-nematic phase transitions. The model is used to investigate spinodal decomposition of platelets in the melt. We obtain a new type of spinodal decomposition patterns with an anisotropic structure factor. Results are studied as a function of the platelet concentration.

DY 17.4 Wed 10:45 H47

Density functional theory for hard polyhedra — •Matthieu Marechal[1] and Hartmut Löwen[2] — [1]Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Heinrich Heine Universität Düsseldorf, Düsseldorf, Germany

The ready availability of polyhedral nanoparticles and colloids as a result of recent advances in synthesis methods have allowed experimental observations of crystals of polyhedra. While this realization of polyhedra spurred simulation work on the structure of hard particles, theoretical approaches, so far, have been limited. Using the framework of geometry-based fundamental-measure theory, we develop a classical density functional (DFT) for hard polyhedra and their mixtures. We apply the DFT to Platonic solids (tetrahedra, cubes, octahedra, dodecahedra and icosahedra) and perform Monte Carlo simulations.

Knowledge of the structure of colloids or nanoparticles near a wall is important for understanding heterogeneous nucleation. Furthermore, the density profile near a hard wall provides a standard test case for DFT by comparing with simulation results. The faceted shape of the polyhedra leads to complex layering and orientational ordering near the wall already for a one-component system which is excellently reproduced by our theory. We also considered a 2:1 mixture of tetrahedra and octahedra, which is interesting because it can form a close packed crystal with unit packing fraction. Surprisingly, the local structure in the fluid near the wall for this binary mixture is not similar to the best-packed structure. These effects can be verified in real-space experiments on polyhedral colloids.

DY 17.5 Wed 11:00 H47

Glassy dynamics of Brownian particles close to walls — •Matthias Kohl — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany

By using Brownian dynamics simulations, we study the slowdown of the dynamics of spherical particles at small temperatures or high densities. In our model system, the particles interact via finite-ranged repulsive interactions. In the limit of small overlaps the dynamics of the soft spheres corresponds to the overdamped dynamics of hard spheres. We determine the relaxation time as a function of temperature and pressure. The dynamics in the vicinity of a wall is compared to the dynamics in bulk.

DY 17.6 Wed 11:15 H47

Structure and Dynamics of Suspensions of Colloidal Dumbbells — •Nils Heptner[1,2], Fangfang Chu[1,2], Miriam Siebenbürger[1], Matthias Ballauff[1,2], and Joachim Dzubiella[1,2] — [1]Helmholtz-Zentrum Berlin — [2]Humboldt-Universität zu Berlin, Germany

We investigate the static and dynamic equilibrium structures of a suspensions of colloidal dumbbells by means of Brownian dynamics (BD) computer simulations and linear response theory. These suspension exhibit an elaborate equilibrium phase diagram[1,2]. The particular focus is the study of bulk translational and orientational structure and near-equilibrium transport coefficients at different colloid packing fractions and anisotropy parameters for a better understanding of material properties in and out-of equilibrium.

Crystal structures in the plastic crystal (PC) phase are identified and the PC-liquid transition is investigated. We present structural properties in form of static and dynamic structure factors $S(q, w)$ and pair distribution functions $g(r)$. Furthermore we calculate frequency-dependent rotational and translational self-diffusion constants as well as shear viscosities from equilibrium autocorrelation functions. In addition we will present preliminary results of non-equilibrium simulations imposing oscillatory and steady simple shear flow. All results are compared to the hard sphere reference system as well as available experimental scattering and rheology data.

(1) Vega, C. et al. J Chem Phys 1992, 96, 9060-9072.
(2) Marechal, M.; Dijkstra, M Phys Rev E 2008, 77, 061405.

DY 17.7 Wed 11:30 H47

Polymer statistics in an attractive sphere — Handan Arkin[1,2] and •Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Germany — [2]Department of Physics Engineering, Faculty of Engineering, Ankara University, Turkey

We analyze the structural behavior of a single polymer chain inside an attractive sphere. Our model is composed of a coarse-grained polymer governed by 12-6 Lennard-Jones interactions of the monomers and an attractive sphere potential which follows by integrating the monomer-monomer interaction over the (inner) surface of the sphere. By means of extensive multicanonical Monte Carlo simulations it is shown that the system exhibits a rich phase diagram in the adsorption strength-temperature ($\epsilon - T$) plane ranging from highly ordered, compact to extended, random coil structures and from desorbed to partially or even completely adsorbed conformations. These findings are identified with different energetic and structural observables including invariant shape parameters such as the asphericity that characterizes the average conformation of the polymer. The resulting phase diagram in the $\epsilon - T$ plane is compared with that for a polymer adsorbing to a plane, attractive substrate obtained previously by Möddel, Bachmann, and one of the authors.

H. Arkın and W. Janke, Phys. Rev. E **85**, 051802 (2012); J. Phys. Chem. B **116**, 10379 (2012); Eur. Phys. J. – Special Topics (in print).

DY 17.8 Wed 11:45 H47

Quantifying shape in heterogeneous media by Minkowski-Tensors — •Michael A. Klatt, Gerd E. Schröder-Turk, and Klaus Mecke — Institut für Theoretische Physik, Universität Erlangen

We describe a novel approach to morphology and anisotropy analysis of complex spatial structure using so-called mixed volumes and Minkowski tensors, which are generalizations of the well-known scalar Minkowski functionals. The tensors are explicitly sensitive to anisotropic aspects of the structure and are relevant for example for elastic moduli or permeabilities of porous materials [1]. A theorem by Alesker (1999) ensures robustness and completeness of a morphological analysis based on Minkowski tensors.

To illustrate the technique we analyze analytically and numerically the spatial structure of the Boolean model of overlapping grains, which is among the most important models for porous and heterogeneous media, leading to good predictions of mechanical and transport properties, e.g., of rock [2]. The morphology of the Boolean model is usually quantified by the mean intercept length for which an analytic expression is presented. However, the commonly used MIL tensor is not well-defined.

An important geometric feature of heterogeneous media is percolation. An accurate estimation of the percolation threshold in Boolean models can be given in terms of mixed volumes and Minkowski tensors.

[1] G. Schröder-Turk et al., Adv. Mater. **23** 2535-2553 (2011).
[2] C. H. Arns et al., Phys. Rev. Lett. **91** 215506 (2003).

DY 18: Statistical Physics Far from Thermal Equilibrium

Time: Wednesday 9:30–12:30 Location: H48

DY 18.1 Wed 9:30 H48

Hardwiring a Maxwell Demon — •Philipp Strasberg[1], Gernot Schaller[1], Tobias Brandes[1], and Massimiliano Esposito[2] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany — [2]Complex Systems and Statistical Mechanics, University of Luxembourg, L-1511 Luxembourg, Luxembourg

We present a physical implementation of a Maxwell demon which consists of a conventional single electron transistor (SET) capacitively coupled to another quantum dot detecting its state. Altogether, the system is described by stochastic thermodynamics. We identify the regime where the energetics of the SET is not affected by the detection, and where its coarse-grained entropy production is shown to contain a new contribution compared to an isolated SET. This additional contribution can be identified as the information flow generated by the "Maxwell demon" feedback in an idealized limit.

DY 18.2 Wed 9:45 H48

Quantum efficiency of heat engines coupled to nonequilibrium reservoirs — •Obinna Abah[1,2] and Eric Lutz[1,2] — [1]Department of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Dahlem Center for Complex Quantum Systems, Freie Universit\"at Berlin, Arnimallee 14, D-14195 Berlin, Germany

We derive the efficiency of quantum heat engines coupled to stationary nonequilibrium reservoirs. We discuss the condition under which the quantum efficiency exceeds its classical limit.

DY 18.3 Wed 10:00 H48

Accumulation and replication of biomolecules driven by the flux of heat — •Moritz Kreysing, Christof Mast, Simon Lanzmich, Lorenz Keil, and Dieter Braun — Systems Biophysics, Department of Physics, LMU München

Central to most Origin-of-Life scenarios is the possibility for pre-biotic organic molecules to form increasingly complex, catalytic machinery, ultimately capable of autonomous replication. While strong evidence for the spontaneous generation of single nucleotides [1] recently arose, concentrations required to allow these building blocks to polymerize [2] to gain functionality still seem improbable for early earth conditions.

Here we demonstrate experimentally that temperature gradients across vertical pores, as they occur in submarine hydrothermal vents [3], are sufficient to accumulate oligonucleotides against high entropic costs. In particular we show that, depending on the pores' dimensions, this thermo-gravitation trapping is strongest for long oligonucleotides and thus provides a length selective molecular filter.

We suggest that equivalent systems could have served as meeting point for long and complex molecules, too rare to find each other in a dilute primordial ocean. Furthermore, we discuss under which conditions length sensitivity could trigger the evolutionary selection of molecular replicators driven by convective thermo-cycling [4].

References: 1. M. Powner et al., Nature 459:239 (2009), 2. G. Costanzo et al., ChemBioChem 13:999 (2012), 3. P. Baaske et al., PNAS 104:9346 (2007), 4. C. Mast and D. Braun, PRL, 104:188102 (2010).

DY 18.4 Wed 10:15 H48

Dynamics of wet granular matter — •Marco Mazza — Max Planck Institute for Dynamics and Self-Organization, Dynamics of Complex Fluids - Bunsen Str. 10, Göttingen, Germany

We present results from computer simulations of the dynamics of wet granular matter. The system exhibits far-from-equilibrium transitions from solid- to fluid-like phase. Differences and analogies to the equilibrium transitions and possible extensions of the equilibrium formalism are discussed.

DY 18.5 Wed 10:30 H48

Random perfect lattices and the sphere packing problem — •Alexei Andreanov[1,2] and Antonello Scardicchio[1,3] — [1]The Abdus Salam ICTP, Trieste, Italy — [2]Max-Planck-Institut fur Physik complexer Systeme, Dresden, Germany — [3]INFN, Sezione di Trieste, Trieste, Italy

We study random sets of perfect lattices in dimensions up to $d = 19$. Perfect lattices are relevant for solution of lattice sphere packing problem. In fact the best lattice packing is a perfect lattice and perfect and eutactic lattices are local maxima of the packing fraction. We use a stochastic generating algorithm for perfect lattices and define a random ensemble with an effective temperature (reminiscent of a Monte Carlo simulation) to study typical properties of perfect lattices and show how as the temperature is decreased the best known packers are easily recovered. We find that the typical perfect lattices are denser than known families and propose two hypotheses for typical packing density between which we cannot distinguish: $\phi \sim 2^{-(0.84\pm0.06)d}$ (improvement of the Minkowksi bound), and a competitor $\phi \sim d^{-ad}$ with a very small coefficient $a = 0.06 \pm 0.04$. We also find properties of the random walk which are suggestive of a glassy system already for moderately small dimensions.

15 min. break.

DY 18.6 Wed 11:00 H48

Globally Coupled Stratonovich Models: Self-consistent Theory of a Non-equilibrium Continuous Phase Transition — •Marc Höll[1] and Ulrich Behn[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Institut für Theoretische Physik, Universität Leipzig, Brüderstr. 16, 04103 Leipzig, Germany

We consider a globally harmonically coupled array of N Stratonovich models. The system exhibits a second order non-equilibrium phase transition when crossing a critical value of the control parameter. For strong coupling it is useful to introduce center of mass and relative coordinates since their chararacteristic time scales are clearly separated. We develop a self consistent approximate theory to determine the stationary probability distributions of these coordinates. For infinite coupling strength the relative coordinates relax very fast to zero and the stationary probability distribution is a δ-function, whereas for finite strength it has a nonzero variance which is determined self-consistently. The results for finite systems with strong but finite coupling are compared with data from simulations and a good agreement is observed.

DY 18.7 Wed 11:15 H48

Crooks' Fluctuation Theorem for a Process on a 2D Fluid Field — •Julia Gundermann[1], Jochen Bröcker[2], and Holger Kantz[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Department of Meteorology, University of Reading, UK

We investigate the behavior of two-dimensional inviscid and incompressible flow when pushed out of dynamical equilibrium. We use the 2D vorticity equation with spectral truncation on a rectangular domain. For sufficiently large number of degrees of freedom, the equilibrium statistics of the flow can be described through a canonical ensemble approach with two conserved quantities, energy and enstrophy. To perturb the system out of equilibrium, we change the shape of the domain according to a protocol, which changes the kinetic energy but leaves the enstrophy constant. We interpret this as doing work to the system. Evolving along a forward and its corresponding backward process, we show that the statistics of the work performed satisfies Crooks' relation $P_f(W)/P_b(-W) = e^{\beta(W-\Delta F)}$. The parameters ΔF and β are given by the formal analogy with the canonical ensemble as the free energy difference and, respectively, the inverse temperature $1/k_BT$.

DY 18.8 Wed 11:30 H48

Vortex arrays as emergent collective phenomena for circle swimmers — •Andreas Kaiser and Hartmut Löwen — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany

Collective properties of many rod-like circle swimmers are explored by computer simulations in two spatial dimensions. In the model considered, the center of mass of a single swimmer moves on a circle with radius R. Therefore the model provides an interpolation between an interacting self-propelled-rod model for linear swimmers ($R \to \infty$) [1] and that of interacting passive rotors ($R = 0$) [2]. We map out the state diagram for various swimmer densities and radii R. We charac-

terize vortices of single swimmers and vortices of swimmer pairs using structural and dynamical diagnostics. Furthermore, a simple theory is proposed to predict the topology of the state diagram.

[1] H. H. Wensink and H. Löwen, J. Phys.: Condens. Matter **24**, 464130 (2012).

[2] R. Kirchhoff and H. Löwen, EPL **69**, 291 (2005).

DY 18.9 Wed 11:45 H48

Globally Coupled Nonlinear Systems with Additive Noise — •Rüdiger Kürsten[1,2], Susanne Gütter[1], and Ulrich Behn[1] — [1]Institut für Theoretische Physik, Brüderstr. 16, 04103 Leipzig — [2]Max-Planck-Institut für Mathematik in den Naturwissenschaften, Inselstr. 22, 04103 Leipzig

We consider the overdamped motion of N harmonically coupled particles in a double well potential under the influence of additive Gaussian white noise. System parameters are noise strength, coupling strength and potential barrier height. In the limit $N \to \infty$ the system exhibits a continous phase transition from a symmetric to a non-symmetric state.

Given any two parameters, positive, there exists a unique critical value for the third parameter, separating the symmetric from the non-symmetric parameter regime.

An inequality for the parameters holding for any critical point is shown and the critical potential barrier is asymptotically calculated. The critical potential barrier reaches the bounds of the inequality for strong coupling or weak noise and for weak coupling or strong noise.

The critical exponents for the order parameter and the susceptibility are computed and universality of the amplitude ratio of the susceptibilities is shown.

Invited Talk DY 18.10 Wed 12:00 H48

The physics of information: from Maxwell's demon to Landauer — •Eric Lutz — Freie Universität Berlin

We discuss the intimate connection existing between information theory and thermodynamics. We focus on two complementary aspects: 1) the gain of information with Maxwell's famous demon and 2) the erasure of information with Landauer's principle. We further present recent experiments that have for the first time demonstrated the equivalence between information and thermodynamics.

DY 19: Focus Session: Dynamics of Adaptive Networks (joint session BP/DY/SOE)

Adaptive Networks attracted recent interest through their dynamical properties that emerge from the interaction of two classes of processes (which may include stochasticity): (i) Growth and restructuring of the network topology itself, and (ii) Coupled dynamical systems defined on the network nodes. In this session, an introduction and overview into adaptive networks and their analytical and numerical investigation is complemented by their recent application to socio-economic, biological and epidemologic systems. (Session compiled by Eckehard Schöll, TU Berlin and Jens Christian Claussen, U Lübeck.)

Time: Wednesday 9:30–12:30 Location: H37

Topical Talk DY 19.1 Wed 9:30 H37

Adaptive Networks: Of social interactions and mathematical tools — •Anne-Ly Do — Max-Planck-Institut für Physik komplexer Systeme, Dresden

Adaptive networks are characterized by the co-evolution of local and topological degrees of freedom. Prime examples are networks of social interactions: Individuals are altered and shaped through interaction with others. On the other hand, they can often decide with whom to interact. Adaptive network models of social systems have attracted keen interest as they promise to provide the key to a number of prominently discussed phenomena such as fragmentation of groups into like-minded subgroups, evolution or break-down of social structures promoting cooperation, and emergence of fairness and leadership. In this talk, I review recent studies that link emergent phenomena in social systems to adaptive feedback in the respective interaction nets. Moreover, I discuss the analytical techniques used, thus aiming to outline both, findings and tools.

DY 19.2 Wed 10:00 H37

Controlling cluster synchronization by adaptive network topology — •Judith Lehnert[1], Anton Selivanov[2], Alexander Fradkov[2,3], and Eckehard Schöll[1] — [1]Institut für Theoretische Physik,TU-Berlin, Hardenbergstr 36, 10623 Berlin, Germany, — [2]SPb State University, Universitetskii pr.28, St.Petersburg, 198504 Russia — [3]Institute for Problems of Mechanical Engineering, Russian Academy of Sciences, Bolshoy Ave, 61, V. O., St. Petersburg, 199178 Russia

Adaptive networks are characterized by a complicated interplay between the dynamics on the nodes and a changing topology: The topology evolves according to the state of the system, while at the same time the dynamics on the network and thus its state is influenced by that topology. Here, we present an algorithm for a changing topology that allows us to control the dynamics on the network. In particular, we control zero-lag and cluster synchronization in delay-coupled networks of Stuart-Landau oscillators. Our method is robust towards different initial conditions. Furthermore, it is not necessary to adapt the network as a whole but it is sufficient to apply the method to a subset of the links to control the dynamics of all nodes. Finally, we discuss the topological characteristics of the network after successful control.

DY 19.3 Wed 10:15 H37

Resilience of collective dynamics in fluctuating network environments — •Alexander Grimm — ETH Zürich, Chair of Systems Design, Switzerland

Do totalitarian networks perform better than democratic networks? What is the most appropriate hierarchy level for networks embedded in volatile environments? We use agent-based models to discover the effect of hierarchy on performance in networks located in highly fluctuating environments. We investigate the emergence of collective dynamics of many units embedded in complex network environments which change boundary conditions constantly. The agents have to adopt their behavior due to these constantly changing conditions. Although the individual node properties do not change, the network shows permanently changing structure with enormously differing properties. The fluctuating environments come into force via three different dynamics which happen on different time scales in adiabatic approximations. We show that a synchronization process is a good approach to model information transfer. The information transfer in the model interlinks the three dynamics. First, the link formation process is the most fundamental process. It is driven by centrality. Second, the a synchronization process describes the information transfer among the nodes. And third, an endogenized node churn removes those nodes which deviate from the networks' common culture. In differing hierarchy values we find a phase transition in centrality. Hysteresis effects and trade-off properties make it possible to determine the most appropriate topology of the network, given its operation area.

DY 19.4 Wed 10:30 H37

Absence of epidemic thresholds in a growing adaptive network — •Güven Demirel[1] and Thilo Gross[2] — [1]Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany — [2]University of Bristol, Bristol, United Kingdom

In epidemics on network, a central role is played by the degree distribution, i.e. the distribution of the number of neighbors of nodes. In particular in scale-free networks, where the variance of the degree distribution diverges, no epidemic thresholds exist, such that even diseases with arbitrary low infectiousness can percolate. By contrast, in networks where the variance of the degree distribution is finite, diseases generally need to surpass a threshold infectiousness to persist. In the real world the degree distribution is not independent of epidemics, but is shaped through disease induced behavioral changes and mortality in a complex interplay. Here, we consider the growth of a network from which nodes are simultaneously removed due to disease-induced mortality. We show analytically and numerically that in this system

no epidemic thresholds exists, although the interplay between network growth and epidemic spreading leads to networks in which the degree distribution has a finite variance.

DY 19.5 Wed 10:45 H37

Hierarchical transport structures in the network of *Physarum polycephalum* — •Werner Baumgarten and Marcus J. B. Hauser — Abteilung Biophysik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

The plasmodium of the slime mould *Physarum polycephalum* consists of a single multinucleate giant amoeboid cell that forms a characteristic two-dimensional vein network. Through the entire tubular network protoplasm is transported periodically back and fro. During evolution this transportation network is optimized for efficiency [1].

The vein network of *P. polycephalum* is considered a weighted undirected graph, with veins as edges and branching points as nodes, the weight is given by the local drag of each vein [2]. A graph analysis is performed on the network of *P. polycephalum* based on the conjecture of laminar flow in the veins. Experiments to quantify the structure were carried out on multiple scales. We demonstrate that the network posses a self-similar hierarchic structure which consists of nested loops of veins of decreasing transport efficiency. These results are used to describe the network evolution.

[1] A. Tero, S. Takagi, T. Saigusa, K. Ito, D. P. Bebber, M. Fricker, K. Yumiki, R. Kobayashi, T. Nakagaki, 2010, Science, 327, 439

[2] W.Baumgarten, T. Ueda, M.J.B. Hauser, Phys. Rev. E 2010, 82, 046113

DY 19.6 Wed 11:00 H37

Natural emergence of clusters and bursts in network evolution — •James Bagrow and Dirk Brockmann — Northwestern University

Network models with preferential attachment, where new nodes are injected into the network and form links with existing nodes proportional to their current connectivity, have been well studied for some time. Extensions have been introduced where nodes attach proportional to arbitrary fitness functions. However, in these models attaching to a node increases the ability of that node to gain more links in the future. We study network growth where nodes attach proportional to the clustering coefficients, or local densities of triangles, of existing nodes. Attaching to a node typically lowers its clustering coefficient, in contrast to preferential attachment or rich-get-richer models. This simple modification naturally leads to a variety of rich phenomena, including aging, non-poissonian bursty dynamics, and community formation. This shows that complex network structure can be modeled without artificially imposing multiple dynamical mechanisms.

DY 19.7 Wed 11:15 H37

Evolution of Cooperation on Stochastic Dynamical Networks — •Bin Wu and Arne Traulsen — Research Group for Evolutionary Theory, Max-Planck-Institute for Evolutionary Biology, Plön, Germany

Cooperative behavior that increases the fitness of others at a cost to oneself can be promoted by natural selection only in the presence of an additional mechanism. One such mechanism is based on population structure, which can lead to clustering of cooperating agents. Recently, the focus has turned to complex dynamical population structures such as social networks, where the nodes represent individuals and links represent social relationships. We investigate how the dynamics of a social network can change the level of cooperation in the network. Individuals either update their strategies by imitating their partners or adjust their social ties. For the dynamics of the network structure, a random link is selected and breaks with a probability determined by the adjacent individuals. Once it is broken, a new one is established. This linking dynamics can be conveniently characterized by a Markov chain in the configuration space of an ever-changing network of interacting agents. Our model can be analytically solved provided the dynamics of links proceeds much faster than the dynamics of strategies. This leads to a simple rule for the evolution of cooperation: The more fragile links between cooperating players and non-cooperating players are (or the more robust links between cooperators are), the more likely cooperation prevails. Our approach may pave the way for analytically investigating coevolution of strategy and structure.

Topical Talk DY 19.8 Wed 11:30 H37

Bio-molecular Networks: Structure, Function, Evolution — •Michael Lässig — Institut für theoretische Physik, Universität zu Köln

In biological systems, networks exist at multiple levels. One is structure: components of a system are linked because they are close in space. An example is the adjacency of amino acids in a protein. Another level is function: components are linked because they do something together, such as the genes in a regulatory or metabolic network. In this talk, I discuss how structure and function networks shape the evolutionary dynamics of organisms and species - and conversely, how evolutionary observations can uncover underlying functional networks. I use two examples: the evolutionary properties of gene regulatory networks and the evolution of the human influenza virus.

Topical Talk DY 19.9 Wed 12:00 H37

Adaptive networks and critical dynamics — •Stefan Bornholdt — Institut für Theoretische Physik, Universität Bremen

Dynamical networks have been studied from the perspective of statistical physics, motivated by questions of information processing in neural networks and genetic networks. In both applications, hypotheses have been discussed that relate optimality of information processing to dynamical criticality in the networks. Consequently, toy models for adaptive networks have been constructed that robustly establish criticality in the network. Here I review a particularly simple model class based on models from physics and discuss its application to the phenomenon of criticality in biological neural networks.

[1] M. Rybarsch and S. Bornholdt, Self-organized criticality in neural network models, in: "Criticality in Neural Systems", Niebur E, Plenz D, Schuster HG (eds.) 2013 (in press); arXiv:1212.3106.

[2] M. Rybarsch and S. Bornholdt, Binary threshold networks as a natural null model for biological networks, Phys. Rev. E 86 (2012) 026114.

[3] M. Rybarsch and S. Bornholdt, Self-organization to criticality in neural networks: A minimal model with binary threshold nodes, arXiv:1206.0166.

DY 20: Focus Session: Modern Power Grid, Nonlinear Dynamics and Self-Organization (joint with SOE)

The drastic change from our traditional energy system based on fossil fuels to one based dominantly on renewable sources provides an extraordinary challenge for the robust operation of future power grids. Complementing standard approaches of electric engineering with principles of self-organization and methods from nonlinear dynamics may help us to understand collective dynamical grid features, emerging due to increasing decentralization, line upgrades, and correlated fluctuations. The Focus Session provides a snapshot of current research in this emerging cross-disciplinary field and points to pressing problems to be addressed in the near future. (Organizers Dirk Witthaut and Marc Timme)

Time: Wednesday 15:00–17:30 Location: H44

Invited Talk DY 20.1 Wed 15:00 H44

Energiewende 2.0 * the transformation of energy systems in uncertain times — •Jürgen-Fr. Hake and Wolfgang Fischer — FZ Jülich

The German Energiewende represents a very ambitious national political program. The specific targets range from GHG emissions reduction

motivated by the mitigation of climate change to technology specific goals emphasizing renewable energy in contrast to nuclear energy. The scope of the Energiewende covers a period of time of about 40 years. Scenario-based analyses point out the feasibility of this politically enforced transformation. A closer look at these scenarios also shows their limitations with respect to the socio-economic foundation and the technological differentiation. Moreover, in many cases linear models are used to describe the system under investigation which might be regarded as another weak point. These deficiencies require an integrated assessment covering **in- depth description of the anticipated major socio-political trends, **the economic embedding of the energy sector, and **an detailed well-balanced technology portfolio. A major criterion for all national initiatives is the compatibility with the transformation of the EU system.

Invited Talk DY 20.2 Wed 15:30 H44

Basin Stability and its Consequences for Power Grids — •Jürgen Kurths, Peter Menck, and Peng Ji — Potsdam Institute for Climate Impact Research, P.O. Box 601203, 14412 Potsdam,

The human brain, power grids, arrays of coupled lasers, and the Amazon rainforest contain the same seed of trouble: multistability. With undesired states looming in state space, it matters strongly how stable the desired state is against major perturbations. Surprisingly, this basic question has so far received little attention. Here we claim that the traditional linearization-based approach to stability is too local to answer it. As a complement, we suggest to quantify stability in terms of basin stability, a new measure related to the volume of the basin of attraction. Basin stability is non-local, non-linear, and easily applicable even to high-dimensional systems. Its consequences for evaluating stability of power grids and their will be discussed.

Invited Talk DY 20.3 Wed 16:00 H44

Requirements and Concepts for Self-Organized Agent-Based Control in Smart Distribution Grids — •Astrid Niesse — OFFIS - Institute for Information Technology

Transforming the existing power generation to renewable, distributed generation implicates an increase in complexity for the control of the overall system. We propose a distributed control method to launch products of self-organized coalitions of small active units in a power grid at markets for trading active power as well as ancillary services. Our concept combines the integration of grid restrictions into proactive scheduling of active power with provision of ancillary services, and additionally provides reactive scheduling of active power, e.g. in the case of ancillary service activation.

