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

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Overview of invited talks and sessions

(main lecture rooms HÜL 186, ZEU 118, ZEU 255, and KÖN Farb; poster P1, P3, and P4)

Plenary talk of the division DY

PV III	Mon	9:15–10:00	HSZ 01	**Linear and non-linear mechanics of biopolymer networks** — •David A. Weitz

Invited and topical talks in regular sessions (chronological order)

DY 2.10	Mon	12:45–13:15	ZEU 255	**Trends, questions and methods in molecular magnetism** — •Jürgen Schnack
DY 5.1	Mon	14:00–14:30	HÜL 186	**Collective dynamics in the cytoskeleton and swimming bacteria** — •Falko Ziebert, Sumanth Swaminathan, Shawn Ryan, Leonid Berlyand, Igor Aranson
DY 6.10	Mon	16:30–17:00	ZEU 255	**The multiscale dynamics of lightning and of terrestrial gamma-ray flashes** — •Ute Ebert
DY 13.1	Tue	10:15–10:45	ZEU 118	**Aggregation and Fragmentation of fractal-like particles in synthetic turbulent flows** — •Ulrike Feudel, Jens Zahnow, Joeran Maerz
DY 12.10	Tue	12:45–13:15	ZEU 255	**Non-equilibrium quantum relaxation, thermalization and boundary effects** — •Heiko Rieger, Ferenc Iglói
DY 17.1	Wed	10:15–10:45	ZEU 255	**Nonlinear Dynamics of Complex Hysteretic Systems** — •Günter Radons
DY 18.1	Wed	10:15–10:45	GÖR 226	**Impact of Single Links in Growing Networks** — •Jan Nagler, Marc Timme
DY 23.1	Wed	14:00–14:30	ZEU 255	**Nonlinear waves in localizing media** — •Sergej Flach
DY 34.1	Thu	14:00–14:30	ZEU 255	**Dynamics of particles in turbulent flow: size matters** — •Holger Homann, Jérémie Bec, Rainer Grauer
DY 33.10	Thu	16:30–17:00	HÜL 186	**Motion States in Intracellular Transport** — •Doris Heinrich

Invited talks of the joint symposium SKM-SYBE

See SKM-SYBE for the full program of the symposium.

SKM-SYBE 1.1	Fri	10:30–11:00	TRE Ma	**Microbial evolution in spatially-structured environments** — •Arjan de Visser
SKM-SYBE 1.2	Fri	11:00–11:30	TRE Ma	**Correlated mutations: Facts or artifacts?** — •Amnon Horovitz
SKM-SYBE 1.3	Fri	11:30–12:00	TRE Ma	**Macroscopic laws in bacterial genome evolution** — •Erik van Nimwegen
SKM-SYBE 1.4	Fri	12:00–12:30	TRE Ma	**The role of horizontal gene transfer in the evolution of bacterial genomes** — •Paul Higgs

Invited talks of focus session "Dense granular flow"

DY 1.1	Mon	10:15–10:45	HÜL 186	**Dense Inclined Flows of Granular Materials** — •James Jenkins
DY 1.2	Mon	10:45–11:15	HÜL 186	**Shear localization and shear alignment in granular flows** — •Tamás Börzsönyi, Balázs Szabó, Gábor Törös, Jim N. McElwaine, Robert E. Ecke, Sandra Wegner, Ralf Stannarius
DY 1.3	Mon	11:15–11:45	HÜL 186	**Flow of dense granular suspensions: an experimental study.** — •Anke Lindner, Claire Bonnoit, Eric Clement
DY 1.4	Mon	12:00–12:30	HÜL 186	**Erosion and mobility in granular avalanches over sloping beds** — •Anne Mangeney, Olivier Roche, Oldrich Hungr, Nicolas Mangold
DY 1.5	Mon	12:30–13:00	HÜL 186	**Confined granular materials: stability, chute flows and grain motion** — •Patrick Richard, Jean-Francois Metayer, Alexandre Valance, Renaud Delannay
DY 1.6	Mon	13:00–13:30	HÜL 186	**Convection and segregation of granular mixtures in almost filled containers** — •Ralf Stannarius, Frank Rietz

Invited talks of focus session "Statistical physics and thermodynamics of small systems"

DY 11.1	Tue	10:00–10:30	HÜL 186	**Doing small systems: Concepts, Role of Ensembles, Thermalization and Fluctuation Theorems** — •Peter Hänggi
DY 11.2	Tue	10:30–11:00	HÜL 186	**Microcanonical singularities in finite systems** — •Jörn Dunkel, Stefan Hilbert
DY 11.3	Tue	11:00–11:30	HÜL 186	**Recent progress in fluctuation theorems and free energy recovery** — •Felix Ritort
DY 11.4	Tue	11:45–12:15	HÜL 186	**Efficiencies and fluctuations in small out-of-equilibrium devices** — •Massimiliano Esposito
DY 11.5	Tue	12:15–12:45	HÜL 186	**Quantum Fluctuation Theorems** — •Michele Campisi
DY 11.6	Tue	12:45–13:15	HÜL 186	**Time-reversal symmetry relations: From the multibaker map to open quantum systems** — •Pierre Gaspard

Invited talks of the joint focus session "GPU computing" (with SOE)

DY 7.1	Mon	14:00–14:30	GÖR 226	**Applications of GPU-Computing in Statistical Physics** — •Peter Virnau
DY 7.2	Mon	14:30–15:00	GÖR 226	**Accelerating Monte Carlo Simulations in Statistical Physics with GPU's** — •David Landau, Junqi Yin

Invited talks of the joint focus session "Computational polymer physics - new developments" (with CPP)

DY 24.1	Wed	14:00–14:30	MOL 213	**Multiscale Simulation of Soft Matter: Challenges** — •Florian Müller-Plathe
DY 24.2	Wed	14:30–15:00	MOL 213	**A self-consistent field approach for crosslinked polymer materials** — •Friederike Schmid
DY 24.3	Wed	15:00–15:30	MOL 213	**Mechanical separation of short double stranded DNA: Effect of pulling geometry** — •Sanjay Kumar
DY 24.4	Wed	15:45–16:15	MOL 213	**Soft coarse-grained models for multi-component polymer melts** — •Marcus Müller
DY 24.5	Wed	16:15–16:45	MOL 213	**Simulations of Polymer Electrolytes for Lithium-Ion Batteries Highly Accurate Polarizable Potentials** — •Grant Smith

Sessions

DY 1.1–1.6	Mon	10:15–13:30	HÜL 186	**Focus Session: Dense Granular Flow**
DY 2.1–2.10	Mon	10:15–13:15	ZEU 255	**Statistical Physics (general)**
DY 3.1–3.9	Mon	10:15–13:00	ZEU 250	**Statistical Physics in Biological Systems I (organised by BP)**

DY 4.1–4.8	Mon	10:30–13:00	HSZ 03	**Graphene I (organised by TT)**
DY 5.1–5.11	Mon	14:00–17:00	HÜL 186	**Statistical Physics of Biological Systems II (organised by DY)**
DY 6.1–6.10	Mon	14:00–17:00	ZEU 255	**Quantum Dynamics, Decoherence, and Quantum Information I**
DY 7.1–7.2	Mon	14:00–15:00	GÖR 226	**Focus Session: GPU Computing (with SOE)**
DY 8.1–8.3	Mon	15:00–15:45	GÖR 226	**Focus Session: GPU Computing - Contributed Talks**
DY 9.1–9.16	Mon	14:00–18:30	HSZ 304	**Graphene II (organised by TT)**
DY 10.1–10.47	Mon	17:00–19:00	P4	**Posters I**
DY 11.1–11.6	Tue	10:00–13:15	HÜL 186	**Focus Session: Thermodynamics and Statistical Physics of Small Systems**
DY 12.1–12.10	Tue	10:15–13:15	ZEU 255	**Quantum Dynamics, Decoherence, and Quantum Information II**
DY 13.1–13.9	Tue	10:15–12:45	ZEU 118	**Fluid Dynamics and Turbulence I**
DY 14.1–14.5	Tue	14:00–15:15	ZEU 255	**Delay Dynamics**
DY 15.1–15.30	Tue	18:00–20:00	P1	**ISPS Intersectional Poster Session**
DY 16.1–16.4	Wed	10:30–11:30	HÜL 186	**Statistical Physics II**
DY 17.1–17.10	Wed	10:15–13:15	ZEU 255	**Nonlinear Dynamics I**
DY 18.1–18.1	Wed	10:15–10:45	GÖR 226	**Networks: From Topology to Dynamics I (with BP, SOE)**
DY 19.1–19.9	Wed	10:45–13:15	GÖR 226	**Networks: From Topology to Dynamics II (with BP, SOE)**
DY 20.1–20.11	Wed	10:15–13:00	KÖN Farb	**Glasses I (jointly with DF and CPP)**
DY 21.1–21.6	Wed	11:45–13:15	HÜL 186	**Thermodynamics and Statistical Physics of Small Systems (contributed talks)**
DY 22.1–22.15	Wed	14:00–18:00	HÜL 186	**Granular Matter/ Contact Dynamics**
DY 23.1–23.8	Wed	14:00–16:15	ZEU 255	**Nonlinear Waves/ Nonlinear Lattices**
DY 24.1–24.5	Wed	14:00–16:45	MOL 213	**Focus Session: Computational Polymer Physics - New Developments (jointly with CPP)**
DY 25.1–25.6	Wed	15:30–17:00	GÖR 226	**Networks: From Topology to Dynamics III (with BP, SOE)**
DY 26.1–26.7	Wed	16:30–18:15	ZEU 255	**Nonlinear Dynamics II**
DY 27.1–27.6	Wed	16:30–18:00	HSZ 02	**ISS Transport and Localization of Interacting Bosons I**
DY 28.1–28.11	Thu	10:15–13:15	HÜL 186	**Statistical Physics far from Equilibrium**
DY 29.1–29.9	Thu	10:15–12:30	ZEU 255	**Quantum Chaos I**
DY 30.1–30.9	Thu	10:15–12:30	ZEU 118	**Reaction-Diffusion Systems**
DY 31.1–31.7	Thu	10:45–13:00	ZEU 114	**Glasses and Glass Transition (jointly with CPP, DF)**
DY 32.1–32.9	Thu	10:15–13:00	ZEU 260	**Statistical Physics in Biological Systems III (organised by BP)**
DY 33.1–33.10	Thu	14:00–17:00	HÜL 186	**Brownian Motion, Stochastic Processes, Transport I**
DY 34.1–34.8	Thu	14:00–16:15	ZEU 255	**Fluid Dynamics and Turbulence II**
DY 35.1–35.6	Thu	14:30–16:00	BAR Schön	**ISS Transport and Localization of interacting Bosons II**
DY 36.1–36.10	Thu	14:00–16:45	ZEU 260	**Statistical Physics in Biological Systems IV (organised by BP)**
DY 37.1–37.5	Thu	16:00–17:15	ZEU 118	**Quantum Chaos II**
DY 38.1–38.2	Thu	16:30–17:00	ZEU 255	**Data Analysis and Stochastic Modeling I (jointly with UP)**
DY 39.1–39.6	Thu	17:00–18:30	ZEU 255	**Data Analysis and Stochastic Modeling II (jointly with UP)**
DY 40.1–40.42	Thu	17:00–19:00	P3	**Posters II**
DY 41.1–41.11	Fri	10:15–13:15	HÜL 186	**Brownian Motion, Stochastic Processes, Transport II**
DY 42.1–42.10	Fri	10:15–12:45	ZEU 255	**Critical Phenomena and Phase Transitions**
DY 43.1–43.9	Fri	10:15–12:30	ZEU 118	**Soft Matter**

Annual General Meeting of the Dynamics and Statistical Physics Division

Donnerstag, 17.3.2011 19:15–20:00 HÜL 186

- Bericht
- Verschiedenes

DY 1: Focus Session: Dense Granular Flow

Time: Monday 10:15–13:30 Location: HÜL 186

Invited Talk DY 1.1 Mon 10:15 HÜL 186

Dense Inclined Flows of Granular Materials — •James Jenkins — Cornell University, Ithaca, NY, USA

Hydrodynamic equations that result from classical kinetic theory, modified to incorporated energy lost in collisions, have been applied with success to dilute and moderately dense collisional granular flows. However, for inclined flows of identical sphere with concentrations above 49 per cent, their predictions do not agree with what is seen in numerical simulations and physical experiments. In this talk, we present a slightly modified hydrodynamic theory for inelastic spheres. The modification is the introduction of a length other than the diameter in the expression for the rate of collisional dissipation. This length is determined by a simple algebraic balance between the creation and destruction of particle chains. We apply the theory to dense collisional flows down both erodible and rigid, bumpy inclines and determine profiles of particle concentration, mean velocity, and fluctuation energy for steady, fully-developed flows of identical, frictional spheres. The profiles exhibit the features seen in the numerical simulations, and the integration of the energy balance through the depth of the flow results in an improvement of a velocity scaling employed in the interpretation of the physical experiments.