In this talk, an overview on requirements for distributed control on smart distribution grid is given, along with results on how this ICT-based approach can be realized using software agents.

Invited Talk DY 20.4 Wed 16:30 H44

A 100% renewable power system in Europe — •Martin Greiner[1], Sarah Becker[2], Rolando Rodriguez[1], Tue Jensen[1], Timo Zeyer[1], Anders Soendergaard[1], and Gorm Andresen[1] — [1]Aarhus University, Aarhus, Denmark — [2]FIAS, Frankfurt, Germany

Todays overall macro energy system based on fossil and nuclear resources will transform into a future system dominantly relying on fluctuating renewable resources. At the moment it is not really clear what will be the best transitional pathway between the current and the future energy system. In this respect it makes sense to think backwards, which means in a first step to get a good functional understanding of fully renewable energy systems and then in a second step bridge from there to todays energy system. Based on state-of-the-art high-resolution meteorological and electrical load data, simple spatio-temporal modelling, solid time-series analysis and the physics of complex networks, fundamental properties of a fully renewable pan-European power system are determined. Amongst such characteristics are the optimal mix of wind and solar power generation, the optimal combination of storage and balancing, the optimal extension of the transmission network, as well as the optimal ramp down of fossil and nuclear power generation during the transitional phase. These results indicate that the pathways into future energy systems will be driven by an optimal systemic combination of technologies, and that economy and markets have to follow technology.

DY 20.5 Wed 17:00 H44

Synchronization and Voltage Stability in a Network of Synchronous Machines — •Katrin Schmietendorf and Rudolf Friedrich — Institute for Theoretical Physics, University of Münster, Germany

Since the progressive integration of renewable energy sources involves substantial changes in grid topology and feed-in characteristics, the questions of power system stability and design have to be reconsidered. Power system stability, or more precisely rotor angle stability, is related to synchronization phenomena as the classical synchronous machine representation can be shown to correspond to a modified version of the prominent Kuramoto model. The Kuramoto model describes the dynamics of a population of coupled oscillators displaying a phase transition from incoherence to partial synchronized states. In this talk we extend the classical Kuramoto-like model which assumes constant voltages by adding dynamical voltage equations. This yields a model which allows to treat both rotor angle and voltage stability and involves the feature of rotor angle and voltage stability interplay. We compare the behaviour of small networks of synchronous machines governed by the classical and the extended model during and after being subjected to different types of disturbances and discuss the implications for the simulation of complex power grids.

DY 20.6 Wed 17:15 H44

How trading impacts distribution in complex power grids — •Sebastian Klipp[1], Dirk Witthaut[1], and Marc Timme[1,2] — [1]Network Dynamics, Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen — [2]Faculty of Physics, University of Göttingen

Instabilities in the collective dynamics of power grids may induce transmission line overloads or even large-scale power outages. One possible source of instability is the energy trading market that modifies locations, times, and volumes of electric power generation and demand. Here we investigate how economic factors can influence the distribution of energy-flow in a power-grid. We reveal that and how the interdependence of the economic and the physical network can induce dynamic instabilities and explain the mechanisms underlying them. These results offer a complementary perspective on the development of smart power grids and the integration of renewable energies.

DY 21: Granular Matter / Contact Dynamics

Time: Wednesday 15:00–18:15 Location: H47

DY 21.1 Wed 15:00 H47

Granular Gases of Rodlike Grains in Microgravity Experiments — •Kirsten Harth, Kathrin May, Torsten Trittel, Sandra Wegner, and Ralf Stannarius — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Germany

Understanding the dynamics of granular materials is relevant both in fundamental physics and from the technological point of view, but many well-known phenomena are still insufficiently understood. Granular gases are dilute ensembles of macroscopic grains, interacting by inelastic collisions. Permanent energy supply is required to maintain dynamic equilibrium. Granular gases of spherical grains have been widely investigated theoretically and in experiments in 2 dimensions. Microgravity is necessary for maintaining such a gas in 3 dimensions (3D). Only dynamics in the Knudsen-regime and clustering instabilities were accessible in previous experiments. Our experiment with rodlike grains offers access to statistical dynamics in the rod-rod collision dominated regime as well as the oppotunity to measure the rotational degrees of freedom of the particles. We present recent results from sounding rocket and drop-tower experiments. Ensembles of rods are confined in a 3D container, monitored by video cameras. Individual rods are tracked in consecutive frames. We analyse spatial and temporal density fluctuations, translational and rotational velocity distributions, the partition of kinetic energy and the influence of different experimental parameters.

DY 21.2 Wed 15:15 H47

Shear Alignment Of Shape-Anisotropic Granular Material —

•Sandra Wegner[1], Tamás Börzsönyi[2], Ralf Stannarius[1], and Balázs Szabó[2] — [1]Otto-von-Guericke Universität Magdeburg, Institute for Experimental Physics, D-39016 Magdeburg, Germany — [2]Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Hungarian Academy of Sciences, P.O. Box 49, H-1525 Budapest, Hungary

Flow of large ensembles of elongated and flat granular particles - often encountered in nature or industry - can induce pronounced alignment of the building blocks. This phenomenon is well known, e. g. in geophysics, but hardly understood quantitatively.

We explore the shear induced orientational order and alignment inside the macroscopic material using X-ray computed tomography (CT). The preferred orientation of the long axes of the particles encloses a small angle with the streamlines in the sheared region.

Our observations demonstrate that the effect of shear alignment of dry elongated particles is very similar to the well-studied case of liquid crystals, irrespectively of the completely different types of interparticle forces. Nematic continuum theory can be used to predict some features of grain alignment.

Extracting the orientations of large numbers of particles by CT image analysis enables us to calculate a local order tensor for the system. From the tensor properties we derive the average orientation, the primary and the biaxial order parameters for the stationary state and two types of transients. In addition single particle dynamics are studied.

DY 21.3 Wed 15:30 H47

A local view on sheared granular matter — Jean-François Métayer[1], Annika Döring[1], Song-Chuan Zhao[1], Mario Scheel[2], and •Matthias Schröter[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen — [2]ESRF, Grenoble, France

Whenever granular material flows along a stationary boundary, it is sheared. Examples reach from downhill avalanches to industrial hopper flows. Inside the shear flow, the volume fraction will change depending on the initial density; loose packings will compact when sheared, dense samples will expand. The transition between these two responses is called dilatancy onset. At present our understanding of it is still mostly phenomenological, e.g. there is no theory predicting the volume fraction of dilatancy onset as a function of friction, shape, or pressure.

This talk will present a local view of sheared sphere packings using fast X-ray tomography at the European Synchrotron Radiation Facility ESRF in Grenoble. While we find no scaling of the volume response with the contact number, as stipulated by the Jamming paradigm, we do see a dependence on the local volume fraction and the local strain rate.

DY 21.4 Wed 15:45 H47

Self-organized changes in the transient behavior of sheared granular materials — •János Török[1], Tamás Börzsönyi[2], and Balázs Szabó[2] — [1]institute of Physics, Budapest University of Technology and Economics, H-1111 Budapest, Hungary — [2]Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Hungarian Academy of Sciences, P.O. Box 49, H-1525 Budapest, Hungary

Recently the kinetic elastoplastic model was introduced to describe the shearing of granular material. It is based on the separation of elastic and plastic deformation where the plastic events modify the local shear stress. Here we propose a mesoscopic model which captures the essence of the kinetic elastoplastic model while making it usable for more complicated geometries like modified Couette cell. We show that in the transient phase the flow gets narrower and this is due to the change in the distribution of the material density around the shear zone. The results are tested against CT and surface video measurements which show perfect agreement in both width and density evolution.

DY 21.5 Wed 16:00 H47

Collective Granular Dynamics in a Shaken Container at Low Gravity Conditions — •Jonathan Kollmer, Achim Sack, Michael Heckel, Fabian Zimber, and Thorsten Pöschel — MSS, FAU Erlangen-Nürnberg, Erlangen, Germany

A rectangular container partially filled with steel beads is subjected to sinusoidal motion at a set of frequencies, and amplitudes that are comparable to the length of the container. We observe the dynamics inside during the low gravitational acceleration achieved on a parabolic flight. An optical flow method is used to study the compaction dynamics and particle wall collisions are characterized using a microphone. We see different regimes of excitation from a very loose state to a more ordered "collect & collide" behavior. We compare the experimental data to force-based molecular dynamics simulations and investigate the limits of describing the system using an effective one-particle model. Understanding the dynamics of this kind of system allows for better modeling and optimization of, for example, granular dampers.

DY 21.6 Wed 16:15 H47

Measurement of rotation of individual spherical particles in cohesive granulates — •Jennifer Wenzl[1], Ryohei Seto[1,2], Marcel Roth[1], Hans-Jürgen Butt[1], and Günter K. Auernhammer[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Benjamin Levich Institute for Physico-Chemical Hydrodynamics, New York, NY 10031, USA

To explore dynamical processes in granular matter, we use a combination of 3D imaging and mechanical testing. We analyze structural changes using confocal microscopy while applying a compression load simultaneously. Fluorescently labeled polydisperse silica particles were hydrophobized with long alkyl chains and dispersed in an index-matching liquid. The particles show a weak attraction. Photobleaching the central plane of individual particles generates an optical anisotropy without changing particle interaction. In a series of 3D images, we follow trajectories and rotation of single particles [1]. We focus on particle translation and rotation in dependency of the local volume fraction. During compression, restructuring happens predominantly in regions of low packing density. We show that rotation plays an important role and is hence a key parameter for explaining dynamical processes in granular systems.

[1] Wenzl, et al, Granul. Matter (2012), doi:10.1007/s10035-012-0383-7

15 min. break

DY 21.7 Wed 16:45 H47

Measuring the Mechanical Properties of a Granular Suspension — •Chih-Wei Peng and Matthias Schröter — Max-Planck-Institute for Dynamics and Self-Organization

The mechanical properties of granular suspensions differ from normal liquids. Fluidized beds are often used to study such systems. By changing the flow rate, one can achieve different states, from suspension at high flow rate to solid-like sediment at low flow rate.

Our experiment system is a torsion pendulum which is partially immersed into a fluidized bed. We apply a sinusoidal magnetic field to drive the torsion pendulum. The complex susceptibility $\tilde{\chi}(\omega)$ can be obtained by the ratio of driving torque and the response deflection angle, the latter being measured by a reflected laser beam and a quadrant photodiode. This ratio can be used to determine the viscosity of this system by using the Langevin equation.

Moreover, this method can also be applied to measure an effective granular temperature based on a fluctuation dissipation theorem.

DY 21.8 Wed 17:00 H47

Surface melting of wet granular matter in two dimensions — Christopher May, Ingo Rehberg, and •Kai Huang — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

Surface melting has been a topic of interest since Michael Faraday's observations on regelation, welding of two blocks of ice after contact below 0 degree. From the qualitative idea of surface energy reduction to quantitative experimental tests, it becomes clear nowadays that melting is a continuous process that tends to start from the free surface.

In the present investigation, we address the 'melting' scenario of a monolayer of wet glass beads under horizontally swirling motion experimentally. Due to the cohesion arising from the formation of capillary bridges between adjacent particles, the particles initially form a crystalline structure at moderate driving. As the strength of driving increases, this structure is found to melt with two steps: A reshaping into a circular shape while keeping a locally hexagonal structure, followed by a melting from the surface. Quantitative characterizations on local packing density and bond orientational order parameters both reveal a critical swirling frequency for the start of surface melting, which can be rationalized with a balance between the energy injection and the barrier for the structure change of surface particles.

DY 21.9 Wed 17:15 H47

Equilibration of liquid morphologies in granulates with dif-

ferent wettability — •Marc Schaber[1], Mario Scheel[3], Martin Brinkmann[1,2], Marco Di Michiel[3], and Ralf Seemann[1,2] — [1]Experimental Physics, Saarland University, D-66041 Saarbrücken — [2]MPI for Dynamics and Self-Organization, D-37073 Göttingen — [3]European Synchrotron Radiation Facility, 6 rue Jules Horowitz, F-38000 Grenoble

When adding liquid to dry granulates, the liquid forms individual capillary bridges or a network of liquid morophologies depending on the amount of liquid and the wettability of the granules. Fairly monodisperse glass and basalt microspheres of different diameters are used as granules having small and large contact angle, respectively. By fluidizing the granulate, the packing geometry of the granules is temporarily changed and accordingly the liquid distribution is destroyed. Using ultra-fast X-ray tomography we explore the time resolved re-distribution of liquid after stopping the fluidization and the re-formation of a new equilibrium distribution of the liquid. For non-wettable basalt beads no liquid redistribution was found. For wettable glass beads, however, a characteristic liquid equilibrium distribution is achieved after a time scale which depends on bead diameter, the viscosity and the amount of the added liquid.

DY 21.10 Wed 17:30 H47

Scaling of the normal coefficient of restitution for wet impacts — •Thomas Müller[1], Frank Gollwitzer[1], Christof A. Krülle[2], Ingo Rehberg[1], and Kai Huang[1] — [1]Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Maschinenbau und Mechatronik, Hochschule Karlsruhe - Technik und Wirtschaft, 76133 Karlsruhe, Germany

For the understanding of the dynamics of granular matter, it is important to know about the dissipation of energy due to inelastic collisions at the particle level. For dry granular matter, there are successful examples describing its dynamical behaviour based on appropriate collision models. In contrast, a continuum description for wet granulate, which considers the cohesion arising from the wetting liquid phase, is not yet established.
We investigate the coefficient of restitution (COR) by tracing a freely falling sphere that rebounds from a flat wetted surface. Our goal is to understand the energy dissipation process of a wet impact and to find a collision law which is appropriate for modelling the dynamics of granular matter. The dependence of the COR on the impact velocity as well as the properties of the particles and the liquid film is presented and discussed in terms of dimensionless numbers which characterize the interplay between inertial, viscous and surface forces. In particular, we discuss the scaling of the COR on various density and size ratios between the particle and the liquid film for liquids with different viscosities.

DY 21.11 Wed 17:45 H47

Compaction of Frictional Octahedra — •N Nirmal Thyagu, Max Neudecker, Stephan Herminghaus, and Matthias Schroeter — Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany

We perform experiments with frictional polypropylene octahedra to study the packing properties. Starting with the loose packing, compaction of octahedra is done by two types of forcing - a) tapping and b) shearing. The compaction gives rise to crystallization of octahedra due to heterogenous nucleation from the walls. We obtain the X-ray tomograms of the packing configurations as a function of packing fraction. From the contact geometries we obtain results for the packings such as - pair correlation function, distance to isostaticity, and spatial & angular correlation functions. We contrast these results with a similar study on the simplest platonic solid, the tetrahedron [Ref.1] and the sphere.

Reference: 1. Jammed frictional tetrahedra are hyperstatic, M. Neudecker, S. Ulrich, S. Herminghaus, M. Schroeter. (arXiv:1202.6272v2)

DY 21.12 Wed 18:00 H47

Compaction of Cohesive Granular Matter — •Sebastian Seemann, Alexander Weuster, Lothar Brendel, and Dietrich E. Wolf — Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany

For granular media with grain sizes in and below the μm-range, interparticular cohesion forces have a major influence on the macroscopic behavior of the medium. Especially, the porosity of a granular packing increases with increasing cohesion force. We use molecular dynamics to study the response of cohesive granular matter to uniaxial compression. With increasing pressure, remaining pores within the packing are closed and the porosity therefore decreases. Previous results [1,2] have shown that this dependency (the *compaction law*) is described by a power law. However, a discrepancy regarding the exponent still exists. Our approach to clear up this discrepancy is twofold. On one hand, we study the response of a ballistic aggregate to a fast, pressure-driven compaction and elucidate the effects of particle elasticity. In this case the behavior is more complex. The role of elastic contributions in the case of shock-compaction is discussed. On the other hand, we use a velocity-driven wall to compress the packing in a quasistatic manner. We will show that elastic effects cease to play a role and we present results for the compaction law and its exponent.
[1] D. Kadau. *Porosität in kohäsiven Pulvern und Nano-Pulvern*, Dissertation, Universität Duisburg-Essen (2004)
[2] F. A. Gilabert, J.-N. Roux, and A. Castellanos, Phys. Rev. E **78**, 031305 (2008)

DY 22: Statistical Physics (general)

Time: Wednesday 15:00–18:30 Location: H48

DY 22.1 Wed 15:00 H48

Density fluctuations and self-diffusion along saturation in dense liquids: acoustic data and lattice model — Alexander Goncharov, Vyacheslav Melent'ev, and •Eugene Postnikov — Kursk State Univesity, Kursk, Russia

We consider the density fluctuations in fluids along a saturation line (both liquid and vapour phases) especially in the region closed to the malting point. Corresponding data are extracted from acoustic (speed of sound) and thermophysical (heat capacity ratio) measurements. The analysis of the dependence for reduced fluctuations (ratio of fluctuations of real media and ideal gas under the same PVT conditions) allow to determine the region of exponentially decaying dependencies, which is universal for a large amount of substances (liquid noble gases, chained hydrocarbons and their halogen substituted).

The considered theoretical lattice model (grand canonical statistic ensamble) argues that this region corresponds to absence of structure transitions but the presence of geometrical rearrangements of particles. The derived correspondence between these fluctuational characteristics and self-diffusion properties confirms the outlook about universality of universal scaling law for atomic distribution [Dzugutov, Nature, 381 (1996), 137] non only for simple (spherically symmetric) particles but for constituents of chained hydrocarbons as well.

DY 22.2 Wed 15:15 H48

Method for prediction of thermophysical, acoustic and structure properties of liquids with the framework of cluster model — Gennady Melnikov[2], •Vyacheslav Verveyko[1], Marina Verveyko[1], and Yury Melikhov[1] — [1]Kursk State University, Kursk, Russia — [2]South-West University, Kursk, Russia

The proposed by authors distribution function of clusters with respect to number of particles allows to obtain the isothermal equation of state, which provides the method for prediction of thermophysical, acoustic and structure properties of simple liquids without a knowledge of an explicit form for the radial distribution function and adjustable intermolecular interaction potential. As well, structure and relaxation processes could be analyzed too.

The calculations are evaluated for liquefied noble gases and several hydrocarbons. Their comparison with the known experimental data shows a high exactness of the proposed method and its advances for the prediction of the mentioned properties in a wide range of state parameters.

G.A. Melnikov, V.N. Verveyko et al. Int. J. Therm. 32 (2011), 901.
G.A. Melnikov, V.N. Verveyko et al. High Temperature. 50 (2012), 214.

DY 22.3 Wed 15:30 H48

Common features of simple water models — •Lotta Heckmann and Barbara Drossel — Institut für Festkörperphysik, TU Darmstadt, Germany

The rich phase diagram and the anomalies of water continue to inspire theoretical and numerical studies. Simplified models for water that do not aim at accurately describing molecular structure, but rather at matching general properties of water, have been successful at revealing the mechanisms and principles behind the special behaviour of this substance. In particular, the association of a lower local density with a stronger binding energy is an important ingredient in such models. Several models have been introduced that include this feature and that produce, among other transitions, phase transitions between a high-density and a low-density liquid phase. We compare three of these models, which are at first sight rather different, and investigate in particular the water anomalies and the phase transition line between the two liquid phases of these models. Our objective is to identify common characteristics and to extract the minimal ingredients required for a successful water model.

DY 22.4 Wed 15:45 H48

Grand-Canonical-like molecular dynamics — •Han Wang, Carsten Hartmann, Christof Schuette, and Luigi Delle Site — Institute for Mathematics, Freie Univ. Berlin

In this presentation, we describe a general theoretical analysis, and show numerical tests of the reliability of the adaptive resolution simulation (AdResS) technique in sampling the Grand Canonical ensemble. We demonstrate that the correct density and radial distribution functions in the hybrid region, where molecules change resolution, are two necessary conditions for considering the atomistic and coarse-grained regions in AdResS equivalent to subsystems of a full atomistic system with an accuracy up to the second order with respect to the probability distribution of the system. Moreover, we show that the work done by a thermodynamic force in the transition region, that is a force originally derived on the basis of empirical thermodynamic considerations, is formally equivalent to balance the chemical potential difference between the different resolutions. From these results follows the main conclusion that the atomistic region exchanges molecules with the coarse-grained region in a Grand Canonical fashion with an accuracy up to (at least) second order. Numerical tests, for the relevant case of liquid water at ambient conditions, are carried out to strengthen the conclusions of the theoretical analysis. This fruitful combination of theoretical principles and numerical evidence candidates the adaptive resolution technique as a natural, general and efficient protocol for Grand Canonical Molecular Dynamics for the case of large systems.

DY 22.5 Wed 16:00 H48

Levy flights search in potential — •Vladimir Palyulin, Alexei Chechkin, and Ralf Metzler — Chair for Theoretical Physics, Inst for Physics & Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany

Problem of target search has a long history. There are many theoretical and experimental works which discuss whether Levy flights, Brownian motion or intermittent search strategy is the most efficient way for a particle or predator to find the target. We introduce a new convenient measure of search efficiency and compute it for Brownian and Levy search with and without potential bias. This measure shows non-trivial behavior which depends on Levy flights exponent, initial distance of a particle from the target and drift velocity. Analytical and numerical results show that either Brownian or Levy flights can be efficient depending on the initial conditions. Cumulative probability to reach a target ever is also calculated. Analytical and numerical results are obtained from fractional Fokker-Planck equation and supported by Monte-Carlo simulations.

15 min. break.

Invited Talk DY 22.6 Wed 16:30 H48

Entropy based approaches to transport — •Thomas Christen — ABB Corporate Research, CH-5405 Baden, Schweiz

The quasi-stationary distribution function for a gas of independent particles, which are not in local thermal equilibrium (LTE) but strongly interact with an LTE medium, can often be described by a linear Boltzmann transport equation (BTE). In order to make use of a truncated expansion of the distribution function in terms of moments that satisfy generalized hydrodynamic equations, an appropriate closure method is required. An often used closure method is based on constrained entropy maximization. We show that a closure based on constrained entropy production minimization is superior to entropy maximization, and mitigates some well-known errors of the latter. As an example, we discuss non-LTE radiation in an LTE-plasma and show how average heat transport coefficients can be determined for realistic absorption spectra. As a second example, we illustrate the approach for electric conduction in low-dimensional structures.

DY 22.7 Wed 17:00 H48

Massively parallel Monte Carlo for many-particle simulations on GPUs: Application to the liquid-hexatic transition of hard disks — Joshua A. Anderson, Eric Jankowski, Sharon C. Glotzer, and •Michael Engel — Chemical Engineering, University of Michigan, USA

Parallel algorithms for Monte Carlo simulations of thermodynamic ensembles of particles have received little attention because of the inherent serial nature of the statistical sampling. In this talk, we present a massively parallel method that obeys detailed balance and its implementation for a system of hard disks on the GPU [1]. We reproduce results of serial high-precision Monte Carlo runs to verify the method [2]. This is a good test case because the hard disk equation of state over the range where the liquid transforms into the solid is particularly sensitive to small deviations away from the balance conditions. Our results confirm the first-order nature of the hard disk liquid-hexatic phase transition. Phase coexistence is visualized for individual configurations via the local orientations, and positional correlation functions are computed. The performance of our method to sample configuration space and approach equilibrium is compared with the local Monte Carlo method, the event-chain Monte Carlo algorithm, and event-driven molecular dynamics.

[1] J.A. Anderson et al., arXiv:1211.1646
[2] J.A. Anderson et al., arXiv:1211.1645

DY 22.8 Wed 17:15 H48

From the number of detritus lines to hysteresis memory – On the statistics of dominant extreme values — •Sven Schubert and Günter Radons — Chemnitz University of Technology, 09107 Chemnitz, Germany

We are interested in the statistics of the number of dominant extreme values and its evolution in time. What are dominant maxima? They are to a time series what the pattern of seaweed and detritus residues on the beach is to the amplitudes of the arriving water waves.
In the first part of the talk, results are presented on the statistics of the number of dominant maxima of a sequence of i.i.d. continuous random variables. One finds that the number of dominant maxima is a nonstationary variable. It shows ageing and its expectation value is diverging logarithmically as the time approaches infinity.
The sequence of dominant maxima memorizes certain local maxima from a time series. This decreasing sequence of maxima is a simplified version of the memory of a Preisach model of hysteresis where an alternating series of dominant minima and maxima is stored. The second part of the talk elucidates this connection and discusses the implications of the results presented to the memory length of the Preisach model of hysteresis.

DY 22.9 Wed 17:30 H48

Chaoticity and thermalization in the mean-field disordered Bose-Hubbard model — •Olivier Tieleman[1], Charalampos Skokos[1,2], and Achilleas Lazarides[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Department of Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece

We study chaoticity and thermalization in the mean-field disordered Bose-Hubbard model. A symplectic integration method allows us to obtain both full trajectories through phase space and maximum Lyapunov exponents, characterizing the chaoticity of the trajectory. We then compare long-time averages of some observables to thermal expectation values and study how the system approaches a thermal state, testing the hypothesis that the ergodicity of trajectories through phase space is closely linked to their chaoticity.

DY 22.10 Wed 17:45 H48

Statistical Physics of Lattice Triangulations in Arbitrary Dimensions — •Benedikt Krüger, Johannes F. Knauf, and Klaus Mecke — Institut für Theoretische Physik, FAU Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

Triangulations are a common tool in physics, e.g. for discretization

of complex structures in classical and quantum geometry. They can be used for approximating smooth curved objects with piecewise flat simplices as elementary building blocks. We study the statistical properties of lattice triangulations in arbitrary dimensions numerically. Defining elementary flips between different triangulations, Markov-Chain Monte-Carlo simulation methods can be applied. Using the Wang-Landau algorithm we can directly calculate the density of states (DOS) and the total number of lattice triangulations for different system sizes. By applying different energy functionals we examine canonical partition sums and phase transitions.

DY 22.11 Wed 18:00 H48

Quasiparticle parameterization of meanfields, Galilean invariance and universal conserving response function — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP)Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

The form of meanfield and density functional parameterization in terms of current, energy and density are examined by the restriction of Galilean invariance. It is found that besides a density functional only one parameter remains which is usually condensed in the effective mass. The universal response with respect to density, momentum and energy is found in the sense that the response becomes independent on actual parameterization of the local equilibrium provided the conservation laws are enforced. The sum rules by frequency moments and the compressibility sum rule impose further restrictions which determines the last parameter.

DY 22.12 Wed 18:15 H48

Asymmetry in the search for the best and the worst configurations of complex problems — •Johannes Josef Schneider — Department of Physics, Mathematics, and Computer Science, Johannes Gutenberg University of Mainz, 55099 Mainz, Germany

Usually, the search for exact ground states of complex problems is considered to be as difficult as the search for states with highest cost function values, at least in the absence of symmetry breaking constraints. In this talk, I will show that there are indeed complex problems, for which the worst solution can be determined computationally much easier than the best configuration, although both tasks have to be considered as complex. Computational results are presented for the traveling salesman problem and the portfolio optimization problem.

DY 23: Statistical Physics in Biological Systems II (joint with BP)

Time: Wednesday 15:00–17:30 Location: H43

Topical Talk DY 23.1 Wed 15:00 H43

Challenges of Neurophysics — •Theo Geisel — Max Planck Institute for Dynamics and Self-Organization & Bernstein Center for Computational Neuroscience, Universität Göttingen

As you are reading these lines, millions of neurons are activated in your brain and communicate by sending short pulses to each other. It is a major aim of neurophysics to understand the collective dynamics of large biological neural networks and to determine how they carry out complex computations. Recent progress of experimental techniques allows monitoring the activity of large numbers of cells in parallel and with single cell resolution even in freely moving animals. These techniques together with targeted optogenetic stimulation promise to considerably advance our insight into the function of collective neuronal dynamics in the near future.

On the other hand, these networks exhibit features that let them elude standard theoretical treatment: E.g. the units of the network interact asymmetrically and at discrete times only, i.e. not continuously as in conventional many-body theory in physics. There are significant interaction delays, which formally make the systems infinite-dimensional. Complex connectivities give rise to novel multi-operator problems, for which new methods based on graph theory are devised to reach rigorous analytic results. The talk reviews challenges and recent progress in characterizing the dynamics and function of these networks.

DY 23.2 Wed 15:30 H43

Retinal light collectors enhance underwater vision — •Moritz Kreysing[1], Kristian Franze[2], Mike Francke[3], Andreas Reichenbach[3], and Jochen Guck[4] — [1]Systems Biophysics, Department of Physics, LMU München, Germany — [2]Department of Physiology, Development and Neuroscience, Cambridge University, UK — [3]Paul Flechsig Institute, University of Leipzig, Germany — [4]Biotechnology Center, TU Dresden, Germany

Vision at low light intensities relies on photoreceptors being able to detect individual photons. As an accepted rule, the light sensitive portions of vertebrate rods and cones, namely outer segments, increase in volume the darker the animals' habitat gets, in order to enhance the probability to capture incident photons. Consequently, the biggest outer segments are found in fish living in the deep sea. A peculiar exception to this rule are the eyes of some deep sea fish, as well as fish living in highly turbid rivers. In their retinas relatively short outer segments are bundled into spatially isolated groups, clearly not meant to maximize the probability of photon absorption. Based on a detailed morphological and optical study of multilayer light-collectors surrounding these segments [1], we argue that under extreme conditions in which quantum noise, i.e. the rate of spontaneous photo-pigment activation, becomes comparable to the rate of photon arrival, visual sensitivity cannot be achieved by large outer segments anymore. Instead the retinal focusing of light on very small receptors is the only way to lower the visual threshold further, or to see at near IR wavelengths. Reference: 1. M. Kreysing et al., Science 336(6089):1700-1703 (2012).

DY 23.3 Wed 15:45 H43

Monte Carlo simulation of the patterns of histone acetylation in response to MS-275 — •Davoud Pouladsaz[1] and Azadeh Ebrahimi[2] — [1]Department of Biological Physics, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Department of Neuropathology, Faculty of Medicine, University of Tübingen, Tübingen, Germany

Abnormal activities of histone decaetylases (HDACs) are considered to be associated with various neurological disorders, from oncogenesis, to neurodegenerative and psychiatric disorders. In this scheme, HDACs are potential targets for therapeutic development. HDAC inhibition has been reported in several studies to improve cognitive function and increase neural longevity. A novel HDAC inhibitor is MS-275, a benzamide derivative with in vivo antitumor activity and selectivity against HDAC1 and HDAC3. We perform computer simulations based on Monte Carlo method in order to describe the patterns of histone acetylation in the brain in response to MS-275. According to previous experimental results, MS-275 is a potent brain region-selective HDAC inhibitor. We theoretically produce similar acetylation profiles associated with the measurements in different regions of the brain, and calculate the changes in the acetylation by means of stochastic processes representing the inhibition of HDACs. The theoretical results show significant correlation to experimental measurements.

DY 23.4 Wed 16:00 H43

NAD(P)H Dynamics in Yeast Populations — •André Weber[1,2], Yury Prokazov[2], Werner Zuschratter[2], and Marcus J B Hauser[1] — [1]Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Leibniz-Institut für Neurobiologie Magdeburg, Germany

NAD(P)H is the most important electron carrier in living cells and therefore it plays a key-role in numerous cellular processes. It is directly involved in glycolysis and Krebs cycle and its autofluorescence acts as an indicator for metabolic dynamics and enzyme activity in cells. The amount of NAD(P)H is reflected by its emitted light intensity. Furthermore, it is possible to discriminate between free and protein-bound NAD(P)H through fluorescence lifetimes. Using single photon counting fluorescence microscopy, we study glycolytic oscillations and metabolic changes in yeast cell populations via NAD(P)H imaging.

Yeast cells show synchronised glycolytic oscillations for high population densities which can be detected as global oscillations. These global oscillations become quiescent, when the population density drops be-

low a critical value. Our results show that individual cells remain oscillatory even at very low cell densities (e.g. 1×10^5 cells/ml). The transition from global oscillations to a quiescent population signal is caused by the desynchronisation of the oscillations of individual cells. This is characteristic for a Kuramoto transition to incoherence. Spatially resolved measurements at low cell densities uncover that even cells that adhere to their neighbours oscillate with their own, independent frequencies and phases.

DY 23.5 Wed 16:15 H43

Description of polarity reorientation in the wing of the fruit fly by liquid crystal hydrodynamics — •Matthias Merkel[1], Andreas Sagenr[2], Raphael Etournay[2], Suzanne Eaton[2], and Frank Jülicher[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Max Planck Institute for Molecular Cell Biology and Genetics, Dresden, Germany

Epithelia are two-dimensional sheets of cells, which often exhibit large-scale patterns of planar cell polarity (PCP) in the tissue plane. Within a single cell, PCP is reflected in an anisotropic distribution of a class of proteins, called PCP proteins. We study PCP in the wing epithelium of the fruit fly. During development of the fly, two processes are observed: cell polarity reorients on large scales and a complex flow field reshapes the wing. This flow field includes a stereotypical pattern of tissue shear. We quantify polarity patterns in wild type and mutant wings. To interpret these patterns, we discuss a simple hydrodynamic model for polarity reorientation from liquid crystals theory. Our model consists of local polarity interactions and a coupling of polarity to tissue shear and tissue rotation. We find, that we can fit stationary states of our hydrodynamic description to the polarity patterns of the adult wings. These fits suggest that the sign of the coupling of polarity to tissue shear depends on the local expression of a PCP protein. We underpin our findings by numerical solutions of the polarity dynamics.

DY 23.6 Wed 16:30 H43

Optimization of shape for cargo transport with bead-spring microswimmers — •Jayant Pande and Ana-Sunčana Smith — Cluster of Excellence: EAM, and Institute for Theoretical Physics, Friedrich Alexander University Erlangen-Nürnberg, Germany

Microswimmers are entities that are capable of swimming in fluids at very low Reynolds numbers. A simple model of a microswimmer was introduced by Najafi and Golestanian, and consists of three spheres connected in series by two arms. This model could be used as a basis for constructing cargo-carrying micromachines, with the cargo making up the spheres in the swimmer. To determine whether other shapes for the bodies lead to more efficient swimming, we augment this model by replacing the spheres by general ellipsoids of revolution and including springs between these ellipsoids. The velocities of such three-ellipsoid swimmers acting under the influence of sinusoidal driving forces are calculated, assuming that either the deformations of the arms or the driving forces are known. Comparing the velocities of different swimmers for a given cargo volume leads to a determination of the optimum body shapes and mechanism of propagation. We observe that a rich behaviour for the velocity curve is obtained, depending on the relative magnitudes of the spring constant and the fluid viscosity. The theoretical calculations are supported by simulations using a framework combining "waLBerla", a lattice-Boltzmann method based fluid solver, and "pe", a rigid body physics engine. The simulation results are found to agree well with the calculated values.

DY 23.7 Wed 16:45 H43

On the collective motion of Chlamidomonas cells — •Johannes Greber[1], Salima Rafai[2], Philippe Peyla[2], and Walter Zimmermann[1] — [1]Universität Bayreuth, D-95447 Bayreuth, Germany — [2]Universite Joseph Fourier, F-38402 Grenoble, France

Swimming Chlamydomonas cells have a n eyespot registrating light comming from a light source far away enabling the cell to orient its direction of motion towards the light. This motion is called phototaxis.

During the propelling process, each cell generates a flow field with an atracting part in the direction of motion and a repelling part perpendicular to this direction. Due to this flow field a stable collectiv motion of a cloud of cells is impossible as long as no direction of motion is prefered by the cells.

We present experimental results and a theoretical analysis based on a model called "Puller" on the collectiv motion of Chlamydomonas cells.

DY 23.8 Wed 17:00 H43

Elastic coupling effects in cooperative transport by molecular motors — •Florian Berger, Corina Keller, Stefan Klumpp, and Reinhard Lipowsky — Max Planck Institute of Colloids and Interfaces, Theory & Biosystems, 14424 Potsdam, Germany

Intracellular transport of cargos is achieved by the cooperative action of molecular motors, which pull the cargo along cytoskeletal filaments. To study this mechanism systematically in vitro, engineered constructs coupling a defined number of molecular motors have recently been introduced. These motors are elastically coupled via their common cargo, which may influence the motors' velocity and/or enhances their unbinding from the filament. Starting from the single molecule properties, we introduce a theoretical framework for cooperative transport which is consistent with recent experiments and provides novel testable predictions about the behavior of elastically coupled kinesin, dynein and myosin motors. Such an approach relates the single motor properties directly to the cooperative dynamics. As an example, we show that the overall cargo run length can either increase or decrease as a function of the single motor velocity depending on the single motor unbinding mechanism.

DY 23.9 Wed 17:15 H43

Teams of molecular spiders: Cooperative effects enhance the transport properties — •Matthias Rank, Louis Reese, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München

Molecular spiders are synthetic molecular motors based on DNA nanotechnology. While natural molecular motors have evolved towards very high efficiency, it remains a major challenge to develop efficient designs for man-made molecular motors. Inspired by biological motor proteins like kinesin and myosin, molecular spiders comprise a body and several legs. The legs walk on a lattice that is coated with substrate which can be cleaved catalytically. We propose a novel molecular spider design in which n spiders form a team. Our theoretical considerations show that coupling several spiders together alters the dynamics of the resulting team significantly. Although spiders operate at a scale where diffusion is dominant, spider teams can be tuned to behave nearly ballistic, which results in fast and predictable motion. Based on the separation of time scales of substrate and product dwell times, we develop a theory which utilises equivalence classes to coarse-grain the microstate space. In addition, we calculate diffusion coefficients of the spider teams, employing a mapping of an n-spider team on an n-dimensional random walker on a confined lattice. We validate these results with Monte Carlo simulations and predict optimal parameters of the molecular spider team architecture which makes their motion most directed and maximally predictable.

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

Time: Wednesday 15:45–17:00 Location: H37

DY 24.1 Wed 15:45 H37

Eigenvector centrality as a measure of influence in dynamics on networks — •Konstantin Klemm[1], M. Angeles Serrano[2], Victor M. Eguiluz[3], Maxi San Miguel[3], and Fakhteh Ghanbarnejad[4] — [1]Bioinformatics, Institute for Computer Science, Leipzig University, Germany — [2]Fisica Fonamental, University of Barcelona, Spain — [3]Institute for Cross-Disciplinary Physics and Complex Systems, Palma de Mallorca, Spain — [4]MPI for Physics of Complex Systems, Dresden, Germany

Definitions of centrality aim at quantifying the importance of a node in a given graph. Among many others, the degree, the betweenness and the closeness are examples of frequently used measures of centrality. Here we ask which notion of centrality is best suited for predicting the influence a node has on dynamics. The concept of dynamical influence is made rigorous for a class of dynamical rules that asymptotically lead the system to a stationary state $y(\infty)$ from any initial condition

$y(0)$. Then the influence of node v is the dependence of the asymptotic state on the initial condition $y_v(0)$ at node v. We find that the principal eigenvector of the coupling matrix is an accurate predictor of influence for various kinds of dynamics [1,2], including critical epidemic and Ising models, Boolean networks, the voter model as well as Kuramoto and Rössler oscillators.

[1] Klemm et al., Scientific Reports 2, 292 (2012).
[2] Ghanbarnejad and Klemm, EPL 99:58006 (2012).

DY 24.2 Wed 16:00 H37

A macroscopic view on temporal networks — •Hartmut Lentz[1,2], Thomas Selhorst[1], and Igor M Sokolov[2] — [1]Friedrich-Loeffler-Institute, Federal Research Institute for Animal Health, 16868 Wusterhausen, Germany — [2]Humboldt-University of Berlin, 12489 Berlin, Germany

The concept of accessibility graphs can be extended to temporal networks. An accessibility graph (transitive closure) of a network contains a link, wherever there is a path of arbitrary length between node pairs. Building an accessibility graph by consecutively adding paths of growing length ("unfolding") yields information about the distribution of shortest path durations and reveals characteristic time-scales in temporal networks. Accessibility contributes a key element for a theoretical framework for the macroscopic analysis of temporal networks, because it maps the whole causal path structure of the system onto a single mathematical object. In addition, we define a causal fidelity, measuring the goodness of the static representation of a temporal network. The methods provided here can be implemented efficiently and their capability is demonstrated in applications, as shown by our discussion of three temporal network data sets, namely social contacts, livestock trade and sexual contacts.

Reference: Unfolding accessibility provides a macroscopic approach to temporal networks, arXiv:1210.2283.

DY 24.3 Wed 16:15 H37

Clustering coefficient of temporal networks — •Vitaly Belik[1,2], Igor M Sokolov[3], and Hartmut Lentz[3,4] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen — [2]Massachusetts Institute of Technology, Cambridge, USA — [3]Humboldt-University of Berlin — [4]Friedrich-Loeffler-Institute, Wusterhausen

The science of complex networks has experienced a tremendous development in recent years. Most of the research was devoted to static networks where interactions between nodes are aggregated over time. However with increasing availability of empirical data of high temporal resolution, the dynamics of networks becomes the focus of research. In the present study we generalize the concept of clustering coefficient to temporal networks allowing for arbitrary durations of triangles fulfilling the requirement of causality. In contrast to many algorithmic approaches, we build up on the current advances in the mesoscopic description of temporal networks [1]. We apply our approach to various empirical datasets, in particular a conference contact network and a mobile phone dataset, as well as to their randomized counterparts.

[1] Unfolding accessibility provides a macroscopic approach to temporal networks, H Lentz, T Selhorst, I M Sokolov, arXiv:1210.2283

DY 24.4 Wed 16:30 H37

Devil's Staircases, Crackling Noise and Phase Transitions in Percolation — •Jan Nagler — Max Planck Inst. f. Dyn. & Self-Organization

We identify and study certain phenomena in percolation that can subvert predictability and controllability in networked systems. We establish devil's staircase phase transitions, non-self-averaging, and power-law fluctuations in percolation. We provide exact conditions for percolation that exhibits multiple discontinuous jumps in the order parameter where the position and magnitude of the jumps are randomly distributed - characteristic of crackling noise. The framework is linked to fragmentation processes, where groups or particles repeatedly split up, to susceptible-infected type dynamics, and also to effects in ferromagnetic materials.

DY 24.5 Wed 16:45 H37

Resilience to Leaking - Dynamic Systems Modeling of Information Security — •Kay Hamacher — Department of Computer Science, Department of Physics & Department of Biology, Technische Universitaet Darmstadt, Germany

Leaking of confidential material is a major threat to information security. This insight become popular wisdom since Wikileaks, which hopes to attack 'unjust' systems or 'conspiracies'.

Eventually, such threats to information security rely on a biologistic argument on the benefits and drawbacks that uncontrolled leaking might pose for 'just' and 'unjust' entities. Such biological metaphors are almost exclusively based on the economic advantage of participants.

Here, I introduce a mathematical model of the complex systems dynamics implied by leaking. The complex interactions of adversaries are modeled by coupled logistic equations including network effects of econo-communication networks.

Situations might arise where leaking can strengthen the 'conspiracy'. The only impact leaking can have on an organization originates in the exploitation of leaks by a competing entity. We conclude that leaks can be used as a 'tactical mean' in direct adversary relations, but do not necessarily increase public benefit.

Within the model exploiting the competition between entities seems to be a more promising approach to control malicious organizations: divide-et-impera policies triumph here.

[1] K. Hamacher, "Resilience to Leaking - Dynamic Systems Modeling of Information Security", PLoS One, 2012, accepted

DY 25: Critical Phenomena and Phase Transitions

Time: Thursday 9:30–12:45 Location: H46

DY 25.1 Thu 9:30 H46

Computing melting temperatures of Na, Mg, Al and Si by pinning of solid-liquid interfaces in ab-initio calculations — •Felix Hummel[1], Ulf R. Pedersen[1,2], Georg Kresse[1], Gerhard Kahl[2], and Christoph Dellago[1] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna, Austria — [2]Institute of Theoretical Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10, A-1040 Vienna, Austria

We use a novel approach for computing the Gibbs free energy difference between phases of a material. The force acting on an interface separating two phases of interest is determined by applying an external field biasing two-phase configurations. This force is proportional to the Gibbs free energy difference between the phases.

We demonstrate the accuracy, efficiency and practical applicability of this approach by computing the melting temperature at ambient pressure of Na, Mg, Al and Si using ab-initio calculations with VASP. Whereas predicted melting temperatures are in good agreement with experiment for Na, Mg and Al, the melting temperature of Si is underestimated, in agreement with previous computations.

DY 25.2 Thu 9:45 H46

The role of phonons in the thermodynamics of Fe — •Michael Leitner[1,2], Jürgen Neuhaus[1,2], Karl Nicolaus[1], Winfried Petry[1,2], Bernard Hennion[3], and Arno Hiess[4] — [1]Technische Universität München, Physik Department E13, 85747 Garching, Germany — [2]Technische Universität München, Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), 85747 Garching, Germany — [3]Laboratoire Léon Brillouin, CEA Saclay, 91191 Gif-sur-Yvette Cédex, France — [4]Institut Laue-Langevin, 38042 Grenoble, France, now at European Spallation Source AB, 22100 Lund, Sweden

We report measurements of the phonon dispersions for the three ambient-pressure phases of pure iron (α-Fe, γ-Fe and δ-Fe) by inelastic neutron scattering. Generally, the anharmonic effects lead to a softening of the phonons. Modelling the dispersions by a Born-von Kármán model with temperature-dependent force constants allows us to deduce the vibrational contributions to the energy and entropy differences at the phase transitions. We can conclude that while the latent heats arise mainly from the electronic contributions, the vibrational contributions to the entropy can not be neglected, and especially the $\gamma \leftrightarrow \delta$-transition is driven mainly by the increased vibrational entropy of the open bcc structure.

DY 25.3 Thu 10:00 H46

Critical Casimir forces between homogeneous and chemically striped surfaces — •Francesco Parisen Toldin[1], Matthias Tröndle[2], and Siegfried Dietrich[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg — [2]Max Planck Institute for Intelligent Systems, Heisenbergstr. 3, D-70569 Stuttgart

Recent experiments have measured the critical Casimir force acting on a colloid immersed in a binary liquid mixture near its continuous demixing phase transition, and exposed to a chemically structured substrate. Motivated by these experiments, we study the critical behavior of a system, which belongs to the Ising universality class, for the film geometry with one planar wall chemically striped, such that there is a laterally alternating adsorption preference for the species of the binary liquid mixture. By means of Mean-Field theory, Monte Carlo simulations and finite-size scaling analysis we determine the critical Casimir force and the corresponding universal scaling function.

DY 25.4 Thu 10:15 H46

Online discussions modeled by an evolving Ising-like dynamics — •Julian Sienkiewicz and Janusz Hołyst — Faculty of Physics, Center of Excellence of Complex Systems Research, Warsaw University of Technology, Poland

We present and exactly solve a one-dimensional model for emotional online discussions basing on the Ising-like asymmetrical and evolving dynamics. We restrict ourselves only to interactions with last message's emotions and study the dependence of the chain's average emotion $\langle e \rangle$ on external field h (community tendency toward a selected valence) and temperature T (uncertainty of the emotion). This leads us to an observation of three distinct phases - the first, where discussion evolution is determined by its beginning only, the second, in which the mostly observed emotion is coping the external influence, a finally, the third one, where the outcome is subject to fluctuations. The phases are separable with respect to the parameter that copies participant's uncertainty about their emotional behaviour.

DY 25.5 Thu 10:30 H46

MC test of cluster definitions in nucleation simulations of the lattice gas model — •Fabian Schmitz, Peter Virnau, and Kurt Binder — Johannes Gutenberg-Universität Mainz - Staudingerweg 7, D-55099 Mainz, Germany

The conventional theory of homogeneous and heterogeneous nucleation in a supersaturated vapor is tested by Monte Carlo simulations of the lattice gas (Ising) model with nearest-neighbor attractive interactions on the simple cubic lattice. The theory considers the nucleation process as a slow (quasi-static) cluster (droplet) growth over a free energy barrier ΔF^*, constructed in terms of a balance of surface and bulk term of a "critical droplet" of radius R^*, implying that the rates of droplet growth and shrinking essentially balance each other for droplet radius $R = R^*$.

Comparing different cluster definitions, namely geometrical clusters, Swendsen-Wang clusters and clusters applying the relations from classical nucleation theory, we find that, for all temperatures below the critical temperature, only the definition of "physical" clusters based on the Fortuin-Kasteleyn mapping is consistent with the estimates from the lever rule. The discrepancy between classical nucleation theory and the lever rule is determined for various temperatures.

DY 25.6 Thu 10:45 H46

Phase Transitions in Classical Lattice Gases with Three-Body Interactions — •Georg Maximilian Lohöfer — Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany

We study a classical lattice gas on a honeycomb lattice in the parameter region where three-body interactions are dominant. Employing Monte Carlo simulations utilizing parallel tempering, we explore the complex low energy manifold, where highly-degenerate states for different values of the chemical potential emerge, resulting from the frustrated nature of three-body repulsions on the hexagonal lattice structure. We analyse the thermal phase transitions out of these low-temperature phases and identify a four-states Potts model transition that can be traced back to a partial re-ordering from an extensive ground state degeneracy at finite temperatures.

15 min. break

DY 25.7 Thu 11:15 H46

Continuous replica-symmetry breaking in mean-field spin-glass models: Perturbation expansion without the replica trick — Vaclav Janis, •Anna Kauch, and Antonin Klic — Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 18221 Praha, Czech Republic

The full mean-field solution of spin glass models with a continuous order-parameter function is not directly available and approximate schemes must be used to assess its properties. The averaged physical quantities are to be represented via the replica trick and the limit to zero number of replicas is to be performed for each of them. To avoid this we introduce a perturbation expansion for a mean-field free-energy functional with a continuous order-parameter function without the need to refer to the replica trick. The expansion can be used to calculate all physical quantities in all mean-field spin-glass models and at all temperatures, including zero temperature. The small expansion parameter is a difference between the continuous order-parameter function and the corresponding order parameter from the solution with one level of replica-symmetry breaking. The first correction beyond the approximation with one level of replica-symmetry breaking is explicitly evaluated in the glassy phase of the Sherrington-Kirkpatrick model.

DY 25.8 Thu 11:30 H46

Searching for spin-glass ground states in a transformed energy landscape — •Markus Manssen and Alexander K. Hartmann — Institut für Physik, Carl von Ossietzky Universität Oldenburg

Spin glasses and related models have been of interest to the scientific community for decades due to their inherent disorder and frustration and the resulting complex energy landscape. But this at the same time makes time evolution of these systems particularly slow and finding the ground states very hard (for 3D systems NP-hard in fact [1]). Consequently many elaborate algorithms have been developed to tackle these problems. Karandashev et al. [2] have proposed an inverse approach in which one takes a power of a system's bond matrix, transforming its energy landscape to make finding the new ground state easier for any algorithm of choice. From there the original ground state should be easily reachable using the normal Hamiltonian. We test this method for the 3D binary Edwards-Anderson model with both the original authors preferred search algorithms and also Monte Carlo and parallel tempering simulations. We compare the results to the exact ground states. To evaluate the performance we have to also take the slow down caused by the transformed matrices into account.

[1] F. Barahona, On the computational complexity of Ising spin glass models, (J. Phys. A: Math. Gen. 15 3241, 1982)
[2] Ya.M. Karandashev and B.V. Kryzhanovsky, Transformation of energy landscape in the problem of binary minimization, (Doklady Mathematics, Vol. 80, No. 3, p. 927–931, 2009)

DY 25.9 Thu 11:45 H46

Stochastic Loewner evolution in the 2D Ising spin glass depends on boundary conditions — •Hamid Khoshbakht[1,2], Martin Weigel[1,2], and Jacob D. Stevenson[3] — [1]Institut für Physik, Johannes Gutenberg-Universitaät Mainz, D-55099 Minz, Germany — [2]Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, UK — [3]University Chemical Laboratories, Lensfield Road, Cambridge, CB2 1EW, UK

Domain walls in two-dimensional Ising spin glasses are scale-invariant curves with fractal dimension d_f. Recent works indicate that $d_f \approx 1.27$ for Gaussian bond distribution and $1.09 \lesssim d_f \lesssim 1.39$ for bimodal couplings. In this contribution, we investigate whether the domain wall of this system satisfies Schramm-Loewner evolution (SLE) and is therefore also conformally invariant. Different boundary conditions are considered, and for each case d_f and the SLE diffusion constant κ of the corresponding Brownian motion are calculated. Correlations between different domain-wall segments are explicitly checked for by testing for independence of the increments of the Loewner driving function. The results show that changing the boundary conditions of the system does not change the fractal dimension, but the stronger conditions of SLE are only satisfied for specific choices of boundary conditions. In this sense, SLE is not universal.

DY 25.10 Thu 12:00 H46

Efficient Monte Carlo Simulations of the Random-Cluster Model using a Dynamic Connectivity Algorithm — •Eren M. Elçi and Martin Weigel — Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, England

The simulation of spin models close to points of continuous phase transitions is heavily impeded by the occurrence of critical slowing

down. A number of cluster algorithms usually based on the Fortuin-Kasteleyn representation of the Potts model and suitable generalizations for continuous-spin models has been used to increase simulation efficiency. The first algorithm making use of this representation, suggested by Sweeny in 1983, has not found widespread adoption due to problems in its efficient implementation. It has been shown recently, however, that it is indeed more efficient in reducing critical slowing down that the more well-known variants due to Swendsen/Wang and Wolff. Here, we discuss an efficient implementation of Sweeny's approach using recent algorithmic advances in dynamic connectivity algorithms, and show how these can be used for efficient simulations in the random-cluster model. An extension of this approach, which is also efficient for first order phase transitions, is the combination of the random cluster model and multicanonical simulations. In this framework, we directly sample the combined geometrical bond- and cluster-number density of states of the model. By construction, this approach does not suffer from any (hyper-)critical slowing down.

DY 25.11 Thu 12:15 H46

Determination of line tension in the 3d Ising model using GPUs — •Benjamin Block, Suam Kim, Peter Virnau, and Kurt Binder — University of Mainz, Germany

Heterogeneous nucleation barriers are influenced by line tension effects [1]. We apply an efficient implementation of the Ising model on graphic cards [2] to quantify this effect in detail. In an Ising system with aperiodic boundary conditions in one dimension, a liquid vapor interface can be stabilized between two walls. When wall fields are applied, this leads to a difference in the Free Energy of the system. This change can be quantified in dependence on the linear dimensions of the simulation box and by varying the size of the box in all dimensions, the contribution of line tension can be extracted. [1] D. Winter, P. Virnau, K. Binder, PRL 103, 225703 (2009). [2] B. Block, EPJ-ST 210, 147 (2012).