Invited Talk DY 1.2 Mon 10:45 HÜL 186

Shear localization and shear alignment in granular flows — •Tamás Börzsönyi[1], Balázs Szabó[1], Gábor Törös[1], Jim N. McElwaine[2], Robert E. Ecke[3], Sandra Wegner[4], and Ralf Stannarius[4] — [1]Research Institute for Solid State Physics and Optics, P.O. Box 49, H-1525 Budapest, Hungary — [2]Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK — [3]CNLS, Los Alamos National Laboratory, Los Alamos, NM 87545, USA — [4]Otto-von-Guericke-University, Institute of Experimental Physics, Universitätsplatz 2, D-39106 Magdeburg, Germany

Dense granular flows have been investigated experimentally and numerically in various geometries. For inclined plane flows we determine how the flow density decreases with increasing shear rate and also show, that the effective friction changes non-monotonously with increasing shear rate. This leads to a flow instability and shear localization. An other phenomenon is, that elongated grains get aligned in a simple shear flow. We study this flow alignment at low shear rates and find, that the alignment angle is independent of the shear rate, which is very similar to the flow alignment of liquid crystals. The shear induced orientation leads to a reduction of the effective friction of the material, which we determine experimentally.

T. Börzsönyi, R.E. Ecke and J.N. McElwaine, Phys. Rev. Lett. 103, 178302 (2009)

Invited Talk DY 1.3 Mon 11:15 HÜL 186

Flow of dense granular suspensions: an experimental study. — •Anke Lindner, Claire Bonnoit, and Eric Clement — PMMH-ESPCI, Paris, France

We study experimentally the flow of dense granular suspensions. The suspensions are made of mono-disperse, spherical, non-Brownian polystyrene beads immersed in density matched silicon oil. The volume fraction can be varied from 30 to 61%. We investigate the flow behaviour of these dense granular suspensions by the use of two complementary geometries: shear flow on an inclined plane and elongation flow during the detachment of a suspension droplet. We show that the inclined plane is a useful rheometer suited to explore the continuous transition from an effective viscous flow (high thicknesses) to dense "pseudo-granular" flow (low thicknesses). A mesoscopic length scale separates the two flow regimes and diverges when the volume fraction approaches the jamming limit. This set-up allows for measuring the viscosity directly up to volume fractions as large as 61%, which is impossible with a classical rheometer. In the case of the "pinch-off" experiments, we show that the elongation viscosity is identical to the one measured on an equivalent pure viscous liquid. Nevertheless, the final detachment regime is accelerated by the presence of grains. Moreover, we find a dynamical process independent of the grain concentration, but slightly dependent on the grain size.

15. min. break

Invited Talk DY 1.4 Mon 12:00 HÜL 186

Erosion and mobility in granular avalanches over sloping beds — •Anne Mangeney[1], Olivier Roche[2], Oldrich Hungr[3], and Nicolas Mangold[4] — [1]IPGP et Unviversité Paris Diderot, Paris, France — [2]LMV, IRD, Université de Clermont, Clermont Ferrand, France — [3]University of British Columbia, Vancouver, British Columbia, Canada — [4]LPGN, Université de Nantes, CNRS, France

We describe laboratory experiments of granular material flowing over an inclined plane covered by an erodible bed, designed to mimic erosion processes of natural flows. Two controlling parameters are the inclination of the plane and the thickness of the erodible layer. We show that erosion processes can increase the flow mobility of the grains by up to 40%. Erosion efficiency is shown to strongly depend on the slope of the topography. Entrainment begins to affect the flow at inclination angles exceeding a critical angle. Runout distance increases almost linearly as a function of the thickness of the erodible bed, suggesting that erosion is mainly supply dependent. Two regimes are observed during granular collapse: a first spreading phase with high velocity followed by a slow thin flow, provided either the slope or the thickness of the erodible bed is high enough. Surprisingly, erosion affects the flow mostly during the deceleration phase and the slow regime. The avalanche excavates the erodible layer immediately at the flow front. Waves are observed behind the front that help to remove grains from the erodible bed. Finally, simple scaling laws are proposed making it possible to obtain a first estimate of the deposit and emplacement time of a granular collapse over erodible bed.

Invited Talk DY 1.5 Mon 12:30 HÜL 186

Confined granular materials: stability, chute flows and grain motion — •Patrick Richard, Jean-Francois Metayer, Alexandre Valance, and Renaud Delannay — Institut de Physique de Rennes, Universite de Rennes I, UMR CNRS 6251, Campus de Beaulieu, 263 av. General Leclerc, 35042 Rennes cedex, FRANCE

We present experimental and numerical results of 3D confined granular materials. We address the issue of the role of the lateral boundaries on the stability and on the flow of such systems. In particular, we find that the presence of flat frictional lateral walls greatly alters the flow features as soon as the width of the flowing layer is of the order of the spacing between the walls or greater. The properties of such confined flow differ significantly from those of unconfined flows. The kinematic properties as well as the stress analysis are presented in details. The shear rate is constant and independent of inclination over much of the flowing layer. In the direction normal to the free surface, the solid volume fraction increases on a scale equal to half the flowing layer depth. Beneath a critical depth grains exhibit creeping and intermittent cage motion similar to that in glasses, causing gradual weakening of friction at the walls. These results underline the open problem of defining a single rheology for confined granular flows.

Invited Talk DY 1.6 Mon 13:00 HÜL 186

Convection and segregation of granular mixtures in almost filled containers — •Ralf Stannarius and Frank Rietz — Otto-von-Guericke-Universität Magdeburg, Institut für Experimentalphysik

When the free volume of granular material in a closed container goes to zero, dynamical degrees of freedom become more and more restricted, the system jams. Finally, agitation with external forces does no longer change the compact granulate structure. Interestingly, during this transition qualitatively new dynamical phenomena are observed. Slow processes become effective [1] that are otherwise absent or masked in containers with low fill level. They dominate dynamical processes and restructuring in almost full containers. We describe convection and segregation phenomena and their complex mutual interrelations. Respective to shaken containers with high fluidization, different symmetries of the dynamical structures as well as new coupling effects between segregation and dynamics are found.

[1] F. Rietz and R. Stannarius, Phys. Rev. Lett. 100, 078002 (2008).

DY 2: Statistical Physics (general)

Time: Monday 10:15–13:15 Location: ZEU 255

DY 2.1 Mon 10:15 ZEU 255

A new factorizacion form for the partition function in quantum open systems — •Juan-Diego Urbina and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, D-93053 Regensburg, Germany

We adress the microscopic description of quantum systems strongly coupled with a linear bath (particularly at very low temperatures) in the framework of the Caldeira-Legget model for the environment. By careful revision of the huge literature on the subject, we support our claim that a weak coupling assumption is inconsistenly done at a very critical stage in basically all thermodynamic calculations. This extra assumption (based on its exactness for harmonic systems) is expressed through a factorized form for the full system-plus-environment equilibrium partition funtion $Z(\beta)$, in terms of the partition function of the bath $Z_{B}(\beta)$ and the effective partition function of the system $Z_{eff}(\beta)$. We will show how the explicit construction of the full partition function of a non-harmonic system (the particle in a box interacting with a bath of harmonic oscilators) suggests a different picture where an extra universal factor, representing neither the system nor the bath but the interaction between them, is naturally added to $Z(\beta)$.

DY 2.2 Mon 10:30 ZEU 255

Canonical thermalization — •Peter Reimann — Universität Bielefeld

For quantum systems which are weakly coupled to a much bigger environment, thermalization of possibly far from equilibrium initial ensembles is demonstrated: for sufficiently large times, the ensemble is for all practical purposes indistinguishable from a canonical density operator under conditions that are satisfied under many, if not all, experimentally realistic conditions [1].

[1] P. Reimann, New J. Phys. 12, 055027 (2010); Phys. Rev. Lett. 101, 190403 (2008)

DY 2.3 Mon 10:45 ZEU 255

Generalization of the parQ method to the grand canonical ensemble — •René Haber and Karl Heinz Hoffmann — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

We present the extension of our transition matrix Monte Carlo method parQ[1] to the grand canonical ensemble. It calculates the density of states $g(E, N)$ in a given energy and particle-number range from transition data. The method is easily parallelizeable, as one can fill the transition matrix from independent simulations running on different processors. It is also flexible in terms of the sampling scheme used as it can be adopted to standard Metropolis sampling, parallel tempering, Wang-Landau sampling as well as probably other sampling methods. At the end of the simulation the eigenvector corresponding to the eigenvalue 1 is calculated, which can be identified as the density of states. Results from simulations of simple Lennard-Jones systems as well as more complex hexadecane systems are presented.

[1] F. Heilmann and K. H. Hoffmann. Europhysics Letters, 70(2):155-161, 2005.

DY 2.4 Mon 11:00 ZEU 255

Binary nucleation: molecular dynamics simulation of the n-nonane/methane system — •Stephan Braun and Thomas Kraska — Institute of Physical Chemistry, University of Cologne, Luxemburger Str. 116, D-50939 Köln

Molecular dynamics simulation is employed to investigate the vapour-liquid nucleation of the binary system n-nonane/methane. The supersaturation of the system is achieved by cooling down the system during expansion in order to closely mimic the real process which is in practice applied, for example, to separate heavy compounds from natural gas.

By means of molecular dynamics simulations it is possible to obtain several details of the nucleation process, which are difficult or impossible to obtain from experiments. This regards the early stages of nucleation and growth taking place on the nanosecond time scale. Properties such as the nucleation rates or the critical cluster size can be determined even at high pressures. Furthermore, the determination of the composition of the clusters and the cluster structure can help to understand the nucleation process. Simulations where performed at different temperatures and densities for systems with various mole-fractions. The resulting nucleation rates have been compared to nucleation theory and the obtained clusters where analyzed with regard to structure and composition to understand possible effects on the nucleation process.

DY 2.5 Mon 11:15 ZEU 255

Non-metal-to-metal transition driven by van der Waals forces in an interacting polaronic gas — •Pascal Quémerais[1,2] and Gennady N. Chuev[3,4] — [1]Institut Néel, CNRS-UJF, Grenoble, France — [2]Max-Planck-Institute for Physics of Complex Systems, Dresden, Germany — [3]Russian Academy of Science, Pushchino, Moscow Region, Russia — [4]Max-Planck-Institute for Mathematics in the Sciences, Leipzig, Germany

We develop a model treating non-degenerate Fröhlich polarons with long-range Coulomb interactions at low densities and temperatures. Starting from the dilute regime, we show that at strong electron-phonon coupling, the collective properties of polarons are mainly governed by dipolar interactions in the crystallized state (Polaron Wigner Crystal) at zero temperature. At larger temperature in the liquid state, the dipolar interactions corresponds to the London dispersion forces, i.e. induced dipole-dipole van der Waals interactions. At a critical density, these forces provoke a non-metal to-metal transition by means of a polarization catastrophe which results in a polaron dissociation. The 3D and 2D case will be discussed as well as possible applications to real systems (metal-ammonia solutions, high-Tc cuprates).

[1] G.N. Chuev, P. Quémerais *J. Chem. Phys.* **127**,244501 (2007)
[2] G.N. Chuev, P. Quémerais *J. Chem. Phys.* **128**, 144503 (2008)
[3] P. Quémerais, G.N. Chuev, *New Jour. Phys.* **12** 023030 (2010)

DY 2.6 Mon 11:30 ZEU 255

Domain walls and Schramm-Loewner evolution in the random-field Ising model — •Jacob Stevenson and Martin Weigel — Johannes Gutenberg Universität, Mainz

The concept of Schramm-Loewner evolution provides a unified description of domain boundaries of many lattice spin systems in two dimensions, possibly even including systems with quenched disorder. Here, we study domain walls in the random-field Ising model. Although, in two dimensions, this system does not show an ordering transition to a ferromagnetic state, in the presence of a uniform external field spin domains percolate beyond a critical field strength. Using exact ground state calculations of very large systems, we examine ground state domain walls near this percolation transition finding strong evidence that they are conformally invariant and satisfy the domain Markov property, implying compatibility with Schramm-Loewner evolution with parameter $\kappa = 6$. These results might pave the way for new field-theoretic treatments of systems with quenched disorder.