DY 25.12 Thu 12:30 H46

Anisotropy and universality: Critical Binder cumulant of a two-dimensional Ising model — •Boris Kastening — Institute for Materials Science, Technische Universität Darmstadt, Germany

We reanalyze transfer matrix and Monte Carlo results for the critical Binder cumulant U^* of an anisotropic two-dimensional Ising model on a square lattice in a square geometry with periodic boundary conditions. Spins are coupled between nearest neighboring sites and between next-nearest neighboring sites along one of the lattice diagonals. We find that U^* depends only on the asymptotic critical long-distance features of the anisotropy, irrespective of its realization through ferromagnetic or antiferromagnetic next-nearest neighbor couplings [1]. Our results support our recent claim towards the validity of universality for finite-size scaling in the presence of a weak anisotropy [2].

[1] B. Kastening, arXiv:1209.0105.
[2] B. Kastening, Phys. Rev. E 86, 041105 (2012).

DY 26: Quantum Chaos I

Time: Thursday 9:30–12:00 Location: H47

Invited Talk DY 26.1 Thu 9:30 H47

Genuine quantum interference in interacting bosonic fields: The semiclassical propagator in Fock space — •Juan Diego Urbina[1], Thomas Engl[1], Arturo Arguelles[2,1], Julien Dujardin[2], Peter Schlagheck[2], and Klaus Richter[1] — [1]Institute for Theoretical Physics, University of Regensburg — [2]Department of Physics, University of Liege

We present a semiclassical theory of quantum interference effects in interacting bosonic fields. We make special emphasis on the difference between genuine quantum interference (due to the superposition principle in the many-body Hilbert space), and classical interference effects due to the wave character of the classical limit.

First, we discuss how the usual approaches to this problem are unable to provide the characteristic sum of oscilatory terms, each asociated with a solution of the classical equations of motion, required to semiclassically address interference effects. We show then how to solve this problems by a formal construction of the van Vleck-Gutzwiller propagator for bosonic fields as a sum over paths in the associated Fock space and we identify the classical limit as a Gross-Pitaevskii equation with boundary conditions and multiple solutions.

The theory predicts effects akin to weak localization to take place in Fock space, and in particular the enhancement of quantum probability of return due to interference between time-reversed paths there. We support our claims with extensive numerical calculations for a discrete version of an interacting bosonic field.

DY 26.2 Thu 10:00 H47

Universality in chaotic quantum transport: The concordance between random matrix and semiclassical theories — Gregory Berkolaiko[1] and •Jack Kuipers[2] — [1]Department of Mathematics, Texas A&M University, College Station, TX 77843-3368, USA — [2]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

Electronic transport through chaotic quantum dots exhibits universal, system independent, properties, consistent with random matrix theory. The quantum transport can also be rooted, via the semiclassical approximation, in sums over the classical scattering trajectories. Correlations between such trajectories can be organized diagrammatically and have been shown to yield universal answers for some observables. Here, we develop the general combinatorial treatment of the semiclassical diagrams, through a connection to factorizations of permutations. We show agreement between the semiclassical and random matrix approaches to the moments of the transmission eigenvalues. The result is valid for all moments to all orders of the expansion in inverse channel number for all three main symmetry classes (with and without time reversal symmetry and spin-orbit interaction) and extends to nonlinear statistics. This finally explains the applicability of random matrix theory to chaotic quantum transport in terms of the underlying dynamics as well as providing semiclassical access to the probability density of the transmission eigenvalues.

Phys. Rev. E **85** (2012) 045201

DY 26.3 Thu 10:15 H47

Experimental resonance spectra and field distributions of a dielectric cube — •Marco Masi, Barbara Dietz, Maksim Miski-Oglu, and Achim Richter — Institut für Kernphysik, TU Darmstadt, 64289 Darmstadt, Germany

In the frame of a project which envisages to extend the experimental study from 2D to 3D dielectric microwave resonators, we present the measurement results for a 3D alumina cube resonator. The aim is the understanding of its spectral properties and its electromagnetic field distributions. These are different from those of a 2D flat dielectric microwave resonator since all polarizations have to be taken into account. Its resonance frequencies, the length spectrum of its corresponding classical periodic orbits, the wave vector distribution, the mode symmetry classes, and the polarization states are investigated. A central question is the existence of superscars in 3D resonant structures, and more generally the validity of semiclassical approximations in 3D resonant structures.

This work has been supported within the DFG grant SFB634.

15 min. break

DY 26.4 Thu 10:45 H47

Experimental observation of spectral gap in microwave n-disk systems — Sonja Barkhofen[1], •Tobias Weich[2], Alexander Potzuweit[1], Hans-Jürgen Stöckmann[1], Ulrich Kuhl[3], and Maciej Zworski[4] — [1]Fachbereich Physik, Philipps-Universität Marburg, Renthof 5,35032 Marburg, Germany — [2]Fachbereich Mathematik, Philipps-Universität Marburg, Hans-Meerwein-Straße,35032 Marburg, Germany — [3]Laboratoire de Physique de la Matière Condensée, CNRS UMR 7336, Université de NiceSophia-Antipolis, F-06108 Nice, France — [4]Department of Mathematics, University of California, Berkeley, California 94720, USA

We present experimental studies of the symmetry reduced 3-disk and 5-disk systems using a microwave setup. By extracting the complex resonances from the signal by means of the harmonic inversion we can access the width distribution. A spectral gap is observed for thick as

well as for thin repellers, for thin repellers it is compared with the known topological pressure bounds. Furthermore the maxima of the distributions coincide in a large range with half of the classical escape rate.

DY 26.5 Thu 11:00 H47

Biased diffusion inside regular islands of randomly perturbed quantum maps — •Alexander Schnell[1] and Roland Ketzmerick[1,2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany

We study quantum maps under random parametric perturbations. Similar to the corresponding classical case [1] we find biased diffusion of wave packets inside a regular island. We show that quantum mechanics leads to two additional effects: (i) Due to quantization the innermost states exhibit a different drift velocity and diffusion coefficient, which can be derived from a linearized model. This may enhance or reduce the survival probability in the regular island depending on the parity of the initial wave packet. (ii) Due to dynamical tunneling the escape from the regular island is further enhanced at large times.

[1] A. Kruscha, R. Ketzmerick, and H. Kantz, Phys. Rev. E **85**, 066210 (2012).

DY 26.6 Thu 11:15 H47

Edge states in a rectangular microwave Dirac billiard — •Maksym Miski-Oglu, Barbara Dietz, Christof Cuno, Tobias Klaus, Marco Masi, and Achim Richter — Institut für Kernphysik, Technische Universität Darmstadt, D-64289 Darmstadt, Germany

We present results on the experimental investigation of edge states in a superconducting microwave Dirac billiard. A rectangular microwave billiard is filled with metallic cylinders which form a photonic crystal with a triangular lattice. In the vicinity of a certain frequency, the so called Dirac frequency, the dispersion relation for electromagnetic waves in a photonic crystal is similar to that of a relativistic massless fermion and the Helmholtz equation reduces to the Dirac equation. The localized states, so called edge states, occur in the vicinity of the Dirac frequency. Their resonance frequencies are extracted from the measured transmission spectra and compared with predictons in the context of the semiclassical theory.

DY 26.7 Thu 11:30 H47

Quantum graphs with time dependent bond lengths — •Daniel Waltner and Uzy Smilansky — Department of Complex Systems, Weizmann Institute of Science, Rehovot, Israel

Usually a graph is considered to be built up by vertices connected by bonds with fixed lengths. In experimental realizations of graphs, for example by optical fiber networks, the bonds usually slightly change their lengths randomly caused e.g. by thermal fluctuations. We study perturbatively the effect of these fluctuations on the properties of graphs and discuss the experimental relevance.

DY 26.8 Thu 11:45 H47

Trapping of chaotic orbits in 4D maps — •Steffen Lange[1,2], Martin Richter[1], Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany

Generic Hamiltonian systems with more than two degrees of freedom lead to chaotic zones in phase space which are all interconnected by the Arnol'd web. We study 4D maps with a regular region embedded in a large chaotic sea, i.e. far away from the near-integrable regime. Chaotic orbits show a power-law decay of survival times. We find that the underlying mechanism is clearly different from trapping in 2D maps. Moreover, it is not related to the Arnol'd web. Instead, an anisotropic diffusion near the surface of the regular region is observed.

DY 27: Fluid Dynamics and Turbulence

Time: Thursday 9:30–11:30 Location: H48

DY 27.1 Thu 9:30 H48

Formation of Kinneyia via shear-induced instabilities in microbial mats — Katherine Thomas[1], Stephan Herminghaus[1], Hubertus Porada[2], and •Lucas Goehring[1] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Germany — [2]Univeristy Göttingen, Goewissenschaftliches Zentrum, Göttingen, Germany

Kinneyia are microbially mediated sedimentary fossils with clearly defined ripple structures. They are generally found in areas that were formally littoral habitats and covered by microbial mats. To date there has been no conclusive explanation as to the processes involved in the formation of these fossils. Microbial mats behave like viscoelastic fluids. We propose that the key mechanism involved in the formation of Kinneyia is a Kelvin-Helmholtz instability induced in a viscoelastic film under flowing water. A ripple corrugation spontaneously forms in the film and grows in amplitude over time. Theoretical predictions show that the ripple instability has a wavelength proportional to the thickness of the film. Experiments carried out using viscoelastic films confirm this prediction. The ripple pattern that forms has a wavelength roughly three times the thickness of the film. Laboratory-analogue Kinneyia were formed via the sedimentation of glass beads, which preferentially deposit in the troughs of the ripples. Well-ordered patterns form, with both honeycomb-like and parallel ridges being observed, depending on the flow speed. These patterns correspond well with those found in Kinneyia fossils, with similar morphologies, wavelengths and amplitudes being observed.

DY 27.2 Thu 9:45 H48

Burgers turbulence from the functional renormalisation group: universal properties of momentum dependent correlation functions — •Steven Mathey, Thomas Gasenzer, and Jan Martin Pawlowski — ITP, Philosophenweg 16, 69120 Heidelberg

The stochastic Burgers' equation is studied as a toy model for Navier-Stokes turbulence. Non perturbative scaling of a randomly stirred fluid in a stationary state is investigated with the functional renormalisation group. We make a truncation with a very general, momentum dependent, two points correlation function and write a fixed point condition which is to be solved recursively. We extract scaling exponents that agree with a similar work on the KPZ equation.

DY 27.3 Thu 10:00 H48

Dynamical scaling of the critical velocity for the onset of turbulence in oscillatory superflows — •Wilfried Schoepe[1] and Risto Hänninen[2] — [1]Universität Regensburg — [2]Aalto University Helsinki

The critical velocity for the onset of turbulence in oscillatory superflows v_c is universal and scales as $\sqrt{\kappa\omega}$, where κ is the circulation quantum of the superfluid vortices and ω is the oscillation frequency. This behavior was observed experimentally and can be derived theoretically in various ways, e.g., from dimensional considerations, from the superfluid Reynolds number $R_s = (vl)/\kappa$ (where v is the flow velocity and l is a characteristic length scale), and rigorously by means of dynamical scaling of the equations of motion of vortex dynamics.

DY 27.4 Thu 10:15 H48

Permeability of porous materials determined from the Euler characteristic — •Christian Scholz[1], Frank Wirner[1], Jan Götz[2], Ulrich Rüde[2], Gerd E. Schröder-Turk[3], Klaus Mecke[3], and Clemens Bechinger[1,4] — [1]2. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Lehrstuhl für Systemsimulation, Friedrich-Alexander Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [3]Institut für Theoretische Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [4]Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart, Germany

We present measurements and lattice Boltzmann simulations of the permeability of quasi two-dimensional porous structures of randomly placed overlapping monodisperse circular and elliptical grains. We demonstrate that the permeability can be determined from the Euler characteristic of the fluid phase. The resulting expression is indepen-

dent of the percolation threshold and shows a good agreement with our data over a wide range of porosities. Our results suggest that the permeability depends explicitly on the overlapping probability of grains rather than their shape (Scholz et al., PRL 2012, in press).

15 min. break

DY 27.5 Thu 10:45 H48

Drag coefficient measurements of spheres with different surface patterns — •Daniel Strutz, Hendrik Heisselmann, Joachim Peinke, and Michael Hölling — ForWind - Center for Wind Energy Research, Institute of Physics, University of Oldenburg, Germany

Precise drag force measurements of bluff bodies are an under-estimated challenge and in particular drag coefficients of bodies with rough surface structure are not very well documented in literature. In our contribution, we present a new setup for measurements of the acting drag forces on spheres and other bluff bodies. The examined bodies are attached to a slim supporting rod, which is held by thin steel wires in a cubical rigid frame, and the resulting velocity-dependent forces are measured by means of strain gauges. Besides a detailed description of the achieved experimental setup, we will present results from force measurements using smooth spheres and a sphere with a dimpled surface pattern. Measurements were performed for a Reynolds number range of 2,700 up to 230,000 under laminar inflow conditions as well as in turbulent flows generated by a classical grid. An overview of the calculated drag coefficients will be given for different sphere types and in turbulent flow. The obtained results will be compared to those documented in literature.

DY 27.6 Thu 11:00 H48

Droplet impact on free-standing smectic liquid crystalline films — •Sarah Dölle[1], Thomas John[1,2], and Ralf Stannarius[1] — [1]Department of Nonlinear Phenomena, Faculty of Science, University of Magdeburg, PB 4120, 39016 Magdeburg, Germany — [2]Department of Experimental Physics, Faculty of Science, University of Saarland, 66123 Saarbrücken, Germany

Liquid droplet impact on solid and liquid surfaces, including wetting phenomena and splashing behavior have been in the focus of scientific interest since decades. Experimental and theoretical work so far dealt basically with droplets hitting wet solid substrates, dry solid substrates or deep liquid pools. Mostly, the diameters of the droplets were chosen in the millimeter range. With the development of inkjet printing, however, a strong interest in the impact behavior of picoliter droplets emerged. So far, only few investigations have been carried out on droplet collisions with free-standing liquid films. We present a study on the impact of aqueous droplets with a diameter of about 50 microns on freely suspended, smectic liquid crystalline films. Because of the small dimensions of the droplets, the Weber and Ohnesorge numbers, that describe the ratios of inertial, viscous and surface tension related forces, are smaller than one. In this regime, capillary forces prevail over kinetic effects and viscous forces. Smectic liquid crystals are favorable materials to generate free-standing films. Due to their layered molecule structure, these films remain stable even if the thickness is as low as two molecular layers. The impact process was resolved via high-speed imaging, using rates up to 180000 frames per second.

DY 27.7 Thu 11:15 H48

Thermal convection in thin soap films — Markus Abel[1,2], Luca Biferale[3,4], •Henning Krüsemann[5], and Mauro Sbragaglia[3,4] — [1]LEMTA UdL, Nancy, France — [2]Ambrosys GmbH, Potsdam, Germany — [3]University of Rome, Tor Vergata, Italy — [4]INFN, Rome, Italy — [5]University of Potsdam, Germany

In recently published experiments it was shown that turbulent convection in a vertically suspended foam film with a nanometer thickness speeds up thinning enormously. The effects that govern the resulting turbulent flows have not been described theoretically, so far. At the nanoscale,mesoscopic and microscopic forces start to play a role, which are unimportant for thicker films.

The presented work concerns a theory for the dynamics of a vertically oriented foam film, including external forcing, in particular thermal effects. The aim is to describe convection in vertical foam films. A closed two-dimensional model for the fluid flow is derived, considering capillary effects, as well as van-der-Waals interaction between the amphiphile surfactants and other forces.

The resulting equations are simulated using a Lattice Boltzmann scheme, which was specially developed for this case. An outline of the development of this model is given and some results considering the analysis of the flow are presented.

DY 28: Symposium: Computational Challenges in Scale-Bridging Modeling of Materials (SYMM)

Time: Thursday 9:30–12:00 Location: H1

Invited Talk DY 28.1 Thu 9:30 H1

Challenges for first-principles based computation of properties of oxide materials — •Karsten Albe — TU Darmstadt, FB 11, FG Materialmodellierung, Petersenstr. 32, D-64287 Darmstadt

Calculations based on density functional theory (DFT) have been the mainstay of theoretical studies of the properties of semiconductor and oxide materials over the past few decades. Despite of their significant successes, challenges remain in adapting these methods for predictive simulations that are quantitatively useful in predicting complex device properties. Increasing computing power and improved theoretical methods taking advantage of ever more powerful computer hardware offer the possibility that computational modelling may finally allow a virtual materials design by truly predictive simulations. In this contribution, I will give examples for successes and failures in calculating bulk, point defect and surface properties of transparent conducting as well as ferroelectric oxides and describe the remaining challenges.

Invited Talk DY 28.2 Thu 10:00 H1

Deformation and Fracture of Solids: Tough Nuts at Atomic and Continuum Scales — •Peter Gumbsch[1,2], Matous Mrovec[1,2], Kinshuk Srivastava[1], and Daniel Weygand[1] — [1]Institut for Applied Materials IAM, Karlsruhe Institute of Technology KIT — [2]Fraunhofer IWM, Freiburg

Multiscale modeling of deformation processes in crystalline materials poses several challenges although the basic physical process, the motion of dislocations, is well understood. I will use the deformation of single crystalline alpha-iron to illustrate these challenges.

To feed dislocation dynamics with realistic atomistic information requires a reliable and computationally efficient description of the atomic interactions. We use a recently developed magnetic bond-order potential (BOP). Dislocation mobility laws for discrete dislocation dynamics (DDD) studies of large dislocation ensembles then require consideration of the full local stress state in a mesoscopic mobility law since it turned out that the effect of non-glide stresses and orientation of the applied loading is crucial for capturing the non-Schmid behavior.

Averaging the behavior of discrete dislocations into continuum mechanical equations is even more difficult. It requires a homogenization of the dislocation fields including a description of their multiplication and mutual interaction. The mathematical framework for such a continuum field theory is still not available. I will present a kinematically consistent continuum description of the dynamics of curved dislocation systems as a first approach to such a continuum field theory.

Invited Talk DY 28.3 Thu 10:30 H1

Crucial Issues and Future Directions of Through-Process Modeling — •Guenter Gottstein — RWTH Aachen University, Institut of Physical Metallurgy and Metal Physics, Aachen, Germany

Computer simulation of materials processing and properties has advanced to an established field and indispensible research topic in materials science and engineering during the past decade. Moreover, it has grown to a powerful and accepted tool for commercial alloy and process development. While the general theory has been laid out, physics based scale-bridging modeling approaches have been developed and are currently employed also in industrial environments, flexible interfacing has become available and automated simulation is currently being tested, there are still bottlenecks that impede the ease of ap-

plication and the predictive power of these tools and urgently need to be addressed. Such needs include reliable experimental databases, the bridging of knowledge gaps on critical phenomena like nucleation, interacting microstructural evolution processes that require vastly different computation times, inverse modeling algorithms etc. Finally, despite of the remarkable advances in available computer power, computer simulation still suffers from too low computational speed to address statistically significant system sizes and to lend itself to process control. More recent concepts will be introduced, in particular in view of the changing philosophy of computer architecture and the increasing availability of massively parallel computing power, which may actually require a departure from conventional and established modeling concepts.

Invited Talk DY 28.4 Thu 11:00 H1
Adaptive Resolution Simulations for Soft Matter: Applications and New Developments — •Kurt Kremer — Max Planck Institute for Polymer Research

The relation between atomistic structure, architecture, molecular weight and material properties is a basic concern of modern soft matter science. A typical additional focus is on surface and interface aspects or the relation between structure and function in nanoscopic molecular assemblies. Here computer simulations on different levels of resolution play an increasingly important role. To progress further, adaptive schemes are being developed, which allow for a free exchange of particles (atoms, molecules) between the different levels of resolution. The lecture will concentrate on these methods to couple particle based simulations. In addition first approaches to connect particle based simulations to continuum as well as to include quantum effects will be presented. Furthermore the extension to open systems MD as well as new recent methodology advances will be explained. A general review on the first part can be found in M. Praprotnik, L. Delle Site, and K. Kremer, Ann. Rev. Phys. Chem. 59, (2008) and recent advances in S. Fritsch et al. Phys. Rev. Lett. 108, 170602 (2012)

Invited Talk DY 28.5 Thu 11:30 H1
Materials by design — •Markus Buehler — MIT, 77 Mass. Ave, Cambridge, MA 02139

Biological materials are synthesized, controlled and used for an astonishing variety of purposes including structural support, force generation, mass transport, catalysis, or energy conversion. By incorporating concepts from biology and engineering, computational modeling has led the way in identifying the core principles that link the molecular structure of biomaterials at scales of nanometers to physiological scales at the level of tissues. The use of the world's fastest supercomputers allows us to predict properties of complex materials from first principles, realized in a multiscale modeling approach that spans massive ranges in scale. Combined with experimental studies, such in silico models allow us to simulate disease, understand catastrophic failure of tissues, and enable us to translate concepts from the living world into material designs that blur the distinction between the living and non-living systems. We discuss challenges and opportunities in new methods of scale bridging.

DY 29: Focus Session: Rayleigh Benard System and Convective Turbulence

It is one of the outstanding problems to understand the interplay between the formation of structured pattern and turbulent disorder. For convective problems these emerging nonlinear structures are dominating the transport properties and they have manifold impact in nature. (Organizers Jörg Schumacher and Joachim Peinke)

Time: Thursday 15:00–17:00 Location: H44

Invited Talk DY 29.1 Thu 15:00 H44
Transitions in rotating Rayleigh-Benard convection at high Rayleigh numbers — •Andreas Tilgner — Institute of Geophysics, University of Göttingen

In geo- and astrophysics, convective flows are mostly studied in rotating frames of reference and are subject to the Coriolis force. Depending on the control parameters, the flow is either well approximated as non-rotating convection, familiar from numerous simulations and experiments, or it is in a rather less well understood regime in which the flow structures and the turbulence are organized by the global rotation of the frame of reference. The question immediately arises at which parameters the transition form rotating to non-rotating flows occurs. This talk will review characteristic features introduced by rotation. Much work has been done on pattern formation in rotating convection near onset. This talk will on the contrary focus on disordered and turbulent flows and explain the criteria separating rotating from non-rotating convection at high Rayleigh numbers.

Invited Talk DY 29.2 Thu 15:30 H44
Connecting Statistics and Dynamics of Turbulent Rayleigh–Bénard Convection — •Johannes Lülff[1], Michael Wilczek[1,2], Rudolf Friedrich[1], Richard Stevens[3,2], Detlef Lohse[3], Klaus Petschel[4], and Ulrich Hansen[4] — [1]Institute for Theoretical Physics, WWU Münster, Germany — [2]Turbulence Research Group, Johns Hopkins University, Baltimore, USA — [3]Physics of Fluids Group, University of Twente, Enschede, Netherlands — [4]Institute for Geophysics, WWU Münster, Germany

Turbulent Rayleigh–Bénard convection as an ubiquitous phenomenon remains in the central interest of scientists and engineers alike. Though major advances from experimental, numerical and theoretical side have been achieved in recent years, there is no full theory of turbulent convection; especially a comprehensive connection between coherent flow patterns, small-scale fluctuations and the statistics has not been established so far.

To tackle this problem, we apply statistical methods to turbulent Rayleigh–Bénard convection, which lead to insights into the dynamics of the system. We investigate from first principles the temperature statistics in the context of PDF equations, which gives rise to the average transport behavior and flow structures in phase space, and also examine the statistics of flow reversals with methods borrowed from the theory of stochastic processes. The methods are applied to data which is provided by different direct numerical simulations that are briefly summarized.

Invited Talk DY 29.3 Thu 16:00 H44
Temperature statistics near the ultimate state of turbulent Rayleigh-Bénard convection * — •Xiaozhou He[1], Dennis van Gils[1], Eberhard Bodenschatz[1], and Guenter Ahlers[1,2] — [1]MPI-DS, Goettingen, Germany — [2]UCSB, USA

We report on the study of temperature statistics in turbulent Rayleigh-Bénard convection (RBC) for Ra up to 10^{15} and for Pr $\simeq$ 0.8. The experiment had been conducted in a pressure vessel known as the "Uboot" of Göttingen with compressed sulfur hexafluoride (SF_6) at a pressure up to 19 bars. We used two upright cylindrical RBC samples with the same diameter $D = 112$ cm but different heights $L = 112$ and 224 cm, corresponding to aspect-ratios $\Gamma \equiv D/L = 1.00$ and 0.50 respectively.

Using the elliptical approximation, we derived local velocities from temperature space-time cross-correlation functions $C_T(r, \tau)$ and found a Gaussian distribution for velocity fluctuations. We also determined an effective Reynolds number in both samples and observed a transition from the classical state to the ultimate state of turbulent RBC[1] near Ra $\simeq 10^{14}$, which agrees with the prediction by GL [2]. Finally, we observed the Kolmogorov $-5/3$ scaling in temperature energy spectra $E(k)$, $E(k) \sim k^{-5/3}$, above Ra $\simeq 10^{14}$ in both samples.

[1] X. He, D. Funfschilling, H. Nobach, E. Bodenschatz and G. Ahlers, Phys. Rev. Lett. **108**, 024502 (2012)
[2] S. Grossmann and D. Lohse, Phys. Rev. E **66**, 016305 (2002)
* Supported by the Max Planck Society, the Volkswagen Stiftung, the DFG SFB963, and NSF grant DMR11-58514.

Invited Talk DY 29.4 Thu 16:30 H44
Cloud formation studies in moist Rayleigh-Benard convection — •Jörg Schumacher — TU Ilmenau, Ilmenau, Germany

Conditionally unstable convection occurs when the stratification is stable for unsaturated air parcels but unstable for saturated air parcels. This leads to the development of isolated convective plumes or clouds which are separated by an extended unsaturated dry environment. Here the statistical behavior of conditionally unstable convection is studied in a model of moist turbulent convection with a simplified thermodynamics of cloudy air. It is closely related to the classical Rayleigh-Benard dry convection problem, but includes phase transitions between the gaseous and liquid phase and the effect of latent heat release on the buoyancy of air parcels. We demonstrate that this simplified model is not only capable to simulate cloud formation processes, but also indicates that the complex dynamics of moist convection results in the emergence of new convective regimes that do not exist in the absence of phase transition. The transition to self-aggregated convection is however highly sensitive to the diffusivity and viscosity used in the model, with the aspect ratio necessary for the transition increasing as the viscosity and diffusivity are decreased. In addition, it is also found that conditionally unstable moist convection is inefficient at transporting energy. We argue that this weak energy transport is tied to the presence of a diffusive layer near the lower boundary, which remains present even when the diffusivity is small. Furthermore, we investigate the impacts of radiative cooling on the self-sustained convective regimes.

DY 30: Quantum Chaos II

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

DY 30.1 Thu 15:00 H47

Edge-independent formation of localized states in manipulated honeycomb lattices — •Pia Adam and Martina Hentschel — Institut für Physik, Technische Universität Ilmenau, Germany

We investigate finite hexagonal lattice systems with different boundary conditions under the influence of strain and local deformations. To this end, we use a tight-binding model including up to third nearest neighbor coupling. This model allows us to describe real graphene as well as honeycomb photonic crystals. First, we study the effect of unidirectional strain by varying the nearest neighbor coupling in one direction. In a microwave realisation of this problem with armchair boundary conditions a phase transition under increasing strain from a gapless to a gapped phase is predicted and observed. Moreover, localized states form at the edges perpendicular to the strain on a hexagon with armchair edges [1]. We confirm these results and, in particular, find them to hold for zigzag edges as well, i.e. to be independent of the edge termination. Furthermore, we investigate the effect of local deformations simulated by locally changing the nearest neighbor interaction. This leads to states which are strongly localized at the sites adjacent to the deformed bonds with energies at the low and high energy flanks of the spectrum rather than near the Dirac point.

[1] M. Bellec, U. Kuhl, G. Montambaux, F. Mortessagne, arXiv:1210.4642 [cond-mat.mes-hall].

DY 30.2 Thu 15:15 H47

Experimental observation of resonance assisted tunneling in systems with a mixed phase space — •Stefan Gehler[1], Steffen Löck[2,3], Ulrich Kuhl[1,4], Hans-Jürgen Stöckmann[1], Susumu Shinohara[5], Arnd Bäcker[2,5], and Roland Ketzmerick[2,5] — [1]Fachbereich Physik, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [3]OncoRay, Technische Universität Dresden, Fetscherstr. 74, 01307 Dresden, Germany — [4]LPMC, CNRS UMR 7336, Université de Nice Sophia-Antipolis, 06108 Nice, France — [5]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany

In quantum mechanical billiards with a mixed phase space tunnelling from regular islands to the chaotic sea can be strongly increased by resonance-assisted tunnelling [1,2]. This occurs due to nonlinear resonances, which cause different regular states to be close in energy. To experimentally verify this theory we designed a cosine-shaped microwave resonator with suitably placed absorbers destroying the resonances of the chaotic sea but not affecting the stable island. Then the tunnelling rate can be determined via the width of the resonances. Our experimental results are in agreement with theoretical predictions.

[1] O. Brodier, P. Schlagheck, D. Ullmo, Phys. Rev. Lett. 87, 064101 (2001).
[2] S. Löck et al., Phys. Rev. Lett. 104, 114101 (2010).

DY 30.3 Thu 15:30 H47

Quantum Goos-Haenchen effect on wave-packet dynamics — •Soo-Young Lee — Max Planck Institute for the Physics of Complex Systems, Dresden

When an optical beam is totally reflected from a dielectric interface, there exists some lateral shift of the reflected beam from the incident point of the beam, this is called Goos-Haenchen (G-H) shift. This comes from the angle-dependent phase loss appearing upon the total internal reflection.The G-H effect can be also found in quantum mechanical problems. We study the quantum G-H effect in step-potential problem and normal/superconductor (NS) interface. In particular, we focus on how the G-H effect changes wave-packet dynamics in the various interfaces. It turns out that the G-H effect in the NS interface is amplified by the ratio between Fermi energy and the pair gap, and it gives only time delay without any lateral shift.

DY 30.4 Thu 15:45 H47

Are Fresnel filtering and the angular Goos-Hänchen shift the same? — •Jörg Götte[1], Susumu Shinohara[2], and Martina Hentschel[3] — [1]Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, D-01187 Dresden, Germany — [2]NTT Communication Science Laboratories, NTT Corporation, 2-4 Hikaridai, Seika-cho, Soraku-gun, Kyoto 619-0237, Japan — [3]Technische Universität Ilmenau, Institut für Physik, Weimarer Str. 25, D-98693 Ilmenau, Germany

In dielectric billiards ray dynamics have to be amended to account for wave effects, such as the spatial Goos-Hänchen shift. This shift is a small displacement upon transmission or reflection of a light beam of finite width. The idea is to change the reflection coefficients for rays to include wave phenomena in an effective way.

These wave phenomena not only alter the dynamics in the spatial domain, but also in the angular domain. Two effects are known in the literature, Fresnel filtering and the angular Goos-Hänchen shift, which both cause a deflection of the light beam with respect to Snell's law or the law of reflection.. This raises the question which of these two effects is more important for an improved ray-wave correspondence.

We approach this question by highlighting the similarities and differences between the two effects and study the dynamical currents of the optical field upon reflection and transmission.

DY 30.5 Thu 16:00 H47

On the fractal dimension spectrum of open chaotic systems — •Moritz Schönwetter[1], Orestis Georgiou[2], and Eduardo Altmann[1] — [1]MPIPKS, Dresden — [2]Toshiba Research Europe Limited, Bristol, England

Wave and quantum properties of open systems are nowadays understood in terms of the invariant sets of their classically chaotic counterparts as for example in the fractal Weyl law connecting the asymptotic resonance density with the fractal dimension of the classical repeller. In this talk we introduce an efficient and accurate algorithm to numerically compute the full spectrum of Renyi-dimensions (D_q), and use it to investigate physically relevant classes of Hamiltonian systems exhibiting interesting D_q: (i) systems with a non-hyperbolic component, in which case we argue that the dimensions should be considered scale-dependent and the dynamics characterized by effective dimensions; and (ii) open systems in which trajectories are only partially reflected in a region of the boundary and which exhibit a non-constant D_q spectrum (multifractals).

DY 31: Anomalous Diffusion

Time: Thursday 15:00–16:45 Location: H48

DY 31.1 Thu 15:00 H48

A self-consistent theory for the localization transition in the Lorentz model — •Simon Lang[1], Teresa Behl[2], Felix Höfling[3], and Thomas Franosch[1] — [1]Institut für Theoretische Physik, Erlangen-Nürnberg — [2]Fakultät für Physik, LMU München — [3]Institut für Theoretische Physik IV, Universität Stuttgart; MPI für Intelligente Systeme, Stuttgart

The reference system for transport in porous media is the Lorentz model, which mimics the dynamics of a particle in a heterogeneous environment of obstacles randomly distributed in space. For a tracer particle obeying brownian repeated collisions with a single obstacle is sufficient to explain the persistent correlations. Therefore for brownian motion the low-density expansion already reveals the onset of long-time tails for the velocity-auto-correlation function (VACF) in next to leading order in density [1]. Here, we use the results of the low-density approximation to formulate a self-consistent theory for the VACF for brownian dynamics of a tracer particle in two dimensions. For low densities, the theory reduces to the exact expansion of Ref. [1], for higher density a consistent diffusion-localization transition is predicted at an obstacle density, which is close to the percolation threshold found for simulations in two dimensions. We find asymptotic scaling laws in the VACF, which are persistent as one approaches the localization transition, as well as long-time tails within the diffusive regime originating from repeated scattering processes.

[1] T. Franosch, F. Höfling, T. Bauer and E. Frey J. Chem. Phys. 375 (2010).

DY 31.2 Thu 15:15 H48

Subdiffusive exciton motion in systems with heavy-tailed disorder — •Sebastiaan M. Vlaming[1,2,3], Alexander Eisfeld[1], Victor A. Malyshev[2], and Jasper Knoester[2] — [1]Max Planck Institute for Physics of Complex Systems, Dresden, Germany — [2]University of Groningen, Groningen, The Netherlands — [3]Massachusetts Institute of Technology, Cambridge, USA

The optical and excitation transport properties of many systems, such as molecular aggregates, photosynthetic complexes and organic photovoltaics, are determined by the collective properties of the relevant excitations, which are strongly influenced by interactions with their environment. In modeling the behavior of these collective excitations in a disordered environment, one conventionally often considers model parameters as stochastic quantities with Gaussian distributions. However, it has been suggested [1] that the limitation to Gaussian distributions is not necessarily the best choice, and novel effects such as exchange broadening and anomalous exciton localization have been shown to be possible when generalizing to the wider class of Lévy distributions. In this study, we investigate the excitation dynamics in such Lévy disordered systems, where we consider molecular aggregates as a model system. It is shown that the exciton dynamics changes qualitatively when generalizing to Lévy disorder distributions, leading to sub-diffusive (i.e. less mobile than diffusive) behavior of the exciton transport.

[1] AE, SMV, VAM, and JK, Phys. Rev. Lett. 105, 137402 (2010) [2] SMV, AE, VAM, and JK, to be submitted

DY 31.3 Thu 15:30 H48

Spatial-temporal velocity autocorrelation function for random walks. — •Vasily Zaburdaev[1], Sergey Denisov[2], and Peter Hänggi[2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Institute of Physics, Augsburg University, Augsburg, Germany

In this work we borrow the concept of spatial-temporal velocity autocorrelation function from the worlds of many-particle systems and fluid dynamics and adopt it for continuous-time random walks. Assuming that at any instant of time a diffusing particle has a well-defined velocity, we pose a question whether it is possible for the particle to remember its initial velocity at some later time and some distance from the starting point. Results are already remarkable for the regime of standard diffusion and exhibit even more rich behavior as diffusion becomes anomalous. We show that for normal diffusion and superdiffusion regimes with sub-ballistic scaling, spatial-temporal velocity autocorrelation function is equivalent to the time derivative of the particle density. As diffusion becomes faster, correlations decay slower in time and might become comparable to the density itself. It is the coupling of displacement and time via a random walker's velocity that makes a particle to remember its initial velocity far away from the starting point. Spatial-temporal velocity autocorrelation function is an extension of the conventional temporal correlation function for a single particle process and, therefore, provides a new insight into the complex transport phenomena that should find its application in various real world systems.

DY 31.4 Thu 15:45 H48

Distinguishing Between Different Subdiffusive Scenarios. — •Felix Thiel and Igor Sokolov — Institut für Physik der Humboldt-Universität zu Berlin, Deutschland

Subdiffusion can be observed in many theoretical and experimental situations, for instance with proteins diffusing in biological cells or with ion channels moving on the cell membrane. Although one may often be sure, that the process is truly subdiffusive, it is not always clear which physical mechanisms give rise to this behaviour. In particular it is necessary to develop techniques that seperate ergodic and non-ergodic (f.e. ageing) parts of such a process. In this talk, we want to present a quantity, suitable for disorder induced subdiffusion, which is sensitive on the kind of disorder, i.e. structural or energetic disorder. We will present some easy theoretical predictions for this so called fundamental exponent and apply it to some pet models.

DY 31.5 Thu 16:00 H48

Anomalous diffusion in two- and three-dimensional polymer melts — •Hendrik Meyer, Jean Farago, and A.N. Semenov — Intitut Charles Sadron, CNRS UPR22, 67034 Strasbourg, France

Polymers in the melt are known to exhibit subdiffusive monomer dynamics which, for unentangled chains, is well described by the Rouse model. Experiments and simulations have shown that the center of mass of a chain exhibits also subdiffusive behavior, a feature which is not contained in the Rouse model. This feature found recently an unexpected explanation: hydrodynamic interactions are still present in polymer melts and their combination with the viscoelastic properties of the melt explain the observed behavior [1]: there is a short superdiffusive regime followed by subdiffusion until the chain relaxation time. We have now developed the theory of visco-hydrodynamic interactions (VHI) for two-dimensional melts where the superdiffusive regime is strongly enhanced. The theory also takes into account finite-box size effects which strongly modify two-dimensional simulation data. This leads to complex anomalous dynamics which cannot be described by simple power laws [2].

J. Farago et al. Phys. Rev. Lett. **107**, 178301 (2011); PRE **85**, 051806 (2012); H. Meyer and A.N. Semenov, Phys. Rev. Lett. accepted (2012).

DY 31.6 Thu 16:15 H48

Geometric properties of continuous time random walks — •Mirko Lukovic, Theo Geisel, and Stephan Eule — MPI for Dynamics and Self-organization, Goettingen, Germany

We investigate the geometric properties of two-dimensional continuous time random walks. In particular, we determine analytical expressions for the time-evolution of the average perimeter and area of convex hulls of non-Markovian processes such as subordinated random walks and Lévy flights. A convex hull is the minimum convex polygon enclosing a set of monitored points and it proves to be very useful when it comes to estimating the home-range of foraging animals.

DY 31.7 Thu 16:30 H48

Oriented Particles in Porous Media — •Prehl Janett[1], Haber René[1,2], Hoffmann Karl Heinz[1], and Herrmann Heiko[2] — [1]TU Chemnitz, Institut für Physik, Chemnitz, Deutschland — [2]Center for Nonlinear Studies, Institute of Cybernetics at Tallinn University of Technology, Tallinn, Estonia

Diffusion in porous media is a long studied topic. The usual modeling applies point particles without any structure. In this presentation we introduce particles, exhibiting a spatial extension and an orientation, that diffuse in porous media represented by a Sierpinski carpet model. Due to the properties of the applied particles, they interact with their surrounding, i.e. they might get stuck in parts of the structure. There-

fore we modeled a new move class for oriented particles based on the blind ant algorithm. We present the obtained result and we discuss the following upcoming questions: How do the oriented particles move within the porous media? Does the transport of these particles follow the same laws as point particles do? If there are differences, are these only local effects or can they also be observed in the over all behavior? Do we obtain different exponents for the mean squared displacement (MSD) or do we even get a new functional dependence for the MSD?

DY 32: Statistical Physics in Biological Systems III (joint with BP)

Time: Thursday 15:00–17:30 Location: H46

DY 32.1 Thu 15:00 H46

On the Fourier spectra of fitness Landscapes — •Johannes Neidhart, Ivan Szendro, and Joachim Krug — Institut für Theoretische Physik, Universität zu Köln, Deutschland

Fitness Landscapes are a well established tool in the analysis of evolutionary precesses. In order to extract important information, graph theoretical Fourier decomposition has proven to be very useful. In order to compare experimental data with stochastic models, we analyse several models, amongst others Kauffmann's LK model and present exact results for the Fourier spectra as well as a comparison to experimental data.

DY 32.2 Thu 15:15 H46

On the existence of accessible paths in trees — •Stefan Nowak and Joachim Krug — Institute for Theoretical Physics, University of Cologne

The study of accessible paths is a new type of percolation problem which is inspired by evolutionary biology. To each node of the underlying graph a random number is assigned and a path through the graph is called accessible if all random numbers along the path are in ascending order. We will give an exact expression for the second moment of the number of accessible paths from the root to the leafs in n-trees and an asymptotic expression for the probability that there is at least one accessible path. Furthermore, we will show that there is a percolation threshold if the random variables are Gumbel distributed and a linear drift is added.

DY 32.3 Thu 15:30 H46

A new evolutionary food web model — •Korinna T. Allhoff[1], Daniel Ritterskamp[2], Christian Guill[3], and Björn C. Rall[3] — [1]Institute of Condensed Matter Physics, TU Darmstadt — [2]Institute for Chemistry and Biology of the Marine Environment, Carl von Ossietzky University of Oldenburg — [3]J. F. Blumenbach Institute for Zoology and Anthropology, Georg-August-University Göttingen

Understanding the conditions that are required for complex ecosystems to persist despite changes in species composition and anthropogenic perturbations, is of utmost importance in order to conserve these systems. Evolutionary food web models provide a mechanistic tool to understand how complex ecosystems emerge and how they react to changes in their composition. We present such an evolutionary food web model, where each species is characterized by three key traits: its own body mass, its preferred prey body mass, and the width of its potential prey body mass spectrum. The model contains allometric effects on feeding and competition interactions and determines dynamically whether a species is viable or goes extinct. The evolutionary processes that enable new species to enter the system as mutants of already existent ones, also follow allometric rules. The food web structure emerges as a highly nontrivial result from the combined effect of population dynamics and evolution. We present computer simulations of different model modifications and show how they influence network structure and stability.

DY 32.4 Thu 15:45 H46

The influence of chaos on the stability of small food webs — •Fanny Groll and Alexander Altland — Institut für Theoretische Physik, Universität zu Köln, Germany

Ecological networks can show different types of dynamics. Experiments have demonstrated that they can actually be governed by deterministic chaos. In that case the population numbers evolve along a chaotic attractor; they show large fluctuations but do not go extinct.

We examine a mathematical model of a simple food web consisting of two prey and one predator population. In this model a control parameter triggers the onset of chaos via bifurcation. Such dynamics have already been observed in an aquatic system of few competing species.

In studying this system we aim to find a catalogue of techniques to approach such a system and to analyze its features. Starting from a general master equation approach we have explored routes to chaos in few-species ecological systems. Emphasis has been put on the mechanisms leading to chaotic attractors. Under ambient conditions ecological systems are subject to demographic and environmental fluctuations. We explore the stability and persistence of populations in chaotic regimes compared to more regular types of dynamics.

DY 32.5 Thu 16:00 H46

The effect of migration between patches on the stability of foodwebs — •Sebastian Plitzko and Barbara Drossel — Institut für Festkörperphysik, TU Darmstadt, Germany

During recent years, several factors that stabilize food webs have been identified. Among these are allometric scaling of metabolism with body size and adaptive foraging. So far, food web models rarely take space into account. However, it is known that being distributed over several spatial patches can have positive as well as negative effects on the stability of metacommunities.

Using computer simulations for the population dynamics of systems with many species, we investigate the stability of food webs that are distributed over several patches that are connected by migration. We evaluate species persistence in dependence of food-web complexity, patch arrangement, and migration rule. In particular, we study conditions under which migration alone, without the above-mentioned additional stabilizing factors, can increase food-web stability. We also determine whether food webs that already have a high stability can gain further by being distributed over several patches.

DY 32.6 Thu 16:15 H46

The effect of predator limitation on the dynamics of simple food chains — •Christoph Schmitt[1], Stefan Schulz[1], Jonas Braun[1], Christian Guill[2], and Barbara Drossel[1] — [1]Physics Department, TU Darmstadt — [2]Institute for Zoology and Anthropology, University of Göttingen

We investigate the influence of competition between predators on the dynamics of predator-prey systems and of tritrophic food chains. Competition between predators is implemented either as interference competition, or as a density-dependent mortality rate.

With interference competition, the paradox of enrichment is reduced or completely suppressed, but otherwise the dynamical behavior of the system is not fundamentally different from that of the Rosenzweig-MacArthur model, which contains no predator competition.

In contrast, with density-dependent predator mortality the predator-prey system shows a surprisingly rich dynamical behavior. In particular, decreasing the density regulation of the predator can induce catastrophic shifts from a stable fixed point to a large oscillation. Furthermore, the model shows several other types of nonlocal bifurcations, the coexistence of several attractors, and different types of regime shifts. In tritrophic food chains chaos can occur in both models.

DY 32.7 Thu 16:30 H46

Score statistics of multiple sequence alignments — •Pascal Fieth and Alexander K. Hartmann — Institute of Physics, University of Oldenburg

Optimally aligned sequences of amino acids [1] can be studied numerically [2] in the biologically relevant high scoring region by means of parallel tempering simulations [3]. Preceding studies have shown that the scores of gapped pairwise sequence alignments of finite-length sequences follow a Gumbel extreme value distribution, modified by a Gaussian correction [4] rather than a simple Gumbel extreme value distribution as previously predicted for ungapped pairwise alignments. In this study these methods are applied to the case of multiple sequence alignment (MSA). Here the distributions of the sum-of-pair scores of the MSA of more than two sequences are studied. In particular the distribution of protein MSA-scores using different common substitution

matrices (BLOSUM and PAM) are analysed for protein background frequencies of real sequences.

[1] R. Durbin et al., *Biological sequence analysis*, (Cambridge University Press, 1998)
[2] A.K. Hartmann, *Practical Guide to Computer Simulations*, (World Scientific, 2009)
[3] A.K. Hartmann and Heiko Rieger, *Optimization Algorithms in Physics*, (Wiley-VCH, 2001)
[4] S. Wolfsheimer et al., *Local Sequence Alignments Statistics: Deviations from the Gumbel Statistics in the Rare-Event Tail*, (Algorithms for Molecular Biology, 2007)

DY 32.8 Thu 16:45 H46

Understanding evolutionary conserved contacts by structure based models. — •Abhinav Verma[1], Benjamin Lutz[1], Martin Weigt[2], and Alexander Schug[1] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Université Pierre et Marie Curie, Paris, France

The evolution of a protein family leaves a fingerprint in databases of protein sequences. In a recent study, Direct Coupling Analysis (DCA) has been shown to accurately identify co-evolving residue pairs preserved as spatial contacts in their three dimensional fold [1]. Such DCA-derived contacts can be combined with molecular dynamics simulations to predict experimentally inaccessible transiently occupied active states [2]. Only a fraction of a contact map, however, is identified by DCA. Here we attempt to understand the evolutionary constraints leading to the conservation of these specific contacts by native structure based models [3]. We compare simulations with DCA derived contact maps to randomly chosen subsets of contacts.[unpublished data]

[1] Marcos et. al. , PNAS, 2011, 108, E1293
[2] Dago et. al. , PNAS, 2012, 109, E1733
[3] Whitford et al. Proteins, 2009 75, 430

DY 32.9 Thu 17:00 H46

Symmetry Breaking of Sequence Information in Catalytic Polymer Soups — •Shoichi Toyabe and Dieter Braun — Systems Biophysics,Ludwig-Maximilians-University Munich, Munich

One of the most distinguished properties of living systems is that they sustain genetic information and reproduce it. However, its origin remains elusive; how can information emerge in the chaotic molecular soup in the prebiotic earth? We discuss models and preliminary experiments to show the emergence of order in a catalytic polymer solution. We argue that template-directed copolymerization of diverse polymers is a promising route. Autocatalytic copolymerization extends polymers stochastically. Interestingly, a numerical simulation shows that the polymers self-organize into an ordered state where a stochastically chosen small set of sequence motifs become dominant. This spontaneous symmetry breaking occurs because autocatalytic chain reactions in the reaction network interact competitively and amplify strands beyond exponential growth. This amplifies spontaneous fluctuations and sustains it by Darwinian selection against other sequences. The transition to the ordered state is accompanied by a population inversion, i.e. the length distribution of polymers was biased to the longer side at the ordered state. In order to demonstrate the symmetry breaking by experiments, we performed ligase chain reactions of DNA strands with semi-random sequences. Under nonequilibrium driving of material flux and temperature cycles, we observed a population inversion, which implies the breaking of the symmetry. Furthermore, we analyzed the sequences to confirm the symmetry breaking by on the basis of PCR.

DY 32.10 Thu 17:15 H46

Characteristics of the formation of oligomers in a primordial broth — •Sabrina Scherer — Biologische Experimentalphysik, Universität des Saarlandes

We analyse the energetically driven emergence of spontaneous and dynamic states of order in prebiotic, complex systems. We perform Miller-Urey-type experiments: simple anorganic molecules driven by electric discharges and form complex, organic reaction mixtures. The process is analysed by real-time mass spectroscopy. The spectra reveal the formation of a time-dependent order of molecules in the reaction mixture. The peak intensities of several oligomeric molecules oscillate over time. Some oligomers vanish after their first occurence to reform again later. The increase and decrease of these intensities follow exponential and sigmoid courses. This points towards autocatalytic processes. In contrast to the original Miller-Urey-experiment which consists of the constituents methane, ammonia, hydrogen and water, we add other biologically relevant elements like phosphor and sulfur to observe their influence on the stability of the oligomer oscillations.

DY 33: Poster II

Poster contributions from Session Stat. physics far from equilibrium; soft matter, pattern formation, Stat physics general; granular matter; Quantum chaos; Critical phenomena; Fluid Dyn / Rayleigh Benard; Anomalous diffusion; Brownian motion.

Time: Thursday 17:00–19:00 Location: Poster C

DY 33.1 Thu 17:00 Poster C

Efficiency of a Brownian information machine — •Michael Bauer, David Abreu, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

The second law of thermodynamics forbids cyclic engines that extract work from a single heat bath when there is no other interaction with the surrounding medium. By making a gedankenexperiment with a Maxwell demon it became clear that with additional information on the system one can indeed extract work.

We investigate two types of an engine modelled by a Brownian particle in a time dependent harmonic trap [1]. In every cycle we perform a measurement with finite precision before we apply a feedback scheme which depends on the measurement outcome. Since the machine operates at finite time the distribution will not be in equilibrium after the measurement. Hence in every cycle the work will depend on all measurements before. We calculate analytically the average work in the steady state for a large number of cycles. To define a efficiency we calculate the information extracted from on the system by the measurements. In the first type of this engine only the center of the potential moves. Here, one extracts $1/2\ k_BT$ in a quasistatic case with perfect measurements. The maximal power is $1/2$ for short cycle periods but then the efficiency goes to zero. In the second variant, additionally the strength of the potential changes which leads to efficiency 1 for precise measurements in finite time.

[1] M. Bauer, D. Abreu and U. Seifert. J. Phys. A: Math. Theor. 45, 162001 (2012).

DY 33.2 Thu 17:00 Poster C

Brownian dynamics simulations of colloidal assemblies on structured substrates — •Aleksandar Mijailović and Michael Schmiedeberg — Institut für Theoretische Physik 2, Heinrich-Heine-Universität Düsseldorf, Germany

We perform Brownian dynamics simulation in order to investigate colloidal structure formation on incommensurate substrates. We study the growth process of colloidal rims and islands that can be observed on stretched substrates. Furthermore, we want to explore the dynamics of rearrangements that occur in readily grown structures when the geometry of the substrate is changed.

DY 33.3 Thu 17:00 Poster C

Diffusion in inhomogeneous environments — Johannes Müller[1,2] and •Markus Rauscher[1,2] — [1]Max-Planck-Institut für Intelligente Systeme, Stuttgart — [2]Institut für Theoretische Physik IV, Universität Stuttgart

In the vicinity of walls the mobility of colloidal particles depends on the distance from the wall. As a consequence, the noise in the Langevin equation describing the overdamped Brownian dynamics is multiplicative and therefore ill defined. The correct stochastic calculus is determined by equilibrium statistical physics: it is the Klimontovich calculus. However, the underdamped Brownian dynamics is well defined.

We investigate the overdamped limit in the framework of adiabatic elemination and we present a formal solution of the underdamped Langevin equation which allows to perform the overdamped limit on the level of the Kramers-Moyal coefficients.

DY 33.4 Thu 17:00 Poster C

Ratchet effects in magnetic colloidal suspensions — •Teresa Reinhard and Sabine H. L. Klapp — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

We consider a system of dipolar colloids driven by an oscillating magnetic field. Specifically, the regarded field is lacking net rotating components and puts the system in an out-of-equilibrium state. In such a nonequilibrium system the microscopic Brownian motion can result in directed rotational macroscopic motions [1]. This process, which is called the ratchet effect, is analysed on the basis of the dynamical density functional theory. Specifically, we investigate the impact of a dipole-dipole interaction and compare our results with those from a mean-field Fokker-Planck approach [2] and from particle-based computer simulations [3].

[1] A. Engel and P. Reimann, Phys. Rev. Let. 91, 060602 (2003).
[2] V. Becker and A. Engel Phys. Rev. E 75, 031118 (2007).
[3] S. Jäger and S. H. L. Klapp, submitted, arXiv:1210.3479 (2012).

DY 33.5 Thu 17:00 Poster C

Weak ergodicity breaking and ageing in subdiffusive continuous time random walks analyzed with the distribution of generalized diffusivities — •Tony Albers and Günter Radons — Chemnitz University of Technology, Germany

We investigate the continuous time random walk (CTRW) model with an algebraically decaying waiting time distribution which does not have a finite first moment. This subdiffusive process is known to show interesting phenomena such as weak ergodicity breaking and ageing. As a consequence, ensemble- and time-averaged quantities do not coincide, time averages become random variables, and statistical quantities depend on the elapsed time between the start of the process and the start of the measurement. In this contribution we are going to introduce a new analysis tool for anomalous diffusion, the distribution of generalized diffusivities, which describes the fluctuations during the diffusion process around the generalized diffusion coefficient that can be obtained from the asymptotic behavior of the conventionally investigated mean squared displacement. How this analysis can be used to identify subdiffusive CTRWs in the experiment and how it leads to a deeper understanding of weak ergodicity breaking and ageing will be shown.