15 min. break.

DY 2.7 Mon 12:00 ZEU 255

Monte Carlo simulations without detailed balance — •Martin Weigel[1] and Heitor Fernandes[2] — [1]Institut für Physik, KOMET 331, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55127 Mainz — [2]Instituto de Física, Universidade Federal do Rio Grande do Sul, CP 15051, 91501-970 Porto Alegre RS, Brazil

Monte Carlo simulations are used to study simple systems where the underlying Markov chain satisfies the necessary condition of global balance but does not obey the more restrictive condition of detailed balance. Here, we show that non-reversible Markov chains can be set up that generate correct stationary distributions, but reduce or eliminate the diffusive motion in phase space typical of the usual Monte Carlo dynamics. Our approach is based on splitting the dynamics into a set of replicas with each replica representing a biased movement in reaction-coordinate space. This introduction of an additional bias in a given replica is compensated for by choosing an appropriate dynamics on the other replicas such as to ensure the validity of global balance. First, we apply this method to a mean field Ising model, splitting the system into two replicas: one trying to increase magnetization and

the other trying to decrease it. For this simple test system, our results show that the altered dynamics is able to reduce the dynamical critical exponent. Generalizations of this scheme to simulations of the Ising model in two dimensions are discussed.

DY 2.8 Mon 12:15 ZEU 255

Magnetic Friction: Stokes to Coulomb — •Sebastian Angst, Martin P. Magiera, Alfred Hucht, and Dietrich E. Wolf — Fakultät für Physik, Universität Duisburg-Essen, D-47057 Duisburg

In recent years, the interest in magnetic contribution to friction due to spin correlations has been increased. One intriguing aspect is the energy dissipation by reason of spin waves induced by a moving tip above a substrate of Heisenberg spins [1], modeled with the Landau-Lifshitz-Gilbert equation. In addition, magnetic friction occurs in a driven Ising model [2] investigated by using Monte-Carlo simulations and analytical methods [3]. Until now the dependency of the friction force f on the velocity v is characterized by a Stokes-like behavior for Heisenberg spins and a Coulomb-like behavior for the Ising model.

Here we show that the qualitative characteristics of $f(v)$ are independent on model details like the spin dimensionality, the model geometry or the simulation methods. Using an Ising model in a moving field of different shapes, we demonstrate that the relevant quantity is the time evolution of the field at a given site [4].

[1] M.P. Magiera et al., EPL 87, 26002 (2009)
[2] D. Kadau et al., Phys. Rev. Lett. 101, 137205 (2008)
[3] A. Hucht, Phys. Rev. E 80, 061138 (2009)
[4] to be published

DY 2.9 Mon 12:30 ZEU 255

Atomistic Modeling of Electromigration — •Andreas Latz and Dietrich E. Wolf — Fakultät für Physik, Universität Duisburg-Essen, D-47057 Duisburg

Strong electric fields lead to a directed movement of atoms in a current carrying conductor. This mass transport is called electromigration and is induced by interactions of the conducting electrons (wind force) and the electric field (direct force) with the atoms. Due to the high current densities (10^6A/cm^2) in integrated circuits, electromigration-induced short circuits and voids are a problem.

We use the Kinetic Monte Carlo method to simulate the dynamics of voids in silver nanowires at the atomic scale. The dependence of the void form on the crystallographic orientation of the nanowire and the direction of the electric field will be shown. In a (001)-oriented silver wire squarelike voids can be observed, in contrast to a (111)-oriented wire, in which voids are triangular and pointed in migration direction. The simulation results are in agreement with experimental observations made with monocrystalline silver nanowires in the SFB 616 "Energy dissipation at surfaces".

Topical Talk DY 2.10 Mon 12:45 ZEU 255

Trends, questions and methods in molecular magnetism — •Jürgen Schnack — Universität Bielefeld, Universitätsstr. 25, D-33615 Bielefeld

The field of molecular magnetism has seen a rapid development during the past 15 years. Initially driven by the discovery of slow magnetic relaxation and magnetic hysteresis on the molecular level, the field nowadays spreads out into several directions as for instance quantum manipulation of molecular qubits, manipulation and investigation of deposited magnetic molecules, rational design of magnetic molecules with large anisotropy barriers or with large ground-state degeneracies for huge magnetocaloric effects. Such activities rise questions of reachable decoherence times or addressability of deposited molecules as well as of methods to theoretically describe both the molecules as well as the desired processes. Theoretical descriptions, that mostly aim at a complete quantum description, have advanced a lot in the field. A few of them will be highlighted.

DY 3: Statistical Physics in Biological Systems I (organised by BP)

Time: Monday 10:15–13:00 Location: ZEU 250

Invited Talk DY 3.1 Mon 10:15 ZEU 250

High throughput microscopy for systems biology: from genome-wide profiling to the analysis of protein complexes — •Jan Ellenberg — EMBL, Heidelberg, Germany

Despite our exponentially growing knowledge about the human genome, we do not know all human genes required for some of the most basic functions of life, such as cell division. Furthermore we do not know how the proteins encoded by these genes work together to carry out the underlying cellular processes. We have developed high throughput microscopy platforms to systematically identify genes and characterize the function of their encoded proteins. For gene identification, we have integrated methods for gene silencing by RNA interference with phenotyping by time-lapse microscopy and computational image processing into one high throughput pipeline. This technology platform allowed us to carry out a genome-wide profiling of each of the ~ 21 000 human protein-coding genes by two day live imaging of fluorescently labeled chromosomes. Quantitative image analysis identified hundreds of human genes involved in several basic biological functions including cell division, migration and survival. Computational clustering of the phenotypic signatures of cell division genes allowed us to group them into different categories and make predictions about their function. To analyze the predicted function of proteins in phenotypic clusters, we are currently developing high throughput fluorescence microscopy and biophysical methods to systematically study their localization, interactions and assembly in the physiological context of the living cell.

DY 3.2 Mon 10:45 ZEU 250

The flow field of an individual bacterium and its implications for cell-cell and cell-surface interactions — Knut Drescher[1], •Jörn Dunkel[1], Luis Cisneros[2], Sujoy Ganguly[1], and Raymond Goldstein[1] — [1]DAMTP, University of Cambridge, Wilberforce Road, Cambridge CB3 0WA, UK — [2]Department of Physics, University of Arizona, 1118 E 4th St, Tucson, AZ 85721, USA

Swimming bacteria create microflows that have been commonly assumed to play an important role in their pair-interactions and during scattering with surfaces. Here, we present the first direct measurement of the bacterial flow field generated by individual *E. coli*. Our experiments allow us to infer the relative importance of fluid dynamics and noise for cell-cell and cell-surface scattering. We find that rotational diffusion due to thermal and intrinsic stochasticity drowns the effects of long-range hydrodynamic pair-interactions, implying that physical interactions between bacteria are dominated by steric collisions and near-field lubrication forces. This closely links collective motion in bacterial suspensions to self-organization in driven granular systems, assemblages of biofilaments, and animal flocks. We further conclude that long-range fluid dynamics is negligible for the scattering of bacteria with surfaces. However, once a bacterium has aligned with the surface through an inelastic collision and swims along the surface at a distance of less than two microns, the self-generated flow traps the bacterium and large fluctuations in orientation are needed to escape. Since our results are based on purely mechanical properties, they are expected to apply to a wide range of bacteria.

DY 3.3 Mon 11:00 ZEU 250

The energy-speed-accuracy tradeoff in sensory adaptation — Ganhui Lan[1], •Pablo Sartori[2], Silke Neumann[3], Viktor Sourjik[3], and Yuhai Tu[1] — [1]IBM T. J. Watson Research Center, Yorktown Heights, NY 10598, USA — [2]Max Planck Institute for the Physics of Complex Systems, Dresden 01187, Germany — [3]Zentrum fur Molekulare Biologie der Universitat Heidelberg, Heidelberg, Germany

Adaptation is a fundamental function of living systems. The benefits of adaptation in sensory systems are well known, but its costs remain poorly understood. By analyzing a stochastic model of the generic feedback circuit responsible for sensory adaptation, we show that adaptation processes are inherently dissipative and continuous energy consumption is required to stabilize the adapted state. We derive a universal relation among energy dissipation rate, adaptation speed, and the maximum adaptation accuracy from our model. We demonstrate how this general energy-speed-accuracy (ESA) relation applies to the E. coli chemosensory system, where hydrolysis of the S-adenosylmethionine (SAM) molecules drives the near-perfect adap-

tation of the system and maintains its high sensitivity in a wide range of backgrounds. We identify the key requirements for an adaptive network to achieve its maximum accuracy with a given energy budget. These requirements are met in the E. coli chemotaxis pathway, making it highly efficient. Moreover, direct measurements confirm that adaptation slows down as cells gradually de-energize in medium without nutrients.

DY 3.4 Mon 11:15 ZEU 250

Looped Star Polymers: Lessons for Bacterial Chromosome Packaging — •Dieter Heermann, Miriam Fritsche, and Pascal Reiss — Institute für Theoretische Physik, Universität Heidelberg

Inspired by the topological organization of the circular Escherichia coli chromosome, which is compacted by separate domains, we study a polymer architecture consisting of a central ring to which either looped or linear arms are attached. A transition from a spherical to a toroidal shape takes place as soon as the inner ring becomes large enough for the attached arms to fit within its circumference. Building up a torus, the system flattens depending on the effective bending stiffness of the chain induced by entropic repulsion of the attached loops and, to a lesser extend, linear arms. We propose that the natural formation of a toroidal structure induced by a specific chromosome topology could be one driving force, among others, that nature exploits to ensure proper packaging of the genetic material within a rod-shaped nucleoid.

15 min. break

DY 3.5 Mon 11:45 ZEU 250

Heterogeneous timing of gene induction as a regulation strategy — •Noreen Walker[1,2], Georg Fritz[1,2], Sonja Westermayer[2], Judith Megerle[2], Joachim Raedler[2], and Ulrich Gerland[1,2] — [1]Arnold Sommerfeld Center for Theoretical Physics — [2]Department of Physics, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 München

Heterogeneity within a genetically homogeneous population is a common phenomenon in nature. While it has long been known that noise in gene expression leads to heterogeneity in protein levels, recent studies also demonstrated heterogeneity in the timing of gene induction. When a colony of E. coli cells is suddenly exposed to a new sugar, the onset time for expression of the specific sugar utilization system is broadly distributed, if the sugar concentration is low [1]. Whereas the underlying mechanism has been characterized [1], it is currently unclear whether this heterogeneous timing is a side effect or a genuine strategy to optimize growth and survival. Here, we first present further experimental evidence for heterogeneous timing. We then perform a theoretical analysis of the cost and benefit of different regulation strategies for gene induction within a coarse-grained growth model. We find that at low sugar concentrations, heterogeneous timing can indeed be an optimal regulation strategy, while a homogeneous response is favorable at high sugar concentrations.

[1] J. Megerle et al., Biophys. J. **95**, 2103-2115 (2008)

DY 3.6 Mon 12:00 ZEU 250

Resolution of gene regulatory conflicts caused by combinations of antibiotics — •Tobias Bollenbach[1,2] and Roy Kishony[1] — [1]Harvard Medical School, Boston, MA, USA — [2]IST Austria, Klosterneuburg, Austria

Regulatory conflicts occur when two signals, which individually trigger opposite cellular responses, are present simultaneously. Here, we investigate how such gene regulation conflicts are resolved in the bacterial response to antibiotic combinations. We use an *Escherichia coli* promoter-GFP reporter library to study the genome-wide transcriptional response to either additive or antagonistic drug pairs at fine two-dimensional resolution of drug concentration. Using principal component analysis (PCA), we find that this complete dataset can be almost fully characterized as a surprisingly simple linear sum of only two components. The first component, accounting for over 70% of the variance in the data set, represents the response to the net effectiveness of the drug combination in inhibiting growth. The second component describes how regulatory conflicts are resolved for genes that respond differently to each of the individual drugs. We find that for the non-interacting drug pair, conflicts are resolved by linearly interpolating the two single drug responses, while for the antagonistic drug pair, the drug that has the stronger impact on growth dominates the transcriptional response. Importantly, for a given drug pair, the same strategy of conflict resolution is used for almost all genes. These results provide a recipe for predicting gene expression responses to drug combinations, which may lead to a more rational design of combination treatments.