DY 33.6 Thu 17:00 Poster C

Selforganization of magnetic particles and biotechnological applications — Claus Fütterer[1,2] and •Florian Rämisch[1] — [1]Fakultät für Physik und Geowissenschaften, In- stitut für Experimentelle Physik I, Universität Leipzig, 04103 Leipzig, Germany — [2]Translationszentrum für Regenerative Medizin (TRM), Universität Leipzig

Superparamagnetic nanoparticles are widely applied in separation technologies, however, their collective behaviour in magnetic fields is poorly understood. We fill this gap by investigating the pattern formation due to magnetic non-linear interactions between spherical particles in static and dynamic homogeneous fields. The interplay between thermal fluctuations, magnetic attraction and repulsion as well as hydrodynamic friction yield a wealth of surprizing and interesting patterns. Our work is mainly experimental but we propose some theoretical ideas as well. Last but not least we explain some biotechnological applications of our results.

DY 33.7 Thu 17:00 Poster C

Orientational order in confined Janus fluid — •Vinothkumar Mohanakrishnan[1] and Martin Schoen[1,2] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Straβe des 17. Juni 135, D-10623 Berlin, Germany — [2]Department of Chemical and Biomolecular Engineering, North Carolina State University, 911 Partners Way, Raleigh, North Carolina 27695, USA

In this study we report, Monte Carlo simulation of Janus fluid confined to a nanoscopic slit pore with an anchoring function planar to the slit pore, where the walls of the slit pore are structureless and non-conducting. The confined system is simulated in the specialized (N,L_z,$P_{||}$,T) isostress-isostrain ensemble. We analyzed the special case of wall separation $L_z = 8\sigma$ in detail where the confined system exhibit spontaneous phase transition from isotropic to polar phase in the pressure range of $1.2 \sim 1.4$. We have computed the density profiles, local dipolar order parameter, in-plane correlation functions at different pressures corresponding to isotropic and polar phases respectively. From the analysis of density profiles, the polar phase is characterized by an additional layer formation (8 layers) as compared to that of the isotropic phase(7 layers). The in-plane correlation function reveals fluid-like behaviour for all the pressure/densities considered. Comparison with the bulk system has been made to study the effect of confinement.

DY 33.8 Thu 17:00 Poster C

Delaying motion in an one-dimensional colloidal system by feedback control — •Sarah Loos, Robert Gernert, and Sabine H. L. Klapp — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

Using feedback control we manipulate the Brownian motion of a colloid in an external tilted sinusoidal potential in one dimension. The mean-squared-displacement (MSD) of the overdamped particle shows a plateau [1], [2]. To stretch this plateau we introduce a feedback control force, where the first moment of the probability density serves as the control target. Preliminary results suggest that this causes a second plateau. We investigate the system by numerically solving the Fokker-Planck-Equation. We further develop a time delayed feedback control as another method to stretch the MSD.

[1] Cecile Dalle-Ferrier, Matthias Krüger, Richard D. L. Hanes, Stefan Walta, Matthew C. Jenkins and Stefan U. Egelhaaf, Soft Matter 7, 2064 (2011)
[2] Clive Emary, Robert Gernert, Sabine H. L. Klapp, arXiv:1209.1504 [cond-mat.stat-mech] (2012)

DY 33.9 Thu 17:00 Poster C

Pore scale modelling of porous media — •Andreas Lemmer and Rudolf Hilfer — Institut für Computerphysik, Universität Stuttgart,70569 Stuttgart, Deutschland

Flow and transport through geological, biological and industrial porous media typically involve multiple length and/or time scales. However, experimental approaches for structural analysis like microcomputertomography are limited in problem size or resolution. Based on a continuum model for porous media[1], we discretize three-dimensional laboratory sized images of porous stones at multiple resolutions[2]. Calculating and analyzing resolution dependent geometric and transport parameters allows quantitative validation of different theoretical approaches and comparison with experiment.

[1] B. Biswal, P.E. Øren, R. Held, S. Bakke, R. Hilfer: Stochastic Multiscale Model for Carbonate Rocks, Phys.Rev.E, 75, 061303 (2007)
[2] R. Hilfer, T. Zauner: High-precision synthetic computed tomography of reconstructed porous media, Phys.Rev.E, 84, 062301 (2011)

DY 33.10 Thu 17:00 Poster C

Generalized theory for multiphase flow in porous media — Oliver Hönig, •Rouven Steinle, and Rudolf Hilfer — Institut für Computerphysik, Universität Stuttgart, 70569 Stuttgart, Deutschland

We study multiphase flow processes, including imbibition and drainage processes, in porous media on macroscopic scales to resolve the shortcomings of the traditional theory. The equations of the fluid percolation model [1] are transformed into a dynamical system with immobile nonpercolating fluid phases. This dynamical system is investigated analytically and numerically. Various classes of travelling wave solutions have been found [2].

[1] R. Hilfer, *Macroscopic capillarity without a constitutive capillary pressure function*, Physica A, vol. 371, pp. 209, (2006)
[2] O. Hönig, F. Doster, R. Hilfer, *Travelling wave solutions in a generalized theory for macroscopic capillarity*, in preparation

DY 33.11 Thu 17:00 Poster C

Residual saturation dynamics and hysteresis in two-phase flow — •Rouven Steinle and Rudolf Hilfer — Institut für Computerphysik, Universität Stuttgart, 70569 Stuttgart, Deutschland

The concepts of relative permeability and capillary pressure are crucial for the accepted traditional theory of two phase flow in porous media. A generalization of the traditional theory does not require these concepts as input [1]. The presentation will describe this novel approach. It allows to predict residual saturations and local spatiotem-

poral changes between imbibition and drainage during two phase immiscible displacement. The Riemann problem for the hyperbolic limit is solved analytically in one dimension by the method of characteristics [2]. Shock fronts and rarefaction waves in both directions in the percolating and the nonpercolating fluids are found, which can be compared directly to experiment [2].

[1] R. Hilfer, *Macroscopic capillarity without a constitutive capillary pressure function*, Physica A, vol. 371, pp. 209, (2006)
[2] F. Doster and R. Hilfer, *Generalized Buckley-Leverett theory for two-phase flow in porous media*, New Journal of Physics, vol. 13, pp. 123030, (2011)

DY 33.12 Thu 17:00 Poster C

Dynamic scaling of a critical binary mixture — Dipanjan Chakraborty, •Felix Höfling, and Siegfried Dietrich — Max Planck Institute for Intelligent Systems, Stuttgart, andInstitute for Theoretical Physics IV, Universität Stuttgart, Germany

A binary mixture near its consolute point exhibits critical fluctuations of the local composition. The static properties of the mixture are well described by the Ising universality class in three dimensions [1], the dynamic properties involving conservation of particles, energy, and momentum are classified as "model H". So far, theoretical work on the critical dynamics has focused mainly on transport coefficients, while studies of the relaxation dynamics of the spatially resolved order parameter have remained elusive.

We present numerical results for the dynamic structure factor of a symmetric binary Lennard-Jones mixture near its demixing transition. To this end, we have performed extensive molecular dynamics simulations in the microcanonical ensemble, employing the immense computing resources of high-end graphics processors [2]. Our simulations cover large systems of 70,000 particles and more than 4 non-trivial orders of magnitude in time. We explore the crossover of the wavenumber-dependent relaxation time from diffusion-like to critical behaviour and find nice agreement with theoretical predictions. Further, dynamic scaling of the full time dependence of the critical relaxation is tested and dynamic scaling functions are deduced.

[1] S. K. Das *et al.*, J. Chem. Phys. **125**, 024506 (2006)
[2] P. Colberg and F. Höfling, Comp. Phys. Comm. **182**, 1120 (2011)

DY 33.13 Thu 17:00 Poster C

Shear banding in drying colloidal dispersions — •Pree-cha Kiatkirakajorn and Lucas Goehring — Max Planck Institute for Dynamics and Self-Organization, Bunsenstrasse 10, D-37075 Göttingen, Germany

During drying, colloidal dispersions undergo complex transformations such as solidification, buckling, cracking and the draining of liquid from pores. These interesting observations suggest how defects and shear localization can arise during the drying of colloidal dispersions. During this process, series of bands appear rapidly behind the solidification front and propagate away from the drying front +/-45°. The emergence of bands have never been explained, although we suggest that these may be the result of shear banding. Here we experimentally show that, during drying, particles of polystyrene dispersion are forced closer to each other so that it crystallizes into a weak solid at some critical volume fraction. Furthermore, solidification is caused by electrostatic charge and Van der Waals force. As this weak solid is further compressed, it responds to the stress during solidification by forming a herringbone pattern of parallel light and dark stripes which can be observed and measured under a microscope. We have measured the film thickness, drying rate, and the band spacing under different drying conditions and salt concentrations, which affect the magnitude of the electrostatic interaction.

DY 33.14 Thu 17:00 Poster C

Colloidal Structures on Quasicrystalline Substrates — •Matthias Sandbrink and Michael Schmiedeberg — Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine-Universität, Düsseldorf

Quasicrystals are structures with long-range order but no periodicity. Therefore, quasicrystals may possess rotational symmetries and other physical properties that cannot occur in conventional periodic crystals. We explore how three-dimensional quasicrystals consisting of monodisperse colloidal particles grow on a substrate. The geometry of the substrate is designed with quasicrystalline symmetry from aperiodic tilings, interference patterns, or Fourier expansions and may contain point defects. By using Monte-Carlo simulations, we study the colloidal structures on the quasicrystalline substrates and investigate the influence of defects on the growth process.

DY 33.15 Thu 17:00 Poster C

Crystallization of Charged Macromolecules using FRESHS — •Kai Kratzer[1], Joshua T. Berryman[2], Rosalind J. Allen[3], and Axel Arnold[1] — [1]Institute for Computational Physics, University of Stuttgart — [2]Theory of Soft Condensed Matter, University of Luxembourg — [3]SUPA, School of Physics, University of Edinburgh

The crystallization of charged macromolecules has a number of important applications in fields such as biology, pharmacology or materials design. For example, proteins are crystallized for purification or structure determination and colloidal crystals are promising candidates for photonic crystals. However, the crystallization of proteins or colloids is still more an art rather than a technique due to the poor understanding of the underlying physical mechanisms. Experimental investigation of nucleation is extremely difficult, which can be facilitated by computer simulations. Since the nucleation of charged macromolecules is a rare event, it is inaccessible to brute force computer simulations and requires special simulation techniques, such as Forward Flux Sampling (FFS). We present our highly efficient FFS implementation FRESHS, the flexible rare event sampling harness system, which allows for massively parallel rare event sampling using conventional Molecular Dynamics codes such as ESPResSo or GROMACS. It features a novel automatic interface placement optimization, so that efficient FFS simulations no longer require expert knowledge. As an example application, we present first results on the nucleation in systems of charged macromolecules with screened Coulomb interactions, a system, that without using FRESHS would have been very challenging to investigate.

DY 33.16 Thu 17:00 Poster C

Form factors of comb polymers — •Christian von Ferber[1], Marvin Bishop[2], Thomas Forzaglia[2], and Cooper Reid[2] — [1]Applied Mathematics Research Centre, Coventry University, UK — [2]Manhattan College, Riverdale, New York, USA

We employ analytical methods and the Monte Carlo Pivot algorithm to investigate continuum, tangent hard-sphere comb polymers both in the ideal and excluded volume regimes.

The mean square radius of gyration, the g-ratio, and the form factors are evaluated. We find that the extrapolated MC g-ratios are in excellent agreement with the theory in the ideal regime. The MC data agree well with the exact form factors. The form factors reveal the influence of the polymer structure at short distances.

DY 33.17 Thu 17:00 Poster C

Excess entropy scaling of viscosity and diffusivity of model polymeric systems — •Evangelos Voyiatzis, Florian Müller-Plathe, and Michael Böhm — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, Technische Universität Darmstadt, Petersenstrasse 22, D-64287 Darmstadt, Germany

The range of validity of empirical excess entropy scalings for diffusivity and viscosity as proposed independently by Rosenfeld and Dzugutov is tested for a model system of monodisperse Lennard-Jones chains. They are long enough to be considered as entangled. Thus, the effect of entanglements on such types of scaling can be quantified. Different ways of estimating the excess entropy based on either conformational or thermodynamic information are explored. The excess entropy is calculated directly by thermodynamic integration. The excess entropy can be approximated via a thermodynamic modeling by employing the self-associating fluid theory. The detected correlations between the various conformational and thermodynamical estimations of the excess entropy are thoroughly investigated. The conformational route for a system with short-range interactions appears to be the more suitable way.The dependence of all parameters appearing in the excess entropy scaling relationships on the chain length is thoroughly examined. The relation of the scaling parameters of the viscosity and diffusion coefficient are in line with the prediction of the Stokes-Einstein law.

DY 33.18 Thu 17:00 Poster C

Bifurcation to cross-stream migration in Poiseuille flow — •Matthias Laumann, Steffen Schreiber, Johannes Greber, and Walter Zimmermann — Universität Bayreuth, Theoretische Physik, 95440 Bayreuth, Germany

The dynamics of asymmetric dumbbells and semiflexible polymers in Poiseuille flow is investigated. We find that asymmetric dumbbells and

semiflexible polymers may migrate towards or away from the center of a Poiseuille flow, depending on the asymmetry of a dumbbell or on the bending stiffness of a semiflexible polymer as well as on the flow parameters. In the case they migrate away from the center of a Poiseuille flow, there are parameter ranges, where they migrate even in the absence of the effects of bounding walls only up to some distance away from the flow center. The distance of the final position of a dumbbell (semiflexible polymer) depends on the flow parameters as well as on the asymmetry and elasticity of the dumbbell (bending stiffness of a semiflexible polymer).

DY 33.19 Thu 17:00 Poster C

The Mechanical Responses of Wet Granulates under Cyclic Shear Deformation — •Somnath Karmakar[1], Marc Schaber[1], Anna-Lena Hippler[1], Marco Di Michiel[2], Mario Scheel[2], Stephan Herminghaus[3], and Ralf Seemann[1,3] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]ESRF, Grenoble, France — [3]MPI-DS, Göttingen, Germany

Adding small amount of wetting liquid to an assembly of dry granulates typically leads to the stiffening of granulates which arises due to the capillary bridge forces. We experimentally study the mechanical properties of wet granulates, composed of monodisperse spherical glass or basalt beads. The glass microspheres are almost perfectly wetted by water whereas the basalt microspheres have a rather large contact angles with water. We investigate the yield strength, measured under cyclic shear deformation for various system parameters like liquid content, bead radius, shear speed, shear amplitude, and absolute pressure. The yield strength of the wettable glass beads is observed to depend on the applied shear rate, leading to a 'shear-thinning-effect'; whereas the yield strength of the non-wetting basalt beads is independent of the applied shear rate. For large absolute pressures the stiffening of a wet compared to a dry granular assembly might be inversed and the liquid might act as a 'lubricant' lowering the yield strength. With time resolved X-ray micro-tomography, we could shed some light on the underlying microscopic mechanisms. We explore the variations in packing geometry during the shear process and the liquid exchange process, occurring between the individual liquid morphologies.

DY 33.20 Thu 17:00 Poster C

Rheology of Frictional Particles — •Matthias Grob[1], Claus Heussinger[1], and Annette Zippelius[1,2] — [1]Institut für Theoretische Physik, Göttingen, Deutschland — [2]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Deutschland

Granular materials are complex fluids with the ability to jam into a solid state. The properties of the jamming transition depend in addition to packing fraction and shear rate on the presence or absence of inter-particle friction. Here, jamming of frictional particles under simple shear is investigated numerically. Various regimes and transitions are observed and discussed. These transitions are influenced by the three control parameters. We find shear banding for dense systems within a certain range of shear rates and coexistence between solid and fluid like states.

DY 33.21 Thu 17:00 Poster C

Compactivity of 2D granular assemblies comprised of polygonal particles — •Volker Becker and Klaus Kassner — Institut für Theoretische Physik, Otto-von-Guericke-Universität Magdeburg, Germany

The theoretical description of granular matter is a subject of current research and scientific discussion [1]. A possible approach was proposed by S.F. Edwards [2]. The central hypothesis in Edwards' approach is that all stable states of a granulate which occupy a specified volume are equally probable. Therefore, the volume of the granulate plays the role of the energy in conventional statistical mechanics. In this framework, an intensive parameter χ called the compactivity, is the analogue to temperature in conventional thermodynamics. One way to determine the compactivity is determining the dependency of the volume fluctuations σ_ϕ on the volume fraction ϕ of the assembly and using a granular version of the fluctuation dissipation theorem[3]. On the other side one can determine χ from the distribution of free volume per particle[4]. Both is following Edwards theory.We will present results of computer simulations for 2D assemblies comprised of polygonal particles and prepared by different protocols(tapping and flow pulses) [3,5]. We compare the resulting compactivities determined by using both methods.

[1] M. P. Ciamarra et. al. *Soft Matter*, **8**, 9731 (2012) [2] Edwards et. al., *Physica A* **157**, 1080 (1989) [3] R. Nowak et al., *Phys. Rev. E* **57**, 1971 (1998) [4] T. Aste et. al., *Eur. Phys. J. B* **64**, 511-517 (2008); F. Lechenault et. al., *J- stat. Mech.*, **P07009** (2006) [5] M. Schröter et. al., *Phys. Rev. E,* **71**, 030301 (2005)

DY 33.22 Thu 17:00 Poster C

Fluctuations and yield stress in sheared granular media — •Seyyede Robabeh Moosavi[1,2], Jeliazko Jeliazkov[3], Michael LeBlanc[3], Karin Dahmen[3], and Matthias Schröter[1] — [1]Max-Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for Advanced Studies in Basic Sciences, Zanjan, Iran — [3]University of Illinois at Urbana Champaign, Illinois, USA

Slowly sheared granular materials show micro-yielding events before a global fracture. These events develop via slip avalanches with a broad range of sizes. We present experiments on the distribution of avalanche sizes in granular media of different packing fractions. We discussed our results in the context of a recently proposed theoretical model of power law for these statistics [1].

1. K. A. Dahmen, Y. Ben-Zion, J. T. Uhl, Nature Physics, 7, 554-557 (2011).

DY 33.23 Thu 17:00 Poster C

Liquid-solid-like transition in two dimensional wet granular matter — •Michael Wild, Christopher May, Ingo Rehberg, and Kai Huang — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

The phase transition of a monolayer of wet granular spheres under horizontally swirling motion is investigated experimentally. Due to the cohesion arising from the formation of capillary bridges between adjacent particles, the particles initially form a crystalline structure at moderate driving. By both increasing and decreasing the swirling frequency, we characterize the transitions between a crystal-like state and a liquid-like state with both local packing density and bond orientational order parameters. The hysteresis between the melting and crystallization threshold will be discussed. Moreover, the dependence of this transition on global fill fraction will be presented. In the limiting case of small crystalline structures, the critical driving frequency to mobilize those structures is found to depend strongly on the the cluster sizes, suggesting a size dependent effective static friction between the wet granular layer and the substance.

DY 33.24 Thu 17:00 Poster C

Tomographic Analysis of Jammed Ellipsoid Packings — •Fabian Schaller[1,2], Max Neudecker[2], Mohammad Saadatfar[3], Klaus Mecke[1], Gerd Schröder-Turk[1], and Matthias Schröter[2] — [1]Institut für theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Germany — [3]Applied Maths, RSPhysSE, The Australian National University, Australia

Disordered packings of ellipsoidal particles are a generalization of disordered sphere packings that can shed light on geometric features of random close packings and structural transitions in granular matter. Here we report the structure of ellipsoid packings in terms of contact numbers and Voronoi cell shapes, for several aspect ratios. Discrete approximations of generalized Voronoi diagrams are extracted from a large number of tomographic data of ellipsoid configurations, obtained by vertical shaking. Their shape is quantified by isotropy indices $\beta_\nu^{r,s}$ based on Minkowski tensors [1]. Contact numbers are discussed in the context of the jamming paradigm [2]. We find that our frictional particles are hyperstatic.

[1] G.E. Schröder-Turk *et al.*, Minkowski Tensor Shape Analysis of Cellular, Granular and Porous Structures, Adv. Mater. **23**, 2535 (2011)
[2] Martin van Hecke, J. Phys.: Condens. Matter (2010)

DY 33.25 Thu 17:00 Poster C

Measuring granular force chains in 3D — •Junaid M. Laskar[1], Stephan Herminghaus[1], Matthias Schröter[1], and Karen E. Daniels[2] — [1]Dynamics of Complex Fluids, Max Planck Institute for Dynamics and Self Organization, Goettingen, Germany — [2]Department of Physics, North Carolina State University, Raleigh, USA

One of the outstanding issues within the area of statistical physics of granular matter is to have better understanding of the statistical properties of forces and force chains. Due to the link to jamming, strain induced yielding and mechanical response; this issue has also technological relevance in civil engineering and geophysics [1, 2]. There have

been pioneering efforts towards experimentally measuring the force chains and their spatial distributions, though these are limited to two dimensions (2D) [1, 2]. For 3D granular systems, till now there are no experimental determinations of the forces on interior grains.

In this regard, an experimental method, based on two photon fluorescence spectroscopy to measure forces in the interior of ensemble of Ruby spheres, is developed. This novel method, which is the extension of the one demonstrated for a single ruby sphere to 3D, will be discussed in detail [3]. The results obtained from the shift in fluorescence peak in response to external compression will be discussed.

References:

[1] T. S. Majumdar and R. P. Behringer, Nature 453, 1079 (2005) [2] Karen E. Daniels and Nicholas W. Hayman, J. of Geophys. Res. 113, B11411 (2008) [3] Y. Chen et al., J. Appl. Phys. 101, 084908 (2007)

DY 33.26 Thu 17:00 Poster C

Pattern formation in agitated wet granular matter — Lorenz Butzhammer, Ingo Rehberg, and •Kai Huang — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

Pattern formation of a thin layer of vertically agitated wet granular matter is investigated experimentally. Due to the strong cohesion arising from the capillary bridges formed between adjacent particles, agitated wet granular matter exhibits a different scenario compared with cohesionless dry particles. Rotating spirals with three arms, which correspond to the kinks between regions with different colliding phases with the vibrating plate, have been found to be the dominating pattern. This preferred number of arms arise from period tripling of the agitated granular layer, which breaks the symmetry and drives the rotation of spiral arms. From both top view snapshots and the laser profilometry method, the rotation frequency of the spiral arms is characterized with image processing procedures. Both methods reveal a finite rotation frequency at a threshold excitation acceleration, which increases linearly with the peak vibration acceleration with a slope strongly dependent on the vibration frequency. As the vibration frequency decreases, a transition from period tripling to doubling bifurcation is observed, which gives rise to 'frozen' spiral arms. The phase diagram of the patterns will be presented and its dependence on various parameters will be discussed.

DY 33.27 Thu 17:00 Poster C

Dynamics of fluid-liquid crystalline interfaces and heterogeneous growth using the Phase Field Crystal Model for Liquid Crystals — •Cristian Vasile Achim and Hartmut Loewen — Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität Düsseldorf

Phase Field Crystal Model for Liquid Crystals is formulated with respect with three position-dependent order parameters, the reduced translational density, the local nematic order parameter, and the mean local direction of the orientations. The free-energy involves local powers of the order parameters up to the fourth order, gradients of the order parameters up to the fourth order, and different couplings among the order parameters. The phase diagram was investigated in Phys. Rev. E 83, 06172 (2011). Among stable phases liquid crystalline states are isotropic, nematic, columnar, smectic-A, and plastic crystalline phases. In this report we present results regarding the dynamics of fluid-liquid crystalline interface and heterogeneous growth obtained by solving numerically the couple equation of motions of the order parameters as presented in J. Phys.: Condens. Matter 22 (2010) 364105.

DY 33.28 Thu 17:00 Poster C

The Origin of Crack Surface Instabilities in silicon crystal — Liron Ben Bashat and •Dov Sherman — Technion, Haifa, Israel

Previous investigations showed micron scale height corrugations instabilities on the fracture surface of the (111) low energy cleavage plane of silicon, when the crack was propagated in the [11] direction at speed below 1100 m/sec. These corrugations were evident in three point bending and tensile experiments, and resemble fluctuations on the (111) and (110) low energy cleavage planes, propagating along the intersection line of both planes.

Recently, the density of these surface corrugations on the same crack system under bending was investigated in specimens having two distinct boron concentrations. Experiments showed that the corrugations density reduced significantly in specimens with low boron concentration. Experiments under ultra-high vacuum were conducted in STM microscope revealed that nano scaled surface instabilities initiate the larger surface corrugations. These instabilities are in the form of atomic steps. Quantum mechanical hybrid multi scale calculations with and without a single boron interstitial verified the latter experimental results in addition to a crack velocity loss at low crack speeds.

The fundamental query is whether the corrugations instabilities are formed due to interactions of the crack front with crystalline defects or is crack surface of defects free crystal always stable. We will present the experimental finding and the origin of the low speed crack surface instabilities and discuss the effect of these perturbations on crack speed.

DY 33.29 Thu 17:00 Poster C

Turing instability in one-component reaction-diffusion systems with fluctuating delay — •Jian Wang and Günter Radons — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

Delay systems used to model retarded actions are relevant in many fields such as optics, mechanical machining, biology or physiology. A frequently encountered situation is that the length of the delay time changes with time. With the presence of fluctuating delay the system dynamics becomes more complex, and sometimes some new phenomena can be obtained. In this study the delay is introduced into the reaction term of the KPP-Fisher-equation. It will be shown, that with a fluctuating delay the Turing instability, which in general is present in more-components systems, can also be obtained in one-component reaction-diffusion systems. The Lyapunov exponents in dependence on spatial perturbations is calculated. The structure and the related spectrum are characterized to prove this phenomenon.

DY 33.30 Thu 17:00 Poster C

Pattern formation in Swift-Hohenberg equation with delayed feedback — •Alexander Kraft and Svetlana Gurevich — Institut for Theoretical Physics, Wilhelm-Klemm-Str. 9, 48149 Münster

We are interested in the stability of periodic patterns in a real Swift-Hohenberg equation subjected to a delayed feedback. We classify different stability regimes of homogeneous solution and discuss how the delayed feedback modifies the stability of periodic patterns. In particular, we show that the delayed feedback induces a spontaneous motion of periodic patterns and leads to the formation of complex structures, including, e.g., traveling zigzag patterns and hexagons.

DY 33.31 Thu 17:00 Poster C

Orientational pattern selection by traveling modulations — •Lisa Rapp, Vanessa Weith, Alexei Krekhov, and Walter Zimmermann — Universität Bayreuth, Theoretische Physik, 95440 Bayreuth, Germany

The process of pattern formation in two-dimensional isotropic systems has been investigated intensively during the last decades. Challenging tasks in these systems are for instance the suppression defects in stripe patterns and the control of the overall orientation of the evolving structures.

We suggest an effective approach to control the pattern morphology by applying a traveling long-wave periodic modulation of the control parameter of the pattern forming system. The model systems we investigate include the Swift-Hohenberg equation (describing e.g. Rayleigh-Bénard convection) and the evolution equation for microphase separation in symmetric diblock copolymers. Studying the onset of the stripe phase we find, that depending on the traveling velocity v different orientations of the stripes with respect to the modulation may be favoured near threshold. In the case of a stationary modulation the wave vector of the stripes is preferentially perpendicular to the wave vector of the forcing. This also holds for velocities smaller than a velocity v_1. For velocities larger than a velocity v_2 a parallel orientation of the wave vectors has the lowest threshold. In the intermediate range $v_1 < v < v_2$ both wave vectors adjust themselves at an angle between 0 and $\pi/2$.

This velocity-dependent (re)orientation effect is confirmed by numerical simulations as well as the fact that the stripe patterns exhibit much less defects than in the unmodulated case.

DY 33.32 Thu 17:00 Poster C

Defect patterns in a model of wrinkles — •Achim Guckenberger, Alexei Krekhov, and Walter Zimmermann — Universität Bayreuth, Theoretische Physik, 95440 Bayreuth, Germany

Anisotropic pattern forming systems may exhibit new scenarios of pattern formation, when the system properties change perpendicularly or obliquely to the direction of the wave vector of the pattern. This is demonstrated for a two-dimensional model of wrinkles, whereby wrin-

kles may form on top of an elastomer, in which the elastic properties are varied in space. Within the model the critical wavenumber changes its value as a function of space in order to mimic the wrinkle formation on top of an inhomogeneous elastomer.

We show, that beyond a certain amplitude of the spatial variation of the critical waven umber the so-called Eckhaus stability-band of the possible wave number of wrinkles vanishes immediately above threshold and defect patterns may occur. Phase diagrams of this transition are presented and discussed.

DY 33.33 Thu 17:00 Poster C

Stochastic POD applied to the Wake of a Wind Turbine — •David Bastine, Matthias Wächter, and Joachim Peinke — ForWind, Institute of Physics, University of Oldenburg, Germany

Since wind turbines operating in the wake of other turbines experience a strongly altered inflow, a good understanding of the wake is crucial for the planing and optimization of large wind farms. In this work the proper orthogonal decomposition (POD) is combined with a Langevin-analysis approach to yield a low order description of spatio-temporal data. The method is applied to large eddy simulation data of a wind turbine wake. In the case of analyzing the data in a plane perpendicular to the mean flow the POD yields clearly structured eigenmodes similar to Fourier modes in the azimuthal direction. The temporal evolution of the modes can be described by time dependent coefficients given by the projection of the velocity field on the eigenmodes. We interpret these coefficients as random variables whose statistics can be modeled by Langevin equations and try to estimate the corresponding drift and diffusion coefficients.

DY 33.34 Thu 17:00 Poster C

Correlation between active grid excitation and generated wind field — •Gerrit Kampers, Nico Reinke, Joachim Peinke, and Michael Hölling — ForWind - Center for Wind Energy Research, Institute of Physics, University of Oldenburg, Germany

Turbulence plays an important role in the field of wind energy conversion. Lift forces and their fluctuations, for example, are strongly influenced by the statistics of the ambient wind field. For realistic wind tunnel investigations, an active grid was build, which allows the generation of wind fields with comparable characteristics to those in the atmospheric boundary layer (ABL). The active grid consists of seven horizontal and nine vertical axes with fixed 7.4×7.4 cm^2 square flaps. Each of these axes can be controlled individually by a step motor.
A challenging part in the work with the active grid is to find the right excitation protocols to control the position in time of the axes, and therefore the stochastical properties of the resulting turbulent flow field. The goal is to create realistic flow fields, e.g. fields with heavy intermittency, which is one of the major properties of the ABL.
To achieve that, the interaction between the active grid excitation and the resulting flow field was investigated experimentally. In the experiments, the angle of attack and the rotation speed of the flaps were successively changed for different wind speeds. The resulting flow field was measured with hot-wires at several downstream positions. Based on the experiments, a model for the excitation - flow field interaction was developed. The model allows for a more systematic creation of excitation protocols for different flow properties.

DY 33.35 Thu 17:00 Poster C

Measurements of LSC dynamics in Rayleigh-Bénard convection with an ultrasonic anemometer — •Katharina Witte and Joachim Peinke — TWiST-Turbulence, Windenergy and Stochastics, University of Oldenburg, Germany

The dynamics of large-scale circulation (LSC) in Rayleigh-Bénard convection are investigated experimentally, particularly with regard to rotations and cessations. The measurements are conducted over the range of the Rayleigh-number from $1 * 10^9$ to $6 * 10^9$. For this a cylindrical cell of aspect ratio $\Gamma = 1$ is used, which is heated from below and cooled from top. Utilization of water enriched with particles as working fluid offers the possibility to applicate an ultrasonic anemometer, which is based on the Doppler effect. With this anemometer velocity profiles of the particles which correspond to those of the fluid are taken. This contact less method is carried out inside the cell by sensors which are recessed into the cell wall.

DY 33.36 Thu 17:00 Poster C

Convection onset in a transient diffusive boundary layer at high Rayleigh numbers — •Stephan Messlinger, Christoph Kramer, Wolfgang Schöpf, and Ingo Rehberg — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth

We observe the onset of Soret driven convection in a colloidal suspension of thermosensitive microgel particles in water. The suspension exhibits a strong positive Soret-effect, resulting in large solutal Rayleigh numbers even for low temperature gradients. When heated from below in a classical convection cell, the convective instability does not set in uniformly over the system height, but starts in the steep concentration profiles established at the cell boundaries. We report on the latency time of the convection onset and the transient behaviour of the fluid motion shortly thereafter.

DY 33.37 Thu 17:00 Poster C

Transitions in double-diffusive finger convection — •Matthias Kellner and Thomas Müller — Institut für Geophysik der Georg-August Universität, Göttingen, Deutschland

An electrodeposition cell is used to sustain a destabilizing concentration difference of copper ions in aqueous solution and a stabilizing temperature gradient between the top and bottom boundaries of the cell. The thermal Rayleigh number was varied for a set destabilizing chemical Rayleigh number. Finger convection is observed, although the overall density gradient is destabilizing ($|\lambda| < 1$). A transition from finger regime to Rayleigh-Benard convection is observed for a fixed ratios of the Rayleigh numbers. This is marked by a change from an anisotropic to an isotropic velocity field. The Sherwood number increases with decreasing Rayleigh number towards its maximum at the transition, after which it will drop again in the convective zone. Numerical simulations concerning this scenario are done.

DY 33.38 Thu 17:00 Poster C

Statistical Physics of Quadrics in Finite Projective Spaces — •Benedikt Krüger, Nils Alex, Felix Winterhalter, Johannes F. Knauf, and Klaus Mecke — Institut für Theoretische Physik, FAU Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

Projective Geometry is an interesting alternative to the usual affine geometry that is typically used in physics. Certain symmetries (e.g. between points and lines in projective planes) lead to a more elegant mathematical description of geometric structures by avoiding case-by-case analysis. A projective space can be seen as an extension of the usual affine space where all parallel hyperplanes intersect on an added "hyperplane at infinity". The analogon to affine conic sections (ellipses, parabolas and hyperbolas) are projective quadrics. This definition holds for projective spaces over finite fields, as well. The emerging properties of these finite quadrics are examined with methods from statistical physics.

DY 33.39 Thu 17:00 Poster C

Quantitative characterisation of capillary rise in nanoscale systems — •Christian Thome and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, Campus E2 6, D66123 Saarbrücken

Considering fluids in confined nanoscale geometries one finds a strong influence of surface effects. Therefore a closer look at the rise of liquid-air interfaces, also called menisci, in nanometer scale capillaries shows the need of modifications of the macroscopic laws like Lucas Washburn. In addition some experiments on the spontaneous imbibition of water in nano-porous vycor glass showed a broadening of the imbibition front. This phenomenon encouraged us to investigate the capillary rise of a simple Lennard-Jones fluid in nano-pores, nano-pore-junctions and nano-pore-intersections using molecular dynamics simulations. Our main interest is the quantitative characterisation of the influence of the interaction strength between the wall particles and the fluid particles. We present results for the fluid propagation, the interface morphology and fluid density profiles.

DY 33.40 Thu 17:00 Poster C

Scaling properties of a parallel implementation of the multicanonical algorithm — •Johannes Zierenberg, Martin Marenz, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Germany

The multicanonical method has been proven powerful for statistical investigations of lattice and off-lattice systems throughout the last two decades. We discuss an intuitive but very efficient parallel implementation of this algorithm and analyze its scaling properties for discrete energy systems, namely the Ising model and the 8-state Potts model. The simple parallelization relies on independent equilibrium simulations in each iteration with identical multicanonical weights, merging their statistics in order to obtain estimates for the successive weights.

With good care, this allows faster investigations of large systems, because it distributes the time-consuming weight-iteration procedure and allows parallel production runs. We show that the parallel implementation scales very well for the simple Ising model, while the performance of the 8-state Potts model, which exhibits a first-order phase transition, is limited due to emerging barriers and the resulting large integrated autocorrelation times. The quality of estimates in parallel production runs remains of the same order at same statistical cost.

DY 33.41 Thu 17:00 Poster C

Local coupling of non-linear oscillators studied in the Bhelousov-Zhabotinsky reaction — •Claudia Lenk[1], Mario Einax[2], Philipp Maass[2], and Michael J Köhler[1] — [1]Institut für Chemie und Biotechnik, Technische Universität Ilmenau, Germany — [2]Fachbereich Physik, Universität Osnabrück, Germany

Pattern formation in reaction-diffusion (RD) systems is important in many areas as, e.g., the embryonic development, catalytic activity or population dynamics. These systems are mostly constituted of many coupled subunits, like the cells of the embryo or catalyst nanoparticles. To get insight into the influence of these modular structure onto the emerging excitation patterns we conduct experiments of the Bhelousov-Zhabotinsky reaction (BZR) in a Nafion membran with a catalyst distribution in form of a micro spots pattern and compare the BZR waves with numerical calculations of the FitzHugh-Nagumo equations.

The influence of the catalyst spot size, their distance and shape on the coupling strength was investigated. We observe a bifurcation into two different patterns, i.e. a spiral wave and a target pattern, in dependence of the distance of catalyst spots. Thereby the initial conditions control which pattern occurs. In further studies, we will investigate the possibility to predict which pattern occurs if only the initial conditions are known.

DY 33.42 Thu 17:00 Poster C

Contemplating coincidences: Rigorous testing for synchrony between time series of discrete events — Jonathan F. Donges[1,2], •Reik V. Donner[1], Katharina Kohl[1,3], and Jürgen Kurths[1,2] — [1]Potsdam Institute for Climate Impact Research, Germany — [2]Department of Physics, Humboldt University, Berlin, Germany — [3]Department of Mathematics, Heinrich Heine University of Düsseldorf, Germany

We present a novel approach to rigorous statistical testing for synchrony between two time series of discrete events. For uncorrelated events, the distribution of the test statistics can be analytically derived under the assumption of rare events. The limits of this analytical approximation are explored by numerical simulations. Subsequently, necessary corrections for correlated events are numerically derived for both short- and long-term correlations. Relationships with existing concepts such as event synchronization are discussed. Finally, the proposed approach is applied to some real-world geoscientific example in order to distinguish signatures of synchrony from insignificant coincidences.

DY 33.43 Thu 17:00 Poster C

Characterization of diffusion processes with non-exponential dwell time distributions by the distribution of diffusivities — •Michael Bauer and Günter Radons — Chemnitz University of Technology, Germany

Many transport phenomena in physical and biological systems can be described by heterogeneous diffusion processes where the diffusive behavior changes during the motion. For instance, diffusion in ultra-thin liquid films is governed by layer-dependent diffusion coefficients and jumps between the liquid layers. Such processes are often characterized by observing individual tracers in single-particle tracking (SPT) experiments. To account for inhomogeneities, we suggested to investigate the distribution of diffusivities and its dependence on the time lag between snapshots [1]. We further studied the relation to ensemble-based measurements obtained from pulsed field gradient nuclear magnetic resonance (PFG NMR) and applied it to the two-compartment exchange (Kärger) model [2]. In our contribution, we extend the investigations to heterogeneous systems where the Kärger model is not applicable. In such systems the dwell time distribution does not decay exponentially but depends on the spatial potential related to, e.g., structured surfaces. We analyze such systems by the time-lag dependence of the distribution of diffusivities and its moments, which characterizes the diffusivity as a fluctuating quantity along a trajectory.

[1] M. Bauer et al., Diffus. Fundam. 11, 104 (2009)

[2] M. Bauer et al., J. Chem. Phys. 135, 144118 (2011)

DY 33.44 Thu 17:00 Poster C

Strong bounds on Onsager coefficients and efficiency for three terminal thermoelectric transport in a magnetic field — •Kay Brandner[1], Keiji Saito[2], and Udo Seifert[1] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Department of Physics, Keio University, 3-14-1 Hiyoshi, Kohoku-ku, Yokohama, Japan 223-8522

For thermoelectric transport in the presence of a magnetic field that breaks time-reversal symmetry, a strong bound on the Onsager coefficients is derived within a general set-up using three terminals. Asymmetric Onsager coefficients lead to a maximum efficiency substantially smaller than the Carnot efficiency reaching only $\eta_C/4$ in the limit of strong asymmetry. Related bounds are derived for efficiency at maximum power, which can become larger than the Curzon-Ahlborn value $\eta_C/2$, and for a cooling device. Our approach reveals that in the presence of reversible currents the standard analysis based on the positivity of entropy production is incomplete without considering the role of current conservation explicitly.

DY 33.45 Thu 17:00 Poster C

Resonant tunnelling and complex paths : 1-d integrable models using normal forms — •Jérémy Le Deunff — MPIPKS, Dresden, Germany

Dynamical tunnelling, defined as a quantum phenomena which is classically forbidden (i.e. which cannot be described by the real classical solutions of the Hamilton's equations), may manifest itself through transition between different regions dynamically disconnected in the classical phase space. It is well-known that the classical nonlinear resonant chains observed in non integrable Hamiltonian systems affect by many order of magnitude the quantum observables describing tunnelling (splittings or decay rates). Here, we introduce a class of 1-d integrable Hamiltonians which reproduce main islands surrounded by (r:s) resonant chains in the phase space. We then propose a semiclassical formula for tunnelling splittings using a complex paths approach. We show that this approach leads to a good agreement with the exact numerical results and we compare with the resonance-assisted-tunnelling theory in different regimes.

DY 33.46 Thu 17:00 Poster C

Multicanonical analysis of the gonihedric Ising model — •Marco Müller[1], Desmond A. Johnston[2], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Germany — [2]Math. Dept., Heriot-Watt University, Edinburgh, United Kingdom

The gonihedric Ising model originates from catching basic properties of fluctuating random surfaces in a bosonic string theory. Formulated as a lattice model of interacting classical spins it can be investigated by means of the multicanonical Monte Carlo algorithm to resolve open questions on the first-order phase transition. The transition temperature has been determined for the model and a dual representation; also the interface tension has been measured for both models and appears to be quite strong.

DY 33.47 Thu 17:00 Poster C

Self-avoiding walks on critical percolation clusters in two to seven dimensions — •Niklas Fricke and Wolfhard Janke — Institut für Theoretische Physik and Centre for Theoretical Sciences (NTZ),
Universität Leipzig, Postfach 100920, D–04009 Leipzig, Germany

Self-avoiding walks (SAWs) on critical percolation clusters are a basic model for polymers in crowded disordered media. The fractal nature of the substrate gives rise to interesting scaling behavior, which, despite considerable efforts in the past, is still poorly understood . We used a recently developed exact enumeration technique [1], which can handle walks of several thousand steps. This enabled us to determine the SAW scaling exponents very accurately. Varying the lattice dimension to the upper critical limit ($D = 6$) allows us to closely check the predictions from field theory and to investigate the influence of the various fractal dimensions of the critical cluster.

[1] N. Fricke and W. Janke, Europhys. Lett. **99**, 56005 (2012).

DY 33.48 Thu 17:00 Poster C

Incommensurate Nematic Fluctuations in 2d Metals —

•Tobias Holder and Walter Metzner — Max-Planck-Institute for Solid State Research, D-70569 Stuttgart

In a homogeneous nematic state an orientational symmetry of the system is spontaneously broken, without breaking the translation invariance. However, in 2010 Metlitski and Sachdev (New J. Phys. **12**, 105007) found a tendency toward formation of a *modulated* nematic state in a two-dimensional metal with strong antiferromagnetic spin-density wave fluctuations.

We investigate the possibility of a modulated nematic state from a model of tight-binding electrons on a square lattice with an interaction that has an attractive d-wave component for forward scattering in the charge channel. Within a random phase approximation (RPA), we find that the wave vector of the nematic quantum fluctuations is generically nonzero at $T = 0$. At finite temperatures the nematic fluctuations are reduced considerably due to their singular momentum dependence, restricting sizable effects of incommensurate fluctuations to very low temperatures.

Ref.: T. Holder and W. Metzner, Phys. Rev. B **85**, 165130 (2012).

DY 33.49 Thu 17:00 Poster C

MERA-networks as holographic duals for the random Heisenberg spin-chain — •Johannes Oberreuter and Stefan Kehrein — Georg-August-Universität Göttingen, Germany

The holographic duality relates a field theory to a theory of (quantum) gravity in one dimension more. A strongly coupled field theory is dual to weakly coupled, classical gravity. This allows to do a calculation of correlation functions for a strongly coupled theory in the weakly coupled counterpart perturbatively. Thereby, the extra (radial) dimension represents the scale of the RG transformation in the field theory. Real space renormalization procedures like the multi-scale-renormalization-ansatz (MERA) can be used to determine the ground state of the field theory. It has been conjectured, that the tensor networks which arise during this procedure are a discretized version of Anti-de Sitter space, which is the background of the gravity theory, for which the duality is established best (AdS/CFT-correspondence). It was so far impossible to construct such a network explicitely. We consider the dual network of a random Heisenberg spin-chain, for which real-space renormalization can be performed analytically. After establishing the form of the network at finite temperature, we examine quenches in the spin-chain to study the relation between the MERA-network and the Heisenberg chain far from equilibrium.

DY 33.50 Thu 17:00 Poster C

Numerical survey of the condensate shape and scaling laws in pair-factorized steady states — Eugen Ehrenpreis, •Hannes Nagel, and Wolfhard Janke — Institut für theoretische Physik, Universität Leipzig, Leipzig, Deutschland

We numerically survey the shapes and scaling laws of extended particle condensates that emerge as a result of spontaneous symmetry breaking in pair-factorized steady states of a stochastic transport process. The specific model based on the zero-range process consists of indistinguishable particles that stochastically hop between sites controlled by a tunable interaction composed of a zero-range and a local-range part. We identify the different condensate shapes within their respective regimes of interaction strengths as well as precisely determine the condensate width scaling. We find good agreement with theoretic predictions [1].

[1] B. Wacław, J. Sopik, W. Janke and H. Meyer-Ortmanns, **Phys. Rev. Lett.** 103, 080602 (2009).

[2] E. Ehrenpreis, H. Nagel and W. Janke, Lepzig preprint (2012).

DY 33.51 Thu 17:00 Poster C

Scaling properties and synchronisation in chaotic networks with multiple delays — •Otti D'Huys[1], Steffen Zeeb[1], Sven Heiligenthal[1], Thomas Juengling[1], Wolfgang Kinzel[1], and Serhiy Yanchuk[2] — [1]Institute of Theoretical Physics, University of Wuerzburg, 97074 Wuerzburg, Germany — [2]Institute of Mathematics, Humboldt University of Berlin, 10099 Berlin, Germany

Delayed complex systems have received much interest in recent years, as delays play an important role in systems as diverse as population dynamics, traffic, communication networks, genetic circuits, and the brain. In general the different interaction delays in a network are not equal, or may even differ by several orders of magnitude.

We consider a hierarchical network of chaotic units: the coupling delay within a subnetwork is much shorter than the delay between the subnetworks. We show that the spectrum of Lyapunov exponents has a typical structure, with different parts of the spectrum scaling with the different delays. We can relate the scaling properties of the maximal Lyapunov exponent to the synchronisation properties of the network: units within a subnetwork can synchronise if the maximal exponent scales with the shorter delay while long range synchronisation between different subnetworks is only possible if the maximal exponent scales with the long delay.

DY 33.52 Thu 17:00 Poster C

Noise enhances information transfer in hierarchical networks — •Agnieszka Czaplicka[1], Janusz A. Hołyst[1], and Peter M.A. Sloot[2,3,4] — [1]Faculty of Physics, Center of Excellence for Complex Systems Research, Warsaw University of Technology, Koszykowa 75, PL-00-662 Warsaw, Poland. — [2]Computational Science, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands. — [3]National Research University of Information Technologies, Mechanics and Optics (ITMO), Kronverkskiy 49, 197101 Saint Petersburg, Russia. — [4]Nanyang Technological University, 50 Nanyang Avenue, 639798 Singapore.

We study the influence of noise on information transmission in a form of packages shipped between nodes of hierarchical networks. Numerical simulations are performed for artificial tree networks, scale-free Ravasz-Barabási networks as well for a real network formed by email addresses of former Enron employees. Two types of noise are considered. One is related to packet dynamics and is responsible for a random part of packets paths. The second one originates from random changes in initial network topology. We find that the information transfer can be enhanced by the noise. The system possesses optimal performance when both kinds of noise are tuned to specific values, this corresponds to the Stochastic Resonance phenomenon. There is a non-trivial synergy present for both noisy components. We found also that hierarchical networks built of nodes of various degrees are more efficient in information transfer than trees with a fixed branching factor.

DY 33.53 Thu 17:00 Poster C

Individual Fractal Weyl Laws in Systems with a Mixed Phase Space — •Martin Körber[1,2], Matthias Michler[1], Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany

In open chaotic systems the number of long-lived states is expected to obey a fractal Weyl law, with the exponent being associated to the fractal dimension of the repeller. For generic open systems with a mixed phase space we demonstrate that there is not just one fractal Weyl law but individual ones. They correspond to states localizing on different regions of the hierarchical phase space. This is illustrated for a designed Markov chain model and the standard map.

DY 33.54 Thu 17:00 Poster C

Integrable Approximation of Regular Islands: The Iterative Canonical Transformation Method — Clemens Löbner[1,2], Steffen Löck[1,3], •Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]Technische Universität Dresden, Institut für Theoretische Physik, 01062 Dresden — [2]MPI für Physik komplexer Systeme, 01187 Dresden — [3]Technische Universität Dresden, OncoRay - National Center for Radiation Research in Oncology, 01307 Dresden

Our aim is to approximate the dynamics of a regular island in a non-integrable Hamiltonian H by an integrable Hamiltonian H_{reg}. We present a new method which allows to find H_{reg} for arbitrarily many degrees of freedom. The method is based on the construction of an integrable approximation in action representation which is then improved in phase-space representation by iterative applications of canonical transformations. These transformations are optimized such that the regular dynamics of H and H_{reg} agree as closely as possible.

We apply this iterative canonical transformation method to the standard map and the cosine billiard. In the second case the resulting integrable Hamiltonian describes a billiard with the same boundary, but a nontrivial time evolution. This provides a basis for the future determination of regular-to-chaotic tunneling rates for generic billiards with the fictitious integrable system approach.

DY 33.55 Thu 17:00 Poster C

Complex paths for regular-to-chaotic tunneling rates — Normann Mertig[1,2], •Steffen Löck[1,2,3], Arnd Bäcker[1,2], Roland Ketzmerick[1,2], and Akira Shudo[2,4] — [1]Institut für Theoretische

Physik, Technische UniversitätDresden, 01062 Dresden — [2]MPI für Physik komplexer Systeme, 01187 Dresden — [3]OncoRay, Technische Universität Dresden, 01307 Dresden — [4]Department of Physics, Tokyo Metropolitan University, Minami-Osawa, Hachioji, Tokyo 192-0397, Japan

For generic non-integrable systems we show that a semiclassical prediction of tunneling rates between regular and chaotic phase-space regions is possible. Our prediction is based on complex paths which can be constructed despite the obstacle of natural boundaries. The semiclassically obtained tunneling rates are in excellent agreement with numerical tunneling rates for the standard map where few complex paths dominate. This gives a semiclassical foundation of the long-conjectured and often-observed exponential scaling with Planck's constant of regular-to-chaotic tunneling rates.

DY 33.56 Thu 17:00 Poster C

Criticality in transport through the quantum Ising chain — •Malte Vogl, Gernot Schaller, and Tobias Brandes — Institut für Theoretische Physik, TU Berlin

We consider thermal transport between two reservoirs coupled by a quantum Ising chain as a model for non-equilibrium physics induced in quantum-critical many-body systems. By deriving rate equations based on exact expressions for the quasi-particle pairs generated during the transport, we observe signatures of the underlying quantum phase transition in the steady-state energy current already at finite and different reservoir temperatures.

Ref.: M.V., G. Schaller, and T. Brandes: arXiv[cond-mat]:1208.5989, to be published in PRL

DY 33.57 Thu 17:00 Poster C

Nonequilibrium dynamics of few–electron systems—A comparison of Green functions and reduced density operator theory — •Sebastian Hermanns and Michael Bonitz — ITAP, Christian–Albrechts–Universität Kiel, Leibnizstr. 15, 24098 Kiel

The dynamics of few–electron systems out of equilibrium are among the most interesting but likewise most challenging problems in theoretical physics for the last 50 years. The complexity lies in the fact that, on the one hand, for more than a few particles, direct numerical solutions of the exact equations of motion are mostly not possible due to the exponentially scaling of the problem size. On the other hand, methods relying on statistical averaging can only be applied successfully for much larger particle numbers. In between these two limiting cases, the approximate methods of nonequilibrium Green functions (NEGFs) and the reduced density operator (NEDO) theory have been widely used. To obtain a closed equation of motion for the main quantities, the single-particle NEGFs and NEDOs, one has to find a suitable truncation of respective hierarchies, the Martin–Schwinger– and the BBGKY–hierarchy.

In this contribution, we compare different strategies of truncation, both for NEGFs and NEDOs, with respect to the representability of different time–dependent processes and the compliance with important conservation laws. A main focus lies on the relation between similar approximations for NEGFs and NEDOs[1].

[1] S. Hermanns, and M. Bonitz, submitted to Jour. Phys. Conf. Ser., arXiv: 1211.6959

DY 33.58 Thu 17:00 Poster C

Green functions approach to the nonequilibrium dynamics of 3D Hubbard nano–clusters — •Sebastian Hermanns[1], Karsten Balzer[2], and Michael Bonitz[1] — [1]ITAP, Christian–Albrechts–Universität Kiel, Leibnizstr. 15, 24098 Kiel, Germany — [2]Max Planck Research Department for Structural Dynamics Hamburg, Building 99 (CFEL), Luruper Chaussee 149, 22761 Hamburg, Germany

The three–dimensional Hubbard model is widely used for the description of narrow–band solid state systems in terms of sites, on which the electrons interact, and hopping amplitudes between these sites. Despite these drastic simplifications, it exhibits many physically relevant phenomena, including phase transitions from Mott–insulator to conductor or the time–dependent dynamics of strongly correlated electrons after an excitation. To describe these classes of processes, the theoretical framework of Nonequilibrium Green functions is very well suited[1], since it provides a controlled way of approximations, is non–perturbative in the exciting field and has shown good results for 1D Hubbard chains[2]. In this contribution, we show results for the response of $2 \times 2 \times 2$ up to $5 \times 5 \times 5$ cubic 3D Hubbard nano–clusters with on–site interaction and nearest–neighbor hopping, after different kinds and strength of excitations and compare with exact as well as other approximate methods.