DY 3.7 Mon 12:15 ZEU 250

Modelling the dynamics of micro-swimmers — •Eva Baresel and Rudolf Friedrich — Insitute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, D-48149 Münster

The motion of self-propelled flagellated bacteria consists of two different modalities: "running" if all flagella rotate counter-clockwise or "tumbling" if at least one flagellum rotates clockwise. As a model for these bacterial motors we consider the dynamics of an ensemble of swimming objects which are composed of two rigidly connected point vortices. The single objects are able to show translation or rotation depending on the circulations of the single point vortices. We discuss the collective behaviour for several of these objects and the resulting velocity fields by means of numerical calculations.

DY 3.8 Mon 12:30 ZEU 250

Onset of Collective Motion due to Escape and Pursuit — •Pawel Romanczuk[1], Vishwesha Guttal[2], Lutz Schimansky-Geier[1], and Iain D. Couzin[2] — [1]Department of Physics, Humboldt Universität zu Berlin, Germany — [2]Department of Ecology and Evolutionary Biology, Princeton University, USA

Recent studies suggest that noncooperative behavior such as cannibalism may be a driving mechanism of collective motion in mass migrating insects such as desert locusts [1]. We have shown in a biologically motivated model of individuals interacting via escape and pursuit interactions associated with cannibalism the emergence of large scale collective motion [2]. Furthermore we were able to reproduce experimental results and make specific prediction from our modelling approach [3]. Here we focus on a generelized model of self-propelled particles interacting via selective attraction or repulsion to approaching or moving-away individuals. We identify conditions for large scale collective motion in our model and discuss the onset of collective motion as an evolutionary stable strategy (ESS) in the context of mass migration of desert locusts under threat of cannibalism.

[1] S. J. Simpson *et. al.*, Proc. Natl. Acad. Sci. USA, 103, 4152 (2006)

[2] P. Romanczuk *et. al.*, Phys. Rev. Lett., 102, 010602 (2009)

[3] S. Bazazi *et. al.*, Proc. Roy. Soc. B, doi 10.1098/rspb.2010.1447

DY 3.9 Mon 12:45 ZEU 250

Spontaneous spiking in presence of an autaptic feedback loop — Yunyun Li[1], •Gerhard Schmid[1], Peter Hänggi[1], and Lutz Schimansky-Geier[2] — [1]Universität Augsburg, Germany — [2]Humboldt Universität zu Berlin, Germany

The effect of intrinsic channel noise on the dynamics of a neuronal cell with a delayed feedback loop is investigated [1]. The loop is based on the so-called autapse phenomenon in which dendrites establish not only connections to neighboring cells but as well to its own axon. The modeling is achieved in terms of a stochastic Hodgkin-Huxley model containing such a built in delayed feedback. The fluctuations stem from intrinsic channel noise, being caused by the stochastic nature of the gating dynamics of ion channels. The delayed feedback manifests itself in the occurrence of bursting and a rich multimodal interspike interval distribution, exhibiting a delay-induced reduction of the spontaneous spiking activity at characteristic frequencies. Moreover, a specific frequency-locking mechanism is detected for the mean interspike interval.

[1] Y. Li, G. Schmid, P. Hänggi, L. Schimansky-Geier, Phys. Rev. E, in press (arXiv:1009.5198)

DY 4: Graphene I (organised by TT)

Time: Monday 10:30–13:00 Location: HSZ 03

Invited Talk DY 4.1 Mon 10:30 HSZ 03

Spin-orbit coupling in graphene: single layer, bilayer, trilayer, and graphite — •Jaroslav Fabian — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

In graphene at the Fermi level the spin-orbit splitting is about 25 μeV. Our first-principles [1] and tight-binding [2] investigations show that the splitting originates from d orbitals that hybridize with the p_z ones and form the π band. In an external transverse electric field there is an additional splitting of the bands (the Bychkov-Rashba effect). This extrinsic splitting is solely due to the hybridization of the σ and π orbitals, and is about 10 μeV for typical fields of 1 V/nm. In bi- and trilayer graphene, and in graphite, the intrinsic splitting is also due to the d electrons. The extrinsic splitting at K points has the intrinsic value, of 25 μeV; somewhat away from K the splitting saturates to the Bychkov-Rashba value similar to the single layer graphene. This work is supported by the DFG SFB 689.

[1] M. Gmitra, S. Konschuh, C. Ertler, C. Ambrosch-Draxl, and J. Fabian, *Band-structure topologies in graphene: spin-orbit coupling effects from first principles,* Phys. Rev. B 80, 235431 (2009).
[2] S. Konschuh, M. Gmitra, and J. Fabian, *Tight-binding theory of the spin-orbit coupling in graphene,* Phys. Rev. B 82, 245412 (2010).
[3] C. Ertler, S. Konschuh, M. Gmitra, and J. Fabian, *Electron spin relaxation in graphene: the role of the substrate,* Phys. Rev. B(R) 80, 041405 (2009)

DY 4.2 Mon 11:00 HSZ 03

Electron transport and spins in graphene — •Jan Bundesmann[1], Michael Wimmer[2], and Klaus Richter[1] — [1]Institut für theoretische Physik, Universität Regensburg, Deutschland — [2]Instituut-Lorentz, TU Leiden, The Netherlands

The weak atomic spin-orbit interaction (SOI) in graphene leads to the assumption of large spin relaxation times. Simulations, taking into account spin-scattering from charged impurities in the substrate, yielded spin relaxation times [1] much larger than spin injection experiments in graphene [2,3].
Still assuming that the model of spins scattered at charged impurities is correct, we implemented a tight-binding model for graphene in the presence of SOI.
In our work the focus lies on the effects of SOI on electron transport (i.e. low energy excitations and the role of symmetry classes manifested, e.g., in weak localization) as well as its influence on spin transport in the diffusive regime.

[1] Ertler, Konschuh, Gmitra and Fabian, Phys. Rev. B **80**, 041405(R) (2009)
[2] Tombros, Josza, Popinciuc, Jonkman and van Wees, Nature **448**, 571 (2007)
[3] Han, Pi, McCreary, Li, Wong, Swartz and Kawakami, Phys. Rev. Lett. **105**, 167202 (2010)

DY 4.3 Mon 11:15 HSZ 03

Electric field control of spin rotation in bilayer graphene — •Paolo Michetti[1], Patrik Recher[1], and Giuseppe Iannaccone[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg — [2]Dipartimento di Ingegneria dell'Informazione, Universita' di Pisa, Via G. Caruso 16 - 56122 - Pisa (Italy)

The manipulation of the electron spin degree of freedom is at the core of the spintronics paradigm, which offers the perspective of reduced power consumption, enabled by the decoupling of information processing from net charge transfer.

Graphene, with its potentially long spin-coherence length, is a promising material for spin-encoded information transport. However, the small spin-orbit interaction is also a limitation for the design of conventional devices based on the canonical Datta-Das spin field-effect transistors. An alternative solution can be found in magnetic doping of graphene or, as discussed in the present work, in exploiting the proximity effect between graphene and ferromagnetic oxides (FOs). Graphene in proximity to FO experiences an exchange proximity interaction, that acts as an effective Zeeman field for electrons in graphene, inducing a spin precession around the magnetization axis of the FO.

Here we show that in an appropriately designed double-gate field-effect transistor, with a bilayer graphene channel and FO used as a gate dielectric, spin-precession of carriers can be turned ON and OFF with the application of a differential voltage to the gates. This feature is directly probed in the spin-resolved conductance of the bilayer.

DY 4.4 Mon 11:30 HSZ 03

Graphene Superlattices Studied by Ab-Initio Methods — •Lars Matthes, Karsten Hannewald, Jürgen Furthmüller, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Jena, Germany

The peculiar electronic properties of graphene have stimulated extensive research towards graphene-based electronics. Hereby, of particular interest are quasi-1D structures such as graphene nanoribbons [1] or, more recently, graphene superlattices [2] which allow a systematic tuning of the band structure. An impressive example for such modifications has been predicted by recent Kronig-Penney-type calculations [2] for a single graphene layer subject to a 1D periodic potential where a rather counterintuitive anisotropic renormalization of the Fermi velocity due to the Klein paradox is expected. Here, we present first-principles DFT calculations of graphene superlattices using the VASP code. The influence of the periodic external potential on the charge-carrier redistribution and corresponding screening effects is investigated in detail. The resulting consequences for the ab-initio band structure including anisotropy effects are studied and compared with analytical calculations based on the Dirac Hamiltonian. Deviations due to self-consistent inclusion of screening effects and nonlinear dispersions are analyzed. Finally, consequences for the practical realization of graphene superlattices with 1D transport properties are discussed.

[1] See, e.g., U. Treske, F. Ortmann, B. Oetzel, K. Hannewald, F. Bechstedt, phys. stat. sol. (a) 207, 304 (2010)
[2] C-H. Park et al., Nature Phys. 4, 213 (2008)

15 min. break

DY 4.5 Mon 12:00 HSZ 03

Nanomachining a Tunneling Barrier in Graphene — •Patrick Barthold and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover, Germany

Utilizing an atomic force microscope, graphene is nanomechanically structured. It is selectively folded in order to produce two dimensional systems that are only a few Angstrom apart. Aditionally, insulating lines are crafted within the sample without inducing any chemical contamination which, in contrast, is inevitable, when traditional structuring methods, e.g. etching procedures, are used. Such manufactured tunneling barriers are characterized by electrical transport measurements at low temperatures on an exemplary few-layer sample. In the conductivity through this barrier we find a gap around zero bias voltage. The conductivity shows a backgate dependent opening of a band gap in the sample. Due to the asymmetric design of the emitter and collector we find an asymmetry in the backgate dependent conductivity through the barrier.

DY 4.6 Mon 12:15 HSZ 03

Evidence for Josephson-coupled superconducting regions at the interfaces of highly oriented pyrolytic graphite — •Ana Ballestar, Jose Barzola-Quiquia, and Pablo Esquinazi — Abteilung für Supraleitung und Magnetismus, Institut für Experimentelle Physik II, Universität Leipzig, Linnéstrasse 5, 04103 Leipzig, Germany

The first observation of superconductivity in doped graphite goes back to 1965 when it was observed in the potassium graphite intercalated compound C8K. A considerable amount of studies had reported this phenomenon in intercalated graphite compounds or doped graphite, however the superconducting properties of pure graphite are still under discussion. Indirect evidences for superconductivity at graphite interfaces have been recently published. In order to better understand these interfaces properties, we prepared micro structured samples (Lamellas) from pure highly oriented pyrolitic graphite. By reducing the dimension in the in plane configuration to $\sim$ 200 nm we can measure the electrical response of graphite interfaces. We obtained evidence for the existence of Josephson-coupled quasi two dimensional superconducting regions. Temperature dependence of the voltage, as well as

I(V) characteristic curves indicate that superconductivity exists even above 150 K. The results support the view that HOPG is a system with interfaces containing non-percolative superconducting domains immersed in a semiconducting graphene-based matrix.

DY 4.7 Mon 12:30 HSZ 03

Tuning the electronic structure of graphene through ac fields: dynamical gaps and polarization effects — •Hernan L. Calvo[1,2], Horacio M. Pastawski[1], Stephan Roche[3], and Luis E. F. Foa Torres[1] — [1]Instituto de Fisica Enrique Gaviola and FaMAF UNC, 5000 Cordoba, Argentina — [2]Institut für Theoretische Physik A, RWTH Aachen University, D-52056 Aachen, Germany — [3]CIN2, CSIC-ICN, Campus UAB, E-08193 Barcelona, Spain

Thanks to its outstanding electrical, mechanical and thermal properties, graphene research is one of the most rapidly advancing fronts ever. Moreover, applications are around the corner, from ballistic transistors to ultracapacitors everything seems possible. Fortunately, there are still many fascinating open problems like the interaction between a laser field and the electrons in graphene. In this work, we discuss this issue within the non-adiabatic regime in terms of both Dirac band and tight-binding models and contrast the obtained results. Notably, we find that the interaction with the field gives rise to back-scattering processes that open dynamical gaps in the electronic structure. The strong dependence of these phenomena on the polarization is emphasized. Our predictions show that these effects should be observable with present laser technology, thereby opening promising prospects for graphene-based opto-electronic devices.

DY 4.8 Mon 12:45 HSZ 03

Relaxation dynamics of graphene in magnetic fields close to the Dirac point — •Martin Mittendorff[1], Stephan Winnerl[1], Paulina Plochocka[2], Piotr Kossacki[2], Harald Schneider[1], Milan Orlita[2], Marek Potemski[2], Mike Sprinkle[3], Claire Berger[3], Walter A. de Heer[3], and Manfred Helm[1] — [1]Institut für Ionenstrahlphysik und Materialforschung, Helmholtz-Zentrum Dresden Rossendorf, Germany — [2]Grenoble High Magnetic Field Laboratory, France — [3]Georgia Institute of Technology, Atlanta, USA

The relaxation dynamics in graphene is of key importance for understanding the basic material properties as well as for high-frequency electronic and opto-electronic device applications. In addition to single colour pump-probe experiments in the THz range (photon energy: 14-30 meV) without magnetic field, we performed experiments at a photon energy of 18 meV in magnetic fields up to 1.34 T. For photon energies larger than twice the Fermi energy (approx. 10 meV) positive pump-probe signals were observed while for smaller photon energies pump-induced absorption occurred due to carrier heating. Relaxation times were around 30 ps. At magnetic fields around 0.23 T the pump-probe signal increases by a factor of 2.5. At this field the splitting of the zeroth to first Landau level is resonant with the photon energy.

DY 5: Statistical Physics of Biological Systems II (organised by DY)

Time: Monday 14:00–17:00 Location: HÜL 186

Topical Talk DY 5.1 Mon 14:00 HÜL 186

Collective dynamics in the cytoskeleton and swimming bacteria — •Falko Ziebert[1,2], Sumanth Swaminathan[3], Shawn Ryan[4,5], Leonid Berlyand[4], and Igor Aranson[5] — [1]PCT - UMR CNRS Gulliver 7083, ESPCI, Paris, France — [2]Physikalisches Institut, Universität Freiburg — [3]Engineering Sciences and Applied Mathematics, Northwestern University, Evanston, U.S. — [4]Department of Mathematics, Pennsylvania State University, U.S. — [5]Materials Science Division, Argonne National Laboratory, Argonne, U.S.

Collective dynamics in active biological materials has attracted much attention in recent years. I will focus on select topics on two systems: i) semi-dilute cytoskeletal solutions where molecular motors induce self-organization of filaments and ii) collective swimming of bacteria solutions. In the first system I propose a model for the semi-dilute case, i.e. the regime of multi-filament interactions. I discuss the order of the isotropic-polar nematic transition - which can not be determined by macroscopic models - as well as the influence of motor fluctuations on the ordering and the respective defect patterns that form. In case of bacterial solutions, recent experimental studies evidenced a decrease in viscosity as a function of density/volume fraction of swimmers in case of pushers (e.g. B. subtilis). In contrast, pullers (e.g. chlamydomonas) lead to an increase in viscosity. To rationalize these findings we performed simulations and analytical work, demonstrating that the viscosity reduction in case of pushers is related to the onset of large-scale collective motion due to interactions between swimmers.

DY 5.2 Mon 14:30 HÜL 186

Stochastic amplification in an epidemic model with seasonal forcing — •Andrew Black and Alan McKane — Theoretical Physics Group, University of Manchester, UK

Stochastic models, subject to external forcing, can capture the regular oscillatory patterns of childhood epidemics, such as measles and whooping cough, but so far the mechanisms generating these pattens have not been well understood. We study the stochastic susceptible-infected-recovered (SIR) model with time-dependent forcing using analytic techniques which allow us to disentangle the interaction of stochasticity and external forcing. The model is formulated as a continuous time Markov process, which is decomposed into a deterministic dynamics together with stochastic corrections, by using an expansion in inverse system size. The forcing induces a limit cycle in the deterministic dynamics, and with the use of Floquet theory, a complete analysis of the fluctuations about this time-dependent solution is given. This analysis is applied when the limit cycle is annual, and after a period-doubling when it is biennial. The comprehensive nature of our approach allows us to give a coherent picture of the dynamics which unifies past work, but which also provides a systematic method for predicting the periods of oscillations seen in both whooping cough and measles epidemics.

DY 5.3 Mon 14:45 HÜL 186

Strong Noise Effects in one-dimensional Neutral Populations — •Luca Dall'Asta[1], Fabio Caccioli[2], and Deborah Beghè[3] — [1]ICTP, Trieste, Italy — [2]Santa Fe Institute, Santa Fe, NM — [3]Università di Parma, Parma, Italy

The dynamics of well-mixed biological populations is studied using mean-field methods and weak- noise expansions. Similar methods have been applied also in spatially extended problems, relying on the fact that these populations are organized in colonies with a large local density of individuals. We provide a counterexample discussing a one-dimensional neutral population with negative frequency- dependent selection. The system exhibits a continuous phase transition between genetic fixation and coexistence that is unexpected from weak-noise arguments. We show that the behavior is a non-perturbative effect of the internal noise that is amplified by presence of spatial correlations (strong- noise regime).

DY 5.4 Mon 15:00 HÜL 186

Active colloidal suspensions exhibit orientational order under gravity — •Mihaela Enculescu und Holger Stark — Technische Universität Berlin, Institut für Theoretische Physik, Hardenbergstr. 36, 10623 Berlin

Recently, the steady state of an active colloidal suspension under gravitational field was studied experimentally in [J.Palacci et al, Phys.Rev.Lett. 105, 088304 (2010)]. It was found that the sedimentation length depends strongly on the velocity of the active Brownian particles. We present a theoretical analysis for the sedimentation of an active colloidal suspension. We find that the change of the sedimentation length is coupled to a partial alignment of the suspension with the mean swimming direction oriented against the gravitational field. Our approach starts from Langevin equations of non-interacting active particles, from which a Smoluchowski equation for the particle distribution is derived. We determine the stationary particle distribution both numerically and by perturbation theory. It agrees very well with the experimental data. The predicted anisotropy in the particle orientational distribution is found to depend on the particle activity, as well as on the gravitational force.

DY 5.5 Mon 15:15 HÜL 186

Fluctuations of intracellular filaments — •Ines-Kristin Weber

and Ludger Santen — Department of Theoretical Physics, Saarland University, 66041 Saarbrücken

The cytoskeleton is an inhomogeneous network of polar filaments consisting of, amongst others, microtubules. These highly dynamic biopolymer filaments are involved in a wide variety of biological processes such as cell division and intracellular transport. Although they are very rigid and form a stiff structural network, it has been shown that they typically exhibit significant bending on all length scales. In this work we describe microtubules as semi-flexible polymers and investigate their fluctuations under thermal and non-thermal forces by means of computer simulations and phenomenological approaches.

DY 5.6 Mon 15:30 HÜL 186

Modelling the African Trypanosome with stochastic rotation dynamics — •Sujin Babu and Holger Stark — Institut für Theoretische Physik Technische Universität Berlin

The dynamics of microorganisms in a viscous fluid has recently received considerable attention in the physics community. It has been reported that the African Trypanosome makes use of hydrodynamic flow fields to evade attack from antibodies in the blood stream. The spindle-shaped flexible cell body of the African Trypanosome possesses some bending rigidity due to its cytoskeleton. A single flagellum runs from the thicker posterior end to the thinner anterior end of the cell body and is firmly attached to it. By propagating a wave along the flagellum from the anterior to the posterior end, the trypanosome moves forward. However, the details of this propulsion mechanism is still under debate. Our goal is to study a model trypanosome in its viscous environment. We model the cell body and the flagellum as a net of vertices connected by springs and also include some resistance to bending. A bending wave passing through the flagellum propels the trypanosome. We simulate the flow field around the model trypanosome using the method of stochastic rotation dynamics, which is an effective solver for the Navier-Stokes equations but also includes thermal fluctuations. We will demonstrate how the model trypanosome is coupled to the effective fluid particles of stochastic rotation dynamics. We will also discuss the propulsion mechanism of the microorganism and demonstrate that our modeling reproduces different shape conformations observed in experiments.

DY 5.7 Mon 15:45 HÜL 186

Explicit Expressions for the Mean First Passage Time of a Diffusing Molecule in Different Two-Dimensional Geometries — •Ronny Straube — Systems Biology Group, Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany

The mean first passage time (MFPT) of a diffusing molecule is an important quantity that describes the first encounter between the molecule and a distant target site. For signaling molecules the MFPT can have a strong impact on the output of a signaling pathway and the inverse of the average MFPT can be used as the diffusion-limited association rate between the molecule and the target site. We have recently shown that in two dimensions the MFPT can be expressed in terms of an associated Neumann function [1] whose regular part can significantly contribute to the average MFPT. Here, I provide simple expressions for the average MFPT in different membrane patch geometries [2] including a square-shaped domain, a cylindrical domain and the surface of a sphere. I also discuss the impact of the presence of multiple target sites on the MFPT. These results can be used to estimate the average MFPT, the foward rate constant or the time scale of receptor clustering for biological membranes of various shapes.

[1] D. Coombs, R. Straube, M. J. Ward, *SIAM J. Appl. Math.* **70**, 302–332 (2009). [2] F. Wei, D. Yang, R. Straube, J. Shuai, submitted to *Phys. Rev. E*

DY 5.8 Mon 16:00 HÜL 186

Perturbation analysis of a reduced model for collective motion: Effects of the initial condition — •Chiu Fan Lee — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

In a system of noisy self-propelled particles with interactions that favor directional alignment, collective motion will appear if the density of particles increases beyond a certain threshold. We argue here that such a threshold may depend also on the profiles of the initial perturbation in the particle directions. Specifically, we perform mean-field, linear stability, perturbative and numerical analyses on an approximated form of the Fokker-Planck equation describing the system. We find that if an angular perturbation to an initially homogeneous system is large in magnitude, it will be amplified even if the density of the system is below the threshold density obtained from mean-field approximation.

Reference: C.F. Lee. Fluctuation-induced collective motion: A single-particle density analysis. Physical Review E **81**, 031125 (2010).

DY 5.9 Mon 16:15 HÜL 186

Active Transport and Cluster Formation on Filament Networks — •Maren Westkott[1], Philip Greulich[2], and Ludger Santen[1] — [1]Department of Theoretical Physics, Saarland University, 66041 Saarbrücken, Germany — [2]Department of Physics & Astronomy, University of Edinburgh, Edinburgh EH9 3JZ, UK

We introduce a model for active transport on inhomogeneous networks embedded in a diffusive environment which is motivated by vesicular transport on actin filaments. In the presence of a hard-core interaction, particle clusters are observed that exhibit an algebraically decaying distribution in a large parameter regime, indicating the existence of clusters on all scales. The scale-free behavior can be understood by a mechanism promoting preferential attachment of particles to large clusters.

We also show that, by applying confining boundary conditions, a self-organization of the network toward a polarized structure is induced, even without explicit regulation and interactions. The polarity, can lead to separation of particle species adjusting to the enclosing geometry. The underlying mechanism can be understood by a linear theory similar to electrostatics. Finally we are discussing active transport phenomena on realistic cellular structures.

[1] P. Greulich and L. Santen, Eur. Phys. J. E 32, 191-208 (2010)

DY 5.10 Mon 16:30 HÜL 186

Modelling the adsorption of biofilms — •Olaf Leidinger and Ludger Santen — Department of Theoretical Physics, Saarland University, 66041 Saarbrücken, Germany

The very first step of the formation of a biofilm at a surface, the adsorption of proteins, is investigated. Therefore a colloidal model is used, in which proteins are described as polydisperse spheres interacting with each other via the framework of the DLVO theory – including steric repulsion, van der Waals and electrostatic interactions. Furthermore an internal degree of freedom, modelled as a change of geometry, is used to represent different conformations of a protein at the surface.

In qualitative agreement with experimental results, the adsorption kinetics of the initial biofilm formation was reproduced by means of Monte Carlo simulations [1,2]. The adsorption kinetics can be divided into three intervals: Initially the adsorption is limited by the flux of particles to the surface. At low concentrations the proteins spread at the surface in order to optimize the binding to the surface. At higher concentrations the adsorbed proteins are compacted due to particle-particle interactions and finally the surface coverage saturates. These dynamical regimes can be identified in experimental and theoretical investigations of the adsorbed amount. The comparison between experimentally and theoretically generated biofilms is completed by a detailed analysis of the point patterns connected to the adsorbed particles, which is carried out by means of integral measures.

[1] Y. Schmitt et al 2010 Biomicrofluidics 4, 032201
[2] A. Quinn et al 2008 EPL 81 56003

DY 5.11 Mon 16:45 HÜL 186

Thermally activated fragmentation of a homopolymer chain — •Simon Fugmann and Igor M. Sokolov — Humboldt-Universität zu Berlin, Department of Physics, Newtonstrasse 15, 12489 Berlin

We consider the thermally activated fragmentation of a homopolymer chain, which can exhibit strongly non-Markovian behavior on the timescale of interest. In our model the dynamics of the intact chain is a Rouse one until a bond breaks and bond breakdown is considered as a first passage problem over a barrier to an absorbing boundary. Using the framework of the Wilemski-Fixman approximation we calculate activation times of individual bonds for free and grafted polymer chains. We show that these times crucially depend on the length of the chain and the location of the bond yielding a minimum at the free chain ends. Going beyond the Wilemski-Fixman approximation we show that a generalized form of the renewal equation for barrier crossings serves to improve the quantitative agreement between numerical simulations and analytical predictions.

DY 6: Quantum Dynamics, Decoherence, and Quantum Information I

Time: Monday 14:00–17:00 Location: ZEU 255

DY 6.1 Mon 14:00 ZEU 255

Attosecond dynamics and decoherence in neutron-H2 scattering — •C. Aris Dreismann[1], Evan Gray[2], and Tom Blach[2] — [1]Institute of Chemistry, TU Berlin, Germany — [2]Griffith University, School of Biomolecular and Physical Sciences, Brisbane, Australia

The standard theory of neutron scattering is based on time-dependent first order perturbation theory (Fermi's Golden Rule); see e.g. [1]. However, the characteristic time-window of neutron Compton scattering (NCS) in the energy transfer range of 1-100 eV lies in the attosecond range, in which the applicability of the Golden Rule becomes questionable. It is argued that, in the NCS physical context, quantum entanglement and decoherence play a significant role [2]. Results of current NCS experiments from H2 and D2 in the gas phase at T = 41 K are reported, showing that the measured Compton profiles reveal new features of quantum dynamics which contradict conventional theoretical expectations. The non-unitary dynamical character of this ultrafast scattering experiments is discussed, and the specific role of decoherence is pointed out. The presented results indicate that the new effect under investigation may play a significant role also in other scattering experimental fiels.

[1] G. L. Squires, Thermal Neutron Scattering, Dover (1996). [2] C. A. Chatzidimitriou-Dreismann and M. Krzystyniak, Laser Physics **20**, 990 (2010).

DY 6.2 Mon 14:15 ZEU 255

Environment-assisted transport and trapping in networks — •Oliver Mülken — Physikalisches Institut, Universität Freiburg, Freiburg, Germany

We study the dynamics and trapping of excitations for a networks with disorder coupled to an external environment. Using a quantum master equation approach, we calculate the survival probability Π(t) of the excitation and define different lifetimes τs of the excitation, corresponding to the duration of the decay of Π(t) in between two predefined values. We show that it is not possible to always enhance the overall decay to the trap. However, it is possible, even for not too small environmental couplings, to decrease certain lifetimes, leading to faster decay of Π(t) in these time intervals: there is an optimal environmental coupling, leading to a maximal decay for fixed disorder strength.

[1] Phys. Rev. E 82, 042104 (2010)

DY 6.3 Mon 14:30 ZEU 255

Quantum walk on a star graph with additional bonds — •Anastasiia Anishchenko, Alexander Blumen, and Oliver Mülken — Physikalisches Institut, Albert-Ludwigs Universität Freiburg; Germany

Continuous-time quantum walks (CTQW) are associated with coherent transport processes of, say, energy, mass or charge. CTQW are applicable to many fields of science from polymer physics to quantum computation. It has been shown in [1] that transfer processes depend on the network topology. Here, we concentrate on CTQW on star graphs, a regular structure that consists of N nodes, where the central node has degree N-1 and the other nodes are leaves with degree 1. There are three discrete eigenvalues for the Hamiltonian of such a system: E(1) = E(2) = ... = E(N-2) = 1; E(N-1) = 0; E(N) = N. For the complete graph of size N, where all the nodes are connected, there are two eigenvalues: E(N-1) = 0, and E(N) = N. The periodicity of regular networks such as stars or rings can be destroyed by adding randomly B additional bonds, see, e.g., Ref. [2]. This creates shortcuts, such that a walker can find a shorter way between pairs of sites than on the regular network. In the following we randomly add bonds to regular star graphs forbidding so-called self-connections, and investigate the transition from the regular star graph to the complete graph [3].

[1] O. Mülken, A. Blumen, Phys. Rev. E 71 (2005) 016101.

[2] O. Mülken, V. Pernice, and A. Blumen, Phys. Rev. E 76 (2007) 051125.

[3] A. Anishchenko, A. Blumen, and O. Mülken, in preparation.

DY 6.4 Mon 14:45 ZEU 255

Environmental induced diffusion in simple networks — •Piet Schijven, Oliver Mülken, and Alexander Blumen — Physikalisches Institut, Albert-Ludwigs Universität Freiburg, Freiburg, BW

This work centers on the behaviour of excitations over simple networks coupled to an external environment. Previous work focussed on the excitonic transport in the presence of a trap (sink) over a dimer, coupled to the environment through the Lindblad formalism [1,2].

A problem with this approach is that larger couplings lead to a quantum Zeno effect. We propose a resolution to this problem by introducing different Lindblad operators such that classical diffusion is obtained for larger coupling strengths. This allows us, in the spirit of the quantum stochastic walk (QSW) [3], to interpolate between classical diffusion and coherent energy transport [4]. To illustrate this process, the influence of tuning the coupling on both a 2-node (dimer) and a 3-node (trimer) network will be discussed.

[1] O. Mülken, L. Mühlbacher, T. Schmid and A. Blumen, Phys. Rev. E 81, 041114 (2010)

[2] O. Mülken and T. Schmid, Phys. Rev. E 82, 042104 (2010)

[3] J.D. Whitfield et. al. Phys. Rev. A 81, 022323 (2010)

[4] P. Schijven, A. Blumen and O. Mülken, in preparation.

DY 6.5 Mon 15:00 ZEU 255

Transition from hopping to band transport in topologically disordered one-particle systems — •Hendrik Niemeyer and Jochen Gemmer — University of Osnabrueck, Physics Departement

As a model system for amorphous materials we investigate a one-particle tight binding model with distance dependent hopping rates whose sites are randomly distributed according to a uniform probability distribution. Diffusion constants and mean free paths for this model can be estimated by integrating over the current autocorrelation function and by mapping the system either onto a linearized Boltzmann equation or onto a discrete diffusion equation. A transition from hopping (small mean free paths and diffusion constants coinciding with a classical random walk) to band transport can be found for increasing hopping ranges.

15 min. break.

DY 6.6 Mon 15:30 ZEU 255

Dynamics of the Rabi model on different time-scales — •Lutz Bakemeier[1], Andreas Alvermann[2], and Holger Fehske[1] — [1]Institut für Physik, Universität Greifswald, Deutschland — [2]Cavendish Laboratory, University of Cambridge, United Kingdom

The generic model of cavity QED, the Rabi model of a two-level system coupled to a quantum oscillator, features a number of interesting dynamical effects if one goes beyond the rotating wave approximation. Depending on the detuning, coupling strength and initial state preparation different types of collapse and revival of Rabi oscillations, as well as spin frequency renormalization or quasi-localization phenomena can be observed. Based on extensive numerical calculations we provide a comprehensive overview over these effects, thus mapping out the 'dynamical phase space' of the Rabi model. In search of a unifying description we ask to which extent the effects can be described with dynamical variational states based on superpositions of coherent oscillator states. The limits of validity of standard approximations, such as the semi-classical approximation and the rotating wave approximation, are also discussed.

DY 6.7 Mon 15:45 ZEU 255

Under what conditions do quantum systems thermalize? New insights from quantum information theory — •Christian Gogolin[1,2,3], Markus P. Müller[1,4], and Jens Eisert[1,5] — [1]Institute for Physics and Astronomy, Potsdam University, 14476 Potsdam, Germany — [2]Fakultät für Physik und Astronomie, Universitä Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Department of Mathematics, University of Bristol, University Walk, Bristol BS8 1TW, UK — [4]Institute of Mathematics, Technical University of Berlin, 10623 Berlin, Germany — [5]Institute for Advanced Study Berlin, 14193 Berlin, Germany

Quantum mechanics is generally regarded as a fundamental theory of physics. As such, it should be able to provide us with a microscopic explanation of all phenomena we observe in macroscopic systems, including irreversible processes such as thermalization. With new mathematical tools from quantum information theory becoming available, there has been a renewed effort to settle the old question of the emer-

gence of classicality and irreversibly. The talk gives an overview over recent progress in the field. In particular it is shown how equilibration and a maximum entropy Jaynes'-principle emerge as a natural consequence of unitary time evolution without any (Markov) approximation, and under which conditions the equilibrium state of a small subsystem is diagonal in the local energy eigenbasis as well as when, and when not, equilibration towards a thermal Boltzmann state can happen.

DY 6.8 Mon 16:00 ZEU 255

The Periodically Driven Dicke Model — •Victor Manuel Bastidas Valencia[1], John Henry Reina[2], Benjamin Regler[1], Clive Emary[1], and Tobias Brandes[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Deutschland — [2]Universidad del Valle, Departamento de Fisica, A. A. 25360, Cali, Colombia

We study the nonequilibrium quantum phase transition (NEQPT) in a periodically-driven Dicke model. The normal-superradiant quantum phase transition in equilibrium conditions has been extensively studied [1,2]. However, the physics of superradiance in nonequilibrium conditions is not completely understood. In order to investigate the nonequilibrium properties of the quantum phase transition in the case of time-dependent atom-field coupling we derive two effective time-independent Hamiltonians by using the rotating wave approximation (RWA) and perturbation theory in the high-driving frequency regime. These effective Hamiltonians allow the description of the quantum phase transition using the well known formulation of quantum phase transitions in time-independent systems. However, in the nonequilibrium case, the character of the quantum phase transition is dynamical and the spectrum of the effective Hamiltonians corresponds to the quasienergy spectrum of the original driven system in perturbation theory.

[1] R. H. Dicke, Phys. Rev. 93, 99 (1954).
[2] C. Emary and T. Brandes, Phys. Rev. E 67, 066203 (2003).

DY 6.9 Mon 16:15 ZEU 255

Gibbs states, exact thermalization of quantum systems, and a certifiable quantum algorithm for preparing thermal states — •Arnau Riera, Christian Gogolin, and Jens Eisert — Institute for Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany

We present three results related to the emergence of thermal states in quantum physics: a) It is known that if a system and its suitable environment are in a microcanonical ensemble, the system is found in a canonical or Gibbs state. Here we introduce precise conditions for the stronger statement of canonical ensembles to emerge for almost all pure states in the subspace corresponding to the energy interval defined by the microcanonical ensemble: This argument makes an idea due to Goldstein et al.\ fully rigorous, including error bounds when employing counting arguments and introducing a precise weak coupling limit, completing an idea going back to Schr{\"o}dinger in 1952.\ b) We establish conditions when subsystems of quenched quantum systems equilibrate to Gibbs states, addressing thermalization – in contrast to equilibration – in non-equilibrium many-body dynamics. c) We finally present a first quantum algorithm for preparing Gibbs states with a certified runtime, including full error estimates, complementing quantum Metropolis algorithms which are expected to be efficient but have no known runtime estimate.

Invited Talk DY 6.10 Mon 16:30 ZEU 255

The multiscale dynamics of lightning and of terrestrial gamma-ray flashes — •Ute Ebert — CWI Amsterdam, The Netherlands — Eindhoven Univ. Techn., The Netherlands

Today most research on cloud-to-ground lightning concentrates on lightning protection. But reserach on lightning physics received a new boost through the discovery of transient luminous events above active thunderstorms in 1990 and of terrestrial gamma-ray flashes from thunderstorms in 1994. In particular, sprite discharges that develop at 40 to 90 km altitude are the first lightning phenomena whose dynamics we now start to understand quantitatively. Sprites are up-scaled versions of streamer discharges, that play an important role in lightning, sparks and high voltage technology.

I will discuss how to bridge the 10 orders of magnitude between the underlying electron-molecule collisions and the km long lightning strokes. I will sketch the hierarchy of dynamical phenomena, and I will focus on: 1. the nonlinear dynamics of sprite and streamer discharges. They are modeled by reaction-drift-diffusion equations and form finger-like structures, that are similar to fingers in two-fluid-flow, in dendritic solidification fronts etc. 2. the single electron dynamics within the streamer. If the field at the finger tip is sufficiently enhanced, the electron density approximation breaks down locally, and electrons run away. This is a possible cause of terrestrial gamma-ray flashes.

Find more information on http://homepages.cwi.nl/~ebert.

DY 7: Focus Session: GPU Computing (with SOE)

Time: Monday 14:00–15:00 Location: GÖR 226

Invited Talk DY 7.1 Mon 14:00 GÖR 226

Applications of GPU-Computing in Statistical Physics — •Peter Virnau — Institut für Physik, Staudinger Weg 7, Uni Mainz

Although simulations and data analysis on Graphic Processing Units require additional programming efforts, and even though not all problems are well-suited for this particular environment, GPU-computing has emerged as a viable low-cost complement to conventional supercomputers in the past three years. In this talk I will highlight recent applications which focus on classical problems of statistical physics and related fields. I will present an extremely fast, freely available Ising code based on multispin coding concepts, which is able to run on multi-GPU clusters, as well as recent results from large-scale molecular dynamics simulations of polymer loops and melts. I will also present interdisciplinary research on econophysics, which focuses on analysis of financial market time series, and discuss future challenges of GPU-computing.

Invited Talk DY 7.2 Mon 14:30 GÖR 226

Accelerating Monte Carlo Simulations in Statistical Physics with GPU's — •David Landau and Junqi Yin — University of Georgia, Athens, GA 30622, U.S.A.

High resolution Monte Carlo simulations are often limited by available resources. This is because long sampling times and large systems are often needed to overcome long correlation times and finite size effects for the systems under study. We will describe how GPU's can be used to formulate multi-threaded algorithms that dramatically accelerate performance of Monte Carlo simulations of condensed matter systems. We give examples of the application to parallel tempering simulation of magnetic lattice models and Wang-Landau sampling of water clusters in the continuum. In both cases a speedup of more than a factor of \$50\$ was achieved compared to a single, current generation CPU; moreover, our implementation scales nearly linearly with the number of GPU's.

DY 8: Focus Session: GPU Computing - Contributed Talks

Time: Monday 15:00–15:45 Location: GÖR 226

DY 8.1 Mon 15:00 GÖR 226

GPU-accelerated analysis of high frequency financial data — •Florian Dittrich[1], Simon Weisseno[1], Lucas Schabhüser[1], and Tobias Preis[2,3] — [1]Spline Consulting e.V., Johannes Gutenberg University Mainz, Staudinger Weg 9, 55099 Mainz, Germany — [2]Center for Polymer Studies, Department of Physics, 590 Commonwealth Avenue, Boston, MA 02215, USA — [3]Artemis Capital Asset Management GmbH, Gartenstr. 14, 65558 Holzheim, Germany

We apply the concept of general-purpose computing on graphics processing units (GPGPU) to the analysis of time series. We use the recently introduced pattern formation conformity [T. Preis et al., New Journal of Physics 11 (2009) 093024], which quantifies pattern-based complex short-time correlations in a time series, for analyzing high-frequency financial data sets. In addition, we evaluate the predictive power for time series using such pattern-based correlations.

DY 8.2 Mon 15:15 GÖR 226

Interacting many-body simulations using graphics processing units — •Tobias Kramer — Institute for Theoretical Physics, Uni Regensburg

Already the solution of the interacting classical many-body problem is difficult to achieve, since the integration of the equations of motions couples all positions of the particles contained in the system. Transport calculations in nanodevices require to include the contacts within the simulation and to study the effect of interactions there.

Classical and quantum-mechanical equations of motions can be related by the time-dependent variational principle as we detail for Coulombic interacting electrons in a magnetic field (1). Interacting systems require to carefully consider the questions of self-consistency, since all particles must be linked together and it is not possible to run one particle trajectory after each other. The emergence of an mean-field potential out of a large (10000 electrons!) many-body calculation is shown in (2). The calculation is only possible due to our usage of graphics processing units, which are ideal tools to study interacting systems.

(1) T. Kramer, Two interacting electrons in a magnetic field: comparison of semiclassical, quantum, and variational solutions, arxiv:1009.6051 (2) T. Kramer, V. Krueckl, E. Heller, and R. Parrott Self-consistent calculation of electric potentials in Hall devices, Phys. Rev. B, 81, 205306 (2010)

DY 8.3 Mon 15:30 GÖR 226

Lattice-Boltzmann Simulations on GPUs — •Dominic Roehm — Institute for Computational Physics Universität Stuttgart

In coarse-grained Molecular dynamics (MD) simulations of large macromolecules, the number of solvent molecules is normally so large that most of the computation time is spent on the solvent. For this reason one is interested in replacing the solvent by a lattice fluid using the Lattice-Boltzmann (LB) method. The LB method is well known and on large length and timescales it leads to a hydrodynamic flow field that satisfies the Navier-Stokes equation. If the lattice fluid should be coupled to a conventional MD simulation of the coarse-grained particles, it is necessary to thermalize the fluid. While the MD particles are easily coupled via friction terms to the fluid, the correct thermalization of the lattice fluid requires to switch into mode space, which makes thermalized LB more complex and computationally expensive.

However, the LB method is particularly well suited for the highly parallel architecture of graphics processors (GPUs). We present a fully thermalized GPU-LB implementation which is coupled to a MD that is running on a conventional CPU using the simulation package ESPResSo (http://www.espressomd.org). This implementation is on a single NVIDIA GTX480 about 50 times faster than on a recent AMD Athlon IIX4 quadcore, therefore replacing a full compute rack by a single desktop PC with a highend graphics card.

DY 9: Graphene II (organised by TT)

Time: Monday 14:00–18:30 Location: HSZ 304

DY 9.1 Mon 14:00 HSZ 304

Radiation-induced quantum interference in graphene based n-p junctions — •Mikhail Fistul[1], Sergey Syzranov[1], Anatoly Kadigrobov[1,2], and Konstantin Efetov[1] — [1]Ruhr-Universität, Bochum, Germany — [2]University of Gothenburg, Göteborg, Sweden

We predict and analyze *radiation-induced quantum interference effect* in low-dimensional graphene based n-p junctions.

In the presence of radiation the ballistic transport of electrons is determined by two processes, namely, by the resonant absorption of photons near the "resonant points", and by the strong reflection from the junction interface, occurring at the "reflection points". There are two paths corresponding to the propagation of electrons through the junction, and the interference between these two paths manifests itself by *large oscillations of the ballistic photocurrent* as a function of the gate voltage or the frequency of the radiation. This coherent quantum phenomenon resembles Ramsey quantum beating and Stueckelberg oscillations well-known in atomic physics.

A suitable radiation frequency may be in the THz or in the infrared optical region. The effect can be observed best in one- and two-dimensional n-p junctions based on carbon nanotubes, monolayer or bilayer graphene nanoribbons.

DY 9.2 Mon 14:15 HSZ 304

Resonant Scattering by Realistic Impurities in Graphene — •Tim Wehling[1], Shengjun Yuan[2], Alexander Lichtenstein[1], Andre Geim[3], and Mikhail Katsnelson[2] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany — [2]Radboud University of Nijmegen, Institute for Molecules and Materials, Heijendaalseweg 135, 6525 AJ Nijmegen, The Netherlands — [3]School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, United Kingdom

We develop a first-principles theory of resonant impurities in graphene and show that a broad range of typical realistic impurities leads to the characteristic sublinear dependence of the conductivity on the carrier concentration. By means of density functional calculations various organic groups as well as adatoms such as H absorbed to graphene are shown to create midgap states within $\pm 0.03\,\mathrm{eV}$ around the neutrality point. A low energy tight-binding description is mapped out. Boltzmann transport theory as well as a numerically exact Kubo formula approach yield the conductivity of graphene contaminated with these realistic impurities in accordance with recent experiments. Consequences for spin-flip scattering are discussed.

DY 9.3 Mon 14:30 HSZ 304

Effect of Coulomb interaction on the gap in monolayer and bilayer graphene — Andreas Sinner and •Klaus Ziegler — Institut für Physik, Universität Augsburg

We study effects of a repulsive Coulomb interaction on the spectral gap in monolayer and bilayer graphene in the vicinity of the charge neutrality point by employing the functional renormalization-group technique. In both cases Coulomb interaction supports the gap once it is open. For monolayer graphene we correctly reproduce results obtained previously by several authors, e.g., an apparent logarithmic divergence of the Fermi velocity and the gap as well as a fixed point corresponding to a quantum phase transition at infinitely large Coulomb interaction. On the other hand, we show that the gap introduces an additional length scale at which renormalization flow of diverging quantities saturates. An analogous analysis is also performed for bilayer graphene with similar results. We find an additional fixed point in the gapless regime with linear spectrum corresponding to the vanishing electronic band mass. This fixed point is unstable with respect to gap fluctuations and can not be reached as soon as the gap is opened. This preserves the quadratic scaling of the spectrum and finite electronic band mass. Ref.:Phys. Rev. B, 82, 165453 (2010).

DY 9.4 Mon 14:45 HSZ 304

Dirac electrons in a spin-orbit periodic potential — •Lucia Lenz[1,2] and Dario Bercioux[1,2] — [1]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universitat, D-79104 Freiburg, Germany

In this talk we present a study of the the band structure of Dirac electrons in graphene in the presence of one-dimensional, periodically modulated spin-orbit interactions. It has been shown that the transmissions of the spin up and spin down channels are strongly dependent on the length of the barrier compared to the spin-precession length [1]. Based on the knowledge of the transfer matrix, we obtain an analytic equation for the band condition using the transfer matrix method [2]. We investigate how the band structure changes compared to potentials with no spin-orbit interactions [3], and give further interpretations to the additional eigenmodes of the transfer matrix.

[1] D. Bercioux, and A. De Martino, Phy. Rev. B **81**, 165410 (2010).
[2] B.H.J. McKellar, G.J. Stepheson, Phy. Rev. C, **35**, 2262 (1987).

[3] M. Barbier, F.M. Peeters, P. Vasilopoulos, J.M. Pereira, Phy.Rev. B **77**, 115446 (2008).

DY 9.5 Mon 15:00 HSZ 304

Transmission through electrostatic and magnetic barriers in the $\mathcal{T}_3$-lattice — •Daniel F. Urban[1], Dario Bercioux[1,2], and Wolfgang Häusler[3] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, D-79104 Freiburg, Germany — [2]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany — [3]Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany

Albeit the $\mathcal{T}_3$-lattice exhibits a reciprocal lattice similar to graphene with two inequivalent Dirac-points at six corners of the hexagonal first Brillouin zone, where relativistic electron-hole symmetric bands touch, $\mathcal{T}_3$ differs and considerably generalizes graphene. A peculiarity of $\mathcal{T}_3$ is the occurance of an additional dispersionless energy band at energy $E = 0$ and an enlarged pseudo-spin $S = 1$ [1] instead of $S = \frac{1}{2}$ as for graphene. As a result, we find enhanced Klein tunneling through rectangular electrostatic barriers, compared to the case of graphene. Moreover, at the particular energy of half the barrier height we find even complete transparency, $T = 1$, irrespective of barrier thickness and of incidence angle. We also investigate rectangular magnetic barriers and in this case identify regimes of zero barrier transparency, qualitatively similar to the case of graphene [2].

[1] D. Bercioux, D. F. Urban, H. Grabert, and W. Häusler, Phys. Rev. A **80**, 063603 (2009).
[2] A. De Martino, L. Dell'Anna, and R. Egger, Phys. Rev. Lett. **98**, 066802 (2007).

DY 9.6 Mon 15:15 HSZ 304

Weak Localization versus Weak Antilocalization in Graphene — •Frank Ortmann[1], Alessandro Cresti[2], Gilles Montambaux[3], and Stephan Roche[4] — [1]INAC/SPRAM, CEA Grenoble, France — [2]IMEP-LAHC, Minatec, Grenoble, France — [3]Laboratoire de Physique des Solides, Université Paris-Sud, Orsay, France — [4]Institut Català de Nanotecnologia and CIN2, Universitat Autònoma de Barcelona, Barcelona, Spain

The understanding of quantum transport phenomena in graphene-based materials is the current subject of great excitation. In the presence of disorder, one of the predicted signatures of pseudospin is the change in sign of the quantum correction to the semiclassical Drude conductivity. This phenomenon, referred to as weak antilocalization (WAL), results from complex quantum-interferences of charge carriers in a disordered potential landscape and has been recently observed experimentally with weak-field magnetotransport measurements.

In this talk we present a numerical weak-field magnetotransport study of huge graphene samples and the influence of a realistic (long-range) disorder potential describing charges trapped in the gate oxide. Our simulations give clearly different magnetoconductance responses in different regimes which are fingerprint of either weak localization or WAL. Depending on the strength of the perturbing potential, the magnetoconductance can be tuned from positive to negative. The gate potential provides a second handle to modify these characteristics. Our results therefore shed new light on experiments and unveil the possible origin of crossovers from positive to negative magnetoconductance.

15 min. break

DY 9.7 Mon 15:45 HSZ 304

Graphene-based electronic spin lenses — •Ali G. Moghaddam[1] and Malek Zareyan[2] — [1]Theoretische Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]Institute for Advanced Studies in Basic Sciences (IASBS), P.O. Box 45195-1159, Zanjan, Iran

We have proposed a solid state electronic spin lens based on a ferromagnetic graphene which has an exchange potential higher than its Fermi energy. The key property is that an interface between such a spin-chiral ferromagnetic (FM) and a nomal (N) graphene region exhibits a negative electronic refractive index which has different signs for electrons with different spin-directions. We have shown that in a corresponding N-FM-N structure, an unpolarized electronic beam can be collimated with a finite spin-polarization producing a point spin accumulation with associated Friedel-like oscillations of spin-dependent local density of states. In this respect, our study reveals that magnetic graphene has the potential to be the electronic counterpart of the recently discovered photonic chiral metamaterials which exhibit a negative refractive index for only one direction of the circular polarization of the electromagnetic wave.

[1] A. G. Moghaddam and M. Zareyan, Phys. Rev. Lett. **105**, 146803 (2010).

DY 9.8 Mon 16:00 HSZ 304

Thermal fluctuations of free standing graphene — •Nils Hasselmann[1,3] and Fabio Braghin[2,3] — [1]MPIFKF Stuttgart — [2]Univ. Fed. de Goias, Goiania, GO, Brazil — [3]IIP, UFRN, Natal, RN, Brazil

We use non-perturbative renormalization group techniques to calculate the momentum dependence of thermal fluctuations of graphene, based on a self-consistent calculation of the momentum dependent elastic constants of a tethered membrane. We find a sharp crossover from the perturbative to the anomalous regime, in excellent agreement with Monte Carlo results for the the out-of-plane fluctuations of graphene, and give an accurate value for the crossover scale. Our work strongly supports the notion that graphene is well described as a tethered membrane. Ripples emerge naturally from our analysis.

DY 9.9 Mon 16:15 HSZ 304

Transport through a quantum-spin-Hall-insulator/normal junction in graphene ribbons — •Georgo Metalidis[1] and Elsa Prada[2] — [1]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Karlsruher Institut für Technologie, D-76128 Karlsruhe, Germany — [2]Instituto de Ciencia de Materiales de Madrid (CSIC), Cantoblanco, 28049 Madrid, Spain

We have investigated a junction between a quantum-spin-Hall insulator and a metallic contact obtained by selectively doping a single graphene ribbon. In the absence of disorder, the transmission of the topological edge states through the junction is perfect due to the orthogonality of left- and right-movers. This is proven analytically by deriving exact wavefunctions for the topological edge states in armchair and zigzag ribbons. The wavefunction character depends fundamentally on the ribbon termination: the edge state width is only dependent on the spin-orbit coupling strength for armchair ribbons, whereas it is only weakly dependent of this parameter for zigzag edge states where the width becomes energy dependent instead. These observations are confirmed in numerical plots of the current density in the sample. When disorder is present, the orthogonality between left- and right-movers is destroyed and backscattering sets in. Nevertheless, the perfect transmission can be restored by increasing the ribbon width.

DY 9.10 Mon 16:30 HSZ 304

Edge magnetism in nanoribbons of graphene — •Hélène Feldner[1,2], Zi Yang Meng[3], Thomas C. Lang[4], Fakher Assaad[4], Stefan Wessel[3], Andreas Honecker[2], and Daniel Cabra[1] — [1]IPCMS, Strasbourg, France — [2]Institut für Theoretische Physik, Göttingen, Germany — [3]Institut für Theoretische Physik III, Stuttgart, Germany — [4]Institut für Theoretische Physik und Astrophysik, Würzburg Am Hubland, Germany

A simple tight-binding model is sufficient to describe most of graphene's properties, but a Hubbard model is needed to account for its magnetic properties. To be able to compute quantities in direct space and for big systems of realistic size with chosen geometry, we use a mean field approximation solved in a self-consistent way in the direct space. In agreement with known results, we find a Mott-Hubbard transition, and a magnetization of the zig-zag edge of finite samples. We have studied the accuracy of the approximation by a comparison of our results with those obtained by exact diagonalization and quantum Monte-Carlo simulations [1]. The main point of our current work consists of a study of the graphene zig-zag ribbons by mean field and quantum Monte-Carlo simulations. First we have looked at the static magnetism of the zig-zag edges and in a second part the local spectral function. These quantities allow us to study the influence of static magnetism on dynamical properties and the local density of states which is a quantity accessible experimentally by STM and shows different behavior on the edge with and without magnetic properties.

[1] Phys. Rev. B 81, 115416 (2010).

DY 9.11 Mon 16:45 HSZ 304

Screening of external electrical fields for different graphene nanoribbons — •Tobias Burnus[1], Gustav Bihlmayer[1], Daniel Wortmann[1], Yuriy Mokrousov[1], Stefan Blügel[1], and Klaus Michael Indlekofer[2] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Hochschule RheinMain, Unter den Eichen 5, 65195 Wiesbaden, Germany

Graphene nanoribbons (GNR) hold great future promise for field-effect transistor and quantum dot (QD) devices. The gate electrodes and the electric field distribution play a crucial role. In this talk the effect of the screening of an in-plane oriented external electric field due to the electrons in graphene nanoribbons is studied in the framework of density functional theory calculations based on the full potential linearized augmented planewave method. These calculations offer a direct link to the static dielectric constant in the ribbon. We compare armchair ribbons of different width to see the effect of the bandgap on the electric response, as well an orientation with zig-zag edges, which show a metallic edge state. The formation of QDs in structures with both types of edges in an external field is considered. The presence of metallic states, e.g. from a substrate, significantly modifies the behavior of QD states in the external field. The work is supported by the DFG Research Unit 912 "Coherence and Relaxation Properties of Electron Spins".

DY 9.12 Mon 17:00 HSZ 304

Color-dependent conductance of graphene with adatoms — •Jörg Schelter[1], Pavel Ostrovsky[2,3], Igor Gornyi[2,4], Björn Trauzettel[1], and Mikhail Titov[2,5] — [1]Institut für Theoretische Physik und Astrophysik, University of Würzburg, 97074 Würzburg, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [3]L. D. Landau Institute for Theoretical Physics RAS, 119334 Moscow, Russia — [4]A. F. Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia — [5]School of Engineering & Physical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, UK

We study ballistic transport properties of graphene with a low concentration of vacancies or adatoms. The conductance of graphene doped to the Dirac point is found to depend on the relative distribution of impurities among different sites of the honeycomb lattice labeled in general by six colors. The conductivity is shown to be sensitive to the crystal orientation if adatom sites have a preferred color. Our theory is confirmed by numerical simulations using recursive Green's functions with no adjustable parameters.

15 min. break

DY 9.13 Mon 17:30 HSZ 304

Edge effects on correlations in quasiparticle spectra of graphene billiards — •Jürgen Wurm[1], Klaus Richter[1], and Inanç Adagideli[2] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg — [2]Faculty of Engineering and Natural Sciences, Sabancı University, Orhanlı - Tuzla, 34956, Turkey

In this work, we study the energy spectrum of quasiparticles in chaotic billiards realized in nanostructured graphene. In particular, we focus on the different types of edges and show how they effect correlations in the spectrum. Previously we have investigated the effects of edges on the transport and spectral properties of graphene quantum dots, as well as on the conductance of graphene nanoribbons numerically [1,2]. Some edges can lead to effective time reversal symmetry breaking, others are effective intervalley scatterers. Here we describe the quasiparticle dynamics in graphene analytically using the effective 2D Dirac Hamiltonian and imposing appropriate boundary conditions that depend on the specific structure of the graphene edges. Starting from the multiple reflection expansion for the exact Green function, we develop a semiclassical theory for graphene and derive a trace formula for the oscillating part of the density of states. We then focus on correlations in the spectrum investigating the spectral form factor and its dependence on the edge structure of the graphene billiard.

[1] J.Wurm, A.Rycerz, I.Adagideli, M.Wimmer, K.Richter and H.U.Baranger. Phys. Rev. Lett. 102, 056806 (2009)
[2] J.Wurm, M.Wimmer, I.Adagideli, K.Richter and H.U.Baranger. New J. Phys. 11, 095022 (2009)

DY 9.14 Mon 17:45 HSZ 304

Transport in Rough Quasi-One-Dimensional Systems — •Otto Dietz[1], Ulrich Kuhl[1,2], Hans-Jürgen Stöckmann[1], Felix M Izrailev[3], and Nykolay M Makarov[3] — [1]Universität Marburg, Germany — [2]Université de Nice, France — [3]Universidad de Puebla, Mexico

Scattering at rough disordered boundaries strongly influence the conductance of nanowires. For rough silicon nanowires a much higher ratio of electric conductivity to thermal conductivity has been reported than expected from the Wiedemann-Franz law [1]. These findings have not been explained yet.

In the case of bulk disorder it is well known that correlations can drastically change conductance properties [2]. Similar effects have been predicted for rough nanowires [3] but drew little attention before their applicability to conductivity in silicon nanowires became evident.

We present a first experimental test of this theory in microwave waveguides with rough walls. Because of the strict analogy between the 2d Schrödinger equation and the Helmholtz equation, the results can be directly applied to electron transport in nano structures. Microwave techniques can be helpful in this respect, since in contrast to real nanowires the surface roughness is both known and controllable. We could confirm that certain rough boundaries can block or enhance wave transport in given frequency windows. \newline [1] A. I. Hochbaum, et. al., Nature 451, 163 (2008). \newline [2] U. Kuhl, et.al., Appl. Phys. Lett. 77, 633 (2000). \newline [3] M. Rendón, et.al., Phys. Rev. B 75, 205404 (2007).

DY 9.15 Mon 18:00 HSZ 304

Strong suppression of thermal conductivity in defected graphene nanoribbons: Order-N methodology and thermoelectric properties — •Hâldun Sevinçli[1], Wu Li[1,2], Stephan Roche[1,3,4], and Gianaurelio Cuniberti[1] — [1]1Institute for Materials Science and Max Bergmann Center of Biomaterials, TU-Dresden, 01062 Dresden, Germany — [2]Institute of Physics, Chinese Academy of Sciences, 100190 Beijing, China — [3]Institut Català de Nanotecnologia (ICN) and CIN2, Campus UAB, 08193 Bellaterra, Barcelona, Spain — [4]Institució Catalana de Recerca Avançats (ICREA), 08010, Barcelona, Spain

We investigate electron and phonon transport through defected graphene nanoribbons (GNRs). For phonon transport, we develop an efficient linear scaling method which is based on the Chebyshev polynomial expansion of the time evolution operator and the Lanczos tridiagonalization scheme, and also use molecular dynamics simulations. We show that edge-defects reduce phonon thermal transport dramatically in both armchair and zigzag GNRs, while in zigzag GNRs edge-defects are only weakly detrimental to electronic conduction. On the other hand, bulk defects suppress both charge and thermal transport for relatively high density of defects. The behavior of the electronic and phononic elastic mean free paths of zigzag GNRs with edge-defects points to the possibility of realizing an electron-crystal coexisting with a phonon-glass.

DY 9.16 Mon 18:15 HSZ 304

Orbital magnetism in ballistic graphene quantum dots — •Lisa Hesse[1], Jürgen Wurm[1], Inanç Adagideli[2], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 — [2]Faculty of Engineering and Natural Sciences, Sabancı University, Orhanlı - Tuzla, 34956, Turkey

We study the magnetic response of quasiparticles in graphene quantum dots. To this end we derive the density of states (DOS) of graphene nanostructures including the effect of a small magnetic field, starting from an exact expansion for the Green function of a graphene flake with arbitrary types of edges. We then consider systems much larger than the Fermi wavelength, for which we can evaluate this expansion in the semiclassical limit and obtain the DOS. For graphene, the structure of the boundary has significant effects on both the average DOS and the DOS oscillations. We then calculate the orbital magnetic susceptibility that is closely related to the DOS and discuss the pecularities that arise due to the different types of edges and the pseudospin degrees of freedom of charge carriers in graphene.

DY 10: Posters I

Time: Monday 17:00–19:00 Location: P4

DY 10.1 Mon 17:00 P4

Zeroth law and fluctuation relations for driven lattice gases in contact: A numerical study — •Robert Ramsperger, Punyabrata Pradhan, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

We numerically study two-dimensional driven lattice