[1] K. Balzer, and M. Bonitz, *Nonequilibrium Green's Functions Approach to Inhomogeneous Systems*, in press (2012)
[2] K. Balzer, S. Hermanns, and M. Bonitz, submitted to J. Phys. Conf. Ser., arXiv: 1211.3036

DY 33.59 Thu 17:00 Poster C

Simulations of the structure formation of Alkyl-Adenine monolayers on graphene — •Oliver Rubner, Markus Bamler, Pritam Kumar Jana, and Andreas Heuer — Institut für Physikalische Chemie, Universität Münster

Recent experiments showed that N9-Alkyl-Adenine molecules can form two different domains when deposited on a graphene surface. These domains consist of networks with different arrangements of head (Adenine) and tail (Alkyl) groups. The formation of the domains and their relative abundance depends in a non trivial way on parameters like temperature or deposition flux. The exact molecular structure of the domains is, however, still unknown. In order to explain the experimental results we first performed quantum-chemical calculations to elucidate the possible network structure and the corresponding energetics. Given these parameters we used Monte-Carlo simulations to investigate the dependence of the structure formation on external parameters. We will present here a model that is consistent with the experimental findings and can be used to tune further experiments to control the network structure on a graphene surface.

DY 33.60 Thu 17:00 Poster C

Ground states of 1D long-range random-field Ising magnets — •Timo Dewenter and Alexander K. Hartmann — Institut für Physik, Carl von Ossietzky Universität Oldenburg

In random-field Ising magnets (RFIMs) Ising spins interact ferromagnetically with each other. Disorder is introduced by local random fields which act on each spin and whose values are drawn from a Gaussian distribution. At zero temperature, at a critical random-field strength h_c the system undergoes a phase transition.

Here, we consider an one-dimensional RFIM with long-range interactions that are only present between spins with a probability that decays like a power-law in the geometric distance between the interacting spins. The parameter σ in the power-law exponent enables us to tune the effective dimension of the model.

Different values of σ are used to investigate numerically [1] the three parameter regions, which are the mean-field, non-mean-field region and the region without a phase transition ($h_c = 0$). Ground states are calculated [2] with graph theoretical algorithms by mapping the system to a directed graph. The critical random-field strength h_c and the critical exponents are obtained by finite-size scaling and then compared to analytical predictions and to results of a hierarchical model [3].

[1] A.K. Hartmann: *Practical Guide to Computer Simulations*, World-Scientific, 2009
[2] A. K. Hartmann and H. Rieger: *Optimization Algorithms in Physics*, Wiley-VCH, 2002
[3] C. Monthus and T. Garel, J. Stat. Mech., P07010, 2011

DY 33.61 Thu 17:00 Poster C

Multifractal analysis of electronic states in corner-sharing tetrahedral lattices — Martin Puschmann, •Philipp Cain, and Michael Schreiber — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz

The corner-sharing tetrahedral lattices appear as a sublattice in different materials, e.g. spinels and pyrochlore. We consider the transport of non-interacting electrons and investigate their electronic states in the vicinity of the localization-delocalization (LD) transitions by analyzing the multifractal properties of the wave functions. The multifractal analysis (MFA) is used to explore the phase diagram, which is then compared to the results obtained by other methods [1]. Furthermore the MFA yields detailed insight into the critical behavior at the LD transition, i.e. the divergence of the correlation length, which is characterized by the value of the universal critical exponent.

[1] F. Fazileh, X. Chen, R. J. Gooding, and K. Tabunshchyk, Phys. Rev. B **73**, 035124 (2006)

DY 33.62 Thu 17:00 Poster C

A State Dependent Potts Model — •Gabriell Máté[1], Ronald Dickman[2], and Dieter W. Heermann[1] — [1]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany — [2]Departamento de Física, ICEx, Universidade Federal de Minas

Gerais, Belo Horizonte, Brazil

Although the resolution of conventional confocal microscopy is limited, the images provided by this technique carry a tremendous amount of information. One of the most straightforward approaches to describe these images is to model them with a Potts model. However, in many cases the detected configurations correspond to a system characterized by a temperature close to the critical point, making it almost impossible to control this model. In this work we present a modified version of the Potts model which might be useful in such situations. The modification consists in introducing arbitrary couplings between different states. We argue that in the simplest case the modified model is equivalent to the original Potts model. We investigate it numerically with respect to criticality and observe a shift of the critical point as we vary the parameters. We also show that the model is capable of exhibiting more exotic behavior.

DY 33.63 Thu 17:00 Poster C

Energy Transfer and Optical Properties of Molecular Aggregates: Application of Non-Markovian Quantum State Diffusion — •Gerhard Ritschel[1], Jan Roden[1,3], Walter T. Strunz[2], and Alexander Eisfeld[1,4] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Technische Universität Dresden, Germany — [3]University of California, Berkeley, USA — [4]Harvard University, Cambridge, USA

The general non-Markovian quantum state diffusion method is used to calculate excitation energy transfer and optical spectra of molecular aggregates for various temperatures. With that approach it is possible to account for structured spectral densities explicitly containing internal vibrational modes of the molecules as well as phonons of an environment. Because the method is very efficient, systematic investigations with respect to parameter variations are possible. We apply the method to the photosynthetic Fenna-Matthews-Olson complex focussing particularly on the role of the recently discovered eighth chromophore, which is believed to play an important role in receiving excitation from the main light harvesting antenna, for excitation energy transfer through the aggregate. It is shown that the energy transfer changes qualitatively when site 8 is excited initially. Instead of the relatively fast transfer that is usually observed when the initial excitation is localized on site 1 or 6, an exponential-like decay of the excitation is found when initialization at site 8 is considered.

DY 34: Annual General Meeting of DY

All members of the Devision – Dynamics and Statistical Physics – are invited to participate in our annual meeting.

Time: Thursday 19:00–20:00 Location: H47

DY 34.1 Thu 19:00 H47

Annual General Meeting of DY — •J. Peinke — Fachverband Dynamik und Statistische Physik

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DY 35: Brownian Motion and Transport

Time: Friday 9:30–11:30 Location: H48

DY 35.1 Fri 9:30 H48

Two-dimensional transport of paramagnetic colloids via an AC-induced ratchet — •Robert Gernert and Sabine H. L. Klapp — Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

Magnetic garnet films are characterized by a striped magnetisation which can be adjusted through an external homogeneous magnetic field. An oscillating field drives paramagnetic colloids, which perform Brownian motion in a plane above the film, out of equilibrium and induces a ratchet effect.[1,2] We investigate the dependence of the arising transport on particle interaction. The Gaussian core model is used to define the interaction potential.

The Brownian motion is assumed to be overdamped. As a framework for solving the equation of motion for the time-dependent probability density, we employ the Dynamical Density Functional Theory (DDFT) where the microscopic particle interactions enter via a free energy functional.[3]

Mean squared displacement, diffusion coefficient and other transport properties are calculated in two dimensions and in a one-dimensional cut perpendicular to the stripes of magnetisation. First results of simulations including attractive magnetic dipole interactions are shown.

[1] P. Tierno, F. Sagues, T. H. Johansen and T. M. Fischer, Phys. Chem. Chem. Phys. **11**, 9615 (2009)

[2] A. Fortini and M. Schmidt, Phys. Rev. E **83**, 041411 (2011)

[3] A. J. Archer and R. Evans, J. Chem. Phys. **121**, 4246 (2004)

DY 35.2 Fri 9:45 H48

Computersimulation of colloidal particles in two-dimensional channel geometries. — •Ullrich Siems and Peter Nielaba — University of Konstanz, Germany

This talk will present the results of Brownian Dynamics Simulations of colloidal particles in external fields confined in two-dimensional channels. Superparamagnetic Brownian particles are well suited 2d model-systems for a variety of problems on different length scales, ranging from pedestrian walking through a bottleneck to ions passing ion-channels in living cells. In such systems confinement into channels can have a great influence on the diffusion and transport properties. In our study interacting colloidal particles were dragged over a washboard potential and are additionally confined in a two-dimensional micro-channel.

DY 35.3 Fri 10:00 H48

Brownian Transport in corrugated narrow channels - inertia effects — •Gerhard Schmid and Peter Hänggi — Universität Augsburg

The transport of Brownian particles through corrugated narrow channels is investigated [1,2]. Interestingly, inertial contributions to the particle dynamics cannot be neglected a priori. Especially, for widths of the channel's bottlenecks smaller than an appropriate particle diffusion length determined by the channel's geometrical parameters and the strength of the forcing, the Smoluchowski approximation breaks down and inertial effects come into play. The inertia corrections to the transport quantifiers, mobility, and diffusivity markedly differ for smoothly and sharply corrugated channels [2].

[1] P.S. Burada, P. Hänggi, F. Marchesoni, G. Schmid, and P. Talkner, ChemPhysChem **10**, 45 (2009).

[2] P.K. Ghosh, P. Hänggi, F. Marchesoni, F. Nori, and G. Schmid, Phys. Rev. E **86**, 021112 (2012).

DY 35.4 Fri 10:15 H48

Determination of eigenvalues of the diffusion tensor in anisotropic systems with orientation change in time and space — •Mario Heidernätsch and Günter Radons — Chemnitz University of Technology, D-09126 Chemnitz, Germany

Anisotropic diffusion is one possible generalization of homogeneous diffusion processes. It occurs typically in systems with anisotropic media such as liquid crystals or in isotropic media when the diffusing particle or molecule has an ellipsoidal shape. It can be formally described by an extended Fokker-Planck-equation using a diffusion tensor. We show how the moments of the distribution of diffusivities [1] can be used in a simple fashion to obtain the eigenvalues of the diffusion tensor from trajectories of such anisotropic processes. For the example of a three-dimensional anisotropic systems with twist, we show how the method regains the principal diffusion coefficients. In such systems, which are

mathematical equivalent to two-dimensional diffusion of an ellipsoid in isotropic media, other methods are harder to accomplish and need better data [2], or might even fail.

[1] M. Bauer et al., J. Chem. Phys. 135, 144118 (2011)
[2] C. Ribrault et al., Phys. Rev. E 75, 021112 (2007)

DY 35.5 Fri 10:30 H48

Fluctuations and equipartition in the dynamics of granular ratchets — •Johannes Blaschke and Jürgen Vollmer — Max Planck Institute for Dynamics and Self-Organization, Göttingen

Collisions involving granular particles exhibit dissipative kinematics. Hence, the motion of granular particles cannot be described using thermodynamics alone, warranting an examination of theories of non-equilibrium steady states and fluctuation theorems.

We examine the motion of a macroscopic wedge-shaped particle (constrained to only move along the x-axis) encountering dissipative collisions with granular gas particles. Based on a general stochastic model, we derive the full PDF of the wedge's motion. Contrary to what is observed for a Maxwell-Boltzmann gas, vanishingly small perturbations to the gas velocity PDF (e.g. via shaking) result in a steady-state drift velocity independent of wedge mass in the limit of a massive particle.

DY 35.6 Fri 10:45 H48

Collective particle dynamics crossing the freezing transition — •Markus Franke[1], Sebastian Golde[1,2], and Hans Joachim Schöpe[1,3] — [1]Johannes Gutenberg-Universität, Institut für Physik, Staudingerweg 7, 55128 Mainz, Germany — [2]Graduate School Material Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [3]Max-Planck-Institut für Polymerforschung, Postfach 3148, 55021 Mainz, Germany

We studied the collective particle dynamics in a hard sphere colloidal modell system of highly cross-linked polystyrene (PS) microgel particles dispersed in the good solvent 2-ethylnaphthalene. We determined the dynamics of the colloidal fluid around the main structure factor peak ($1.7<qR<5$) over a wide concentration range crossing the freezing transition point using dynamic light scattering. This gives access to the intermediate scattering function (ISF) which measures particle number density fluctuations or collecitve particle dynamics respectively. Further analyzation of the ISF dynamics shows that there is a significant difference in the relaxation mechanism of the collective density fluctuations of a fluid in the stable state and in the metastable state. In the nonequilibrium state the dynamics becomes heterogeneous in space and time. Once crossing the freezing point the fluid seperates in two fractions: One shows the dynamic signature of an equilibrium fluid and one displays an unequlibrium collective mode.

DY 35.7 Fri 11:00 H48

Mass loading induced dephasing in nanomechanical resonators — •Juan Atalaya — Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie, Karlsruher, Deutschland.

I study dephasing of an underdamped nanomechanical resonator subject to random mass loading of small particles. I propose a frequency noise model to describe dephasing due to attachment and detachment of particles at random points and particle diffusion along the resonator. This situation is commonly encountered in current mass measurement experiments using nanoelectromechanical (NEM) resonators. I discuss the conditions which can lead to inhomogeneous broadening and fine structure in the vibrational modes absorption spectra. I show that the spectra of the higher-order cumulants of the (complex) vibrational mode amplitude are sensitive to the parameters characterizing the frequency noise process. Hence, measurement of these cumulants can provide information not only about the mass but also about other parameters of the adsorbed particles (diffusion coefficient, attachment and detachment rates).

DY 35.8 Fri 11:15 H48

Brownian motion of a heated colloid — •Dipanjan Chakraborty[1,2], Manuel Gnann[3], Daniel Rings[4], Felix Otto[3], Frank Cichos[5], and Klaus Kroy[4] — [1]MPI-IS,Stuttgart, Germany — [2]IV[th] Physics Institute, University of Stuttgart, Germany — [3]MPI for Mathematics in Sciences, Leipzig, Germany — [4]ITP, University of Leipzig, Germany — [5]EXP-I, University of Leipzig, Germany

We establish a generalized Stokes-Einstein relation and an effective Markovian theory for hot Brownian motion [1-3]. Hot Brownian motion is the stochastic thermal motion of a nanoparticle maintained at an elevated temperature with respect to the ambient fluid, a scenario which is often encountered when a light-absorbing tracer particle diffuses in the focus of a laser. The temperature profile around the nanoparticle can be detected by a second laser, which can be exploited in photothermal particle tracking and spectroscopy techniques [4]. Our effective Markovian description serves as a valuable quantitative descritption for a wide variety applications using hot nanoparticles.

[1] D. Chakraborty, M. V. Gnann, D. Rings, J. Glaser, F. Otto, F. Cichos and K. Kroy, Europhys. Lett. 96(6), 60009 (2012).
[2] D. Rings, D. Chakraborty and K. Kroy, New Journal of Physics, 14(5), 53012 (2012).
[3] D. Rings, R. Schachoff, M. Selmke, F. Cichos, and K. Kroy, Phys. Rev. Lett., 105 (9), 090604 (2010)
[4] R. Radünz, D. Rings, K. Kroy, and F. Cichos, J. Phys. Chem. A 113 (9), 1674-1677 (2009)

DY 36: Statistical Physics in Biological Systems IV (joint with BP)

Time: Friday 9:30–12:45 Location: H44

DY 36.1 Fri 9:30 H44

Range expansions in heterogeneous environments — •Wolfram Möbius[1], Andrew W. Murray[2], and David R. Nelson[1] — [1]Department of Physics and FAS Center for Systems Biology, Harvard University, Cambridge, MA, USA — [2]FAS Center for Systems Biology and Department of Molecular and Cellular Biology, Harvard University, Cambridge, MA, USA

How species invade new territories and how these range expansions influence a population's genetic diversity are important questions in the field of population genetics. While the majority of work addressing these questions focuses on well-mixed environments, populations on a set of islands, or spatially uniform environments, much less is known about the consequences of an expanding population encountering obstacles such as lakes or mountain ranges.

We employ both experimental and theoretical methods to better understand range expansions in such types of environments. In particular, we established a system of bacteriophage T7 and *E. coli* as a bench-scale model system: The bacteriophage population spreads on a lawn of susceptible bacteria while a region of resistant bacteria poses an obstacle to the population wave and determines its shape. We use reaction-diffusion modeling and a phenomenological description to complement the experimental results. In addition, stochastic modeling allows us to study the fate of individual alleles in the course of the range expansion.

DY 36.2 Fri 9:45 H44

Chemical Warfare and Survival Strategies in Bacterial Range Expansions — Gabriele Poxleitner[1], •Markus Felix Weber[2], Elke Hebisch[1], Erwin Frey[2], and Madeleine Leisner[1] — [1]Center for NanoScience, Faculty of Physics, Ludwig-Maximilians-Universität München, Geschwister-Scholl-Platz 1, D-80539 Munich, Germany. — [2]Arnold-Sommerfeld Center for Theoretical Physics and Center for NanoScience, Faculty of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 Munich, Germany.

Bacterial communities represent complex and dynamic ecological systems. Different environmental conditions as well as bacterial interactions determine the establishment and sustainability of bacterial diversity. We study the competition of three Escherichia coli strains during range expansions on agar plates. In this bacterial model system, a colicin E2 producing strain C competes with a colicin resistant strain R and with a colicin sensitive strain S for new territory. Genetic engineering allows us to tune the growth rates of the strains and to study distinct ecological scenarios. These scenarios may lead to either single-strain dominance, pairwise coexistence, or to the coexistence of all three strains. In order to elucidate the survival mechanisms of the individual strains, we developed a stochastic agent-based model to capture the ecological scenarios in silico. In a combined theoretical

and experimental approach we are able to show that the level of biodiversity depends crucially on the composition of the inoculum, on the relative growth rates of the three strains, and on the effective reach of colicin toxicity.

DY 36.3 Fri 10:00 H44

Efficacy of ribosome-targeting antibiotics determined by a non-linear molecular race — •Philip Greulich[1,2], Martin R. Evans[2], and Rosalind J. Allen[2] — [1]Cavendish Laboratory, University of Cambridge — [2]School of Physics and Astronomy, University of Edinburgh

Many antibiotics in current clinical use target bacterial ribosomes. We present a dynamical model for the response of a cell to a ribosome-targeting antibiotic. In this model, the efficacy of the antibiotic is determined by a non-linear "molecular race" between binding of the antibiotic to ribosomes and net production of new ribosomes. The model points to a non-trivial growth-rate dependence of the minimum inhibitory concentration (MIC) and predicts a discontinuous transition at the MIC when the antibiotic concentration is varied: the growth rate abruptly drops to zero at this point. Furthermore, the efficacy of an antibiotic treatment depends on both its intensity and duration, and we can determine the relation to critical pharmacokinetic/-dynamic parameters for cell killing.

DY 36.4 Fri 10:15 H44

Information-theoretic vs. thermodynamic entropy production in autonomous sensory networks — •Andre Cardoso Barato and Udo Seifert — Universität Stuttgart, II. Institut für Theoretische Physik, Pfaffenwaldring 57 / III, D-70550, Stuttgart, Deutschland

Acquiring and processing information about the instantaneous state of the environment is a prerequisite for survival for any living system. Sensory and signal transducting networks have evolved to achieve this task under a variety of external conditions as, e.g., the work on bacteria like Escherichia coli has demonstrated so beautifully [1,2].

We determine the rate with which sensory networks acquire information about the changing external conditions. Comparing this rate with the thermodynamic entropy production that quantifies the cost of maintaining the network, we show that there is no universal bound restricting the rate of obtaining information to be less than this thermodynamic cost. These results obtained within a general bipartite model consisting of a stochastically changing environment that affects the instantaneous transition rates within the system are illustrated with a simple four-states model motivated by cellular sensing. On the technical level, we require and justify a new conjecture on the mutual information rate involving a non-Markovian process.

[1] H. C. Berg and M. Purcell, Biophys. J. 20, 193 (1977).

[2] G. Lan, P. Sartori, S. Neumann, V. Sourjik, and Y. Tu, Nature Phys. 8, 422 (2012).

DY 36.5 Fri 10:30 H44

Optimality principles for bacterial quorum sensing — •Bastian Drees and Ilka Bischofs — BioQuant, Center for Quantitative Analysis of Molecular and Cellular Biosystems at Heidelberg University, Heidelberg

Bacterial signaling networks have to meet the challenge of gathering information from noisy biochemical signals. We introduce a theoretical framework to quantify the accuracy of a signaling process in the presence of noise by defining the resolving power R, the minimal difference between two inputs that is required to separate two outputs. We show that many natural quorum sensing systems - which regulate cell density dependent behavior in bacteria - tend to optimize R at their switching points. We furthermore study how differences in the physical network design affect R as a function of input strength. We find different network architectures to optimize R in different input regimes, which could explain the diversity of quorum sensing architectures that is observed in nature. Together our results suggest the existence of a physics-driven optimal design principle for quorum sensing networks, which could be exploited to facilitate rational design choices in synthetic biology applications.

DY 36.6 Fri 10:45 H44

In vivo facilitated diffusion model — •Maximilian Bauer[1,2] and Ralf Metzler[1,3] — [1]Institute for Physics and Astronomy, Potsdam University, Germany — [2]Physics Department, Technical University of Munich, Germany — [3]Physics Department, Tampere University of Technology, Finland

In vitro transcription factors (TFs) alternate between three-dimensional bulk diffusion and sliding along DNA in order to quickly find their target on DNA. Recent experiments showed that also in the crowded interior of living cells TFs employ this facilitated diffusion mechanism. For a theoretical description of the situation in vivo we use a simple model of the bacterial genome embedded in an experimentally identified subvolume of the cell. Explicitly taking into account the configuration of DNA, our findings agree with experimental results and suggest that cells operate near to conditions which are optimal for target localization.

References: M. Bauer and R. Metzler, Biophys. J. 102, 2321 (2012) and submitted (2012)

DY 36.7 Fri 11:00 H44

Random walks of bacteria: How the motility pattern affects diffusion and chemotaxis — •Johannes Taktikos[1,2], Holger Stark[2], and Vasily Zaburdaev[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [2]Institut für Theoretische Physik, Technische Universität Berlin

The motility patterns of many bacterial species can be described with the help of random walk models. Swimming *E. coli* bacteria alternate almost straight runs with tumbling events, which randomize the direction of cell motion but keep a certain persistence. The majority of marine bacteria fully reverse their swimming direction after a tumbling event. However, the swimming strategy of the marine bacterium *V. alginolyticus* was recently discovered to consist of a strict sequence of reversal and completely randomizing flick events between the runs [Xie *et al.*, PNAS **108**, 2246 (2011)]. Remarkably, all these bacteria are capable to undergo chemotaxis – the ability to adjust their swimming direction to the concentration gradient of certain chemicals. We propose a generalized random walk model describing these motility patterns and use it to characterize the diffusion process of bacteria moving in chemically neutral environments. In the presence of a small gradient of a signaling chemical we calculate the chemotactic drift velocity along the gradient and analyze how it depends on the particular motility pattern. Our calculations show that the motility pattern alone cannot explain experimentally observed differences in the chemotactic behavior of *E. coli* and *V. alginolyticus* bacteria. This result suggests that the chemotactic internal response function of both bacteria differ.

15 min break

DY 36.8 Fri 11:30 H44

Impact of the cell division cycle on the dynamics of gene expression — •Veronika Bierbaum and Stefan Klumpp — Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Am Mühlenberg 1, 14476 Potsdam

Cell growth and division are elementary processes that influcence gene expression: While proteins are being synthesized, the change in cell volume due to cell growth leads to a dilution of protein concentration. To maintain a stable amount of protein, the protein content has to be doubled during the cell cycle. In this way, upon division, each daughter cell initiates the new cycle with the same amount of each protein. Protein synthesis and cell growth are typically not synchronous, such that the protein concentration varies over the cell division cycle. This variation may have an impact on the function of gene regulatory circuits.

We have developed a theoretical description of genetic regulatory systems that explicitly considers the cell division cycle to investigate its impact onto both simple and regulated systems of gene expression. We calculate the cell-to-cell variations in protein content of cells at different stages in the division cycle, and discuss to which extent these variations contribute to the extrinsic noise observed in single-cell experiments. While positive autoregulation can amplify the variation in protein concentration over the division cycle, negative autoregulation buffers against such variation. In addition, we investigate how the variability in the concentration influences the stability phases of bistable autoregulated systems.

DY 36.9 Fri 11:45 H44

Deducing underlying mechanisms from protein recruitment data — •Laurin Lengert and Barbara Drossel — TU Darmstadt, Hessen

The technique of fluorescently labelling proteins made it possible to visualize cellular proteins and to measure their distribution and dynamics within the cell. We focus on protein recruitment to a region in

the cell following a triggering event, such as irradiation. Often mechanistic models are used to fit the recruitment data. In such models, differential equations describe the changes in the concentrations of activated or bound proteins in the region of interest. The aim of such mechanistic models consists in evaluating rate constants, in identifying the proteins and reactions that are essential for the investigated process, and in obtaining evidence for processes that are not directly visible. By analyzing in a systematic way the recruitment curves generated by different simple models, we explain how the features of the recruitment curves reflect the properties of the underlying processes. This analysis also shows that a distinction between different models is not always possible from a given set of data. However, in many cases it is possible to suggest additional experiments with different protein concentrations that allow to distinguish between different models.

DY 36.10 Fri 12:00 H44

Scaling behaviour of knotted polymer rings in semidilute solutions — •Benjamin Trefz and Peter Virnau — Johannes Gutenberg Universität Mainz

Recently, the study of ring polymers and in particular their scaling behaviour in semidilute solutions [1, 2] has attracted considerable attention as a potential model system for the organization of DNA in chromosome territories. Building upon these studies, we investigate the influence of topology in melts of rings, which contain a certain knot type. These molecular dynamics simulations typically require around half a million particles as well as long run times and have been performed on graphic cards. Just like their unknotted counterparts, knotted rings form crumpled globules in the large N-limit. Knots tend to take up a large fraction of the chain for small rings, but become localized in the thermodynamic limit.

[1] J. Halverson, W. Lee, G. Grest, A. Grosberg, and K. Kremer, "Molecular dynamics simulation study of nonconcatenated ring polymers in a melt. I. Statics," The Journal of chemical physics, vol. 134, p. 204904, 2011.

[2] D. Reith, L. Mirny, and P. Virnau, "GPU Based Molecular Dynamics Simulations of Polymer Rings in Concentrated solution: Structure and Scaling," Progress of Theoretical Physics Supplement, vol. 191, pp. 135-145, 2011.

DY 36.11 Fri 12:15 H44

Molecular knots can pass through each other — •Peter Virnau and Benjamin Trefz — Uni Mainz

We propose a novel mechanism in which two molecular knots can pass through each other and effectively swap positions along a polymer strand. Associated free energy barriers in our molecular dynamics simulations only amount to a few k_BT, which may enable the interchange of knots on single DNA strands.

DY 36.12 Fri 12:30 H44

Sequence depending membrane-activity of amphiphilic polymers — •Marco Werner[1,2] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Technische Universität Dresden, Germany

Using the bond fluctuation model with explicit solvent we investigate self-assembled bilayer membranes interacting with random copolymers of hydrophilic/-phobic monomers under variation of the fraction of hydrophobic monomers, H. Our simulation data indicates that polymers localize at the membrane-solvent interface for values of $H \gtrsim 1/2$, where the polymer forms excess blobs in the solvent- and lipid tail phases to increase the number of preferred contacts to both environments. Excess blobs with hydrophobic majority are inhibited to freely expand in the lipid tail phase due to the self-organized packing of lipids. Therefore, the number of preferred polymer-environment contacts is balanced on both sides for values of H slightly larger than $H = 1/2$. Here, the polymer shows the largest membrane-activity as indicated by a maximum of polymer-induced permeability for solvent. Testing a larger population of random polymer sequences we demonstrate that heterogeneity of the amphiphilic components of the polymer on a scale smaller than the lipid tail length is a key feature for polymer-induced bilayer perturbations. This seems to be confirmed by testing polymers with alternating sequences with hydrophobic blocks of size smaller than the lipid tail length, for which the polymer-induced membrane permeability for solvent is larger than on average for the population of random copolymers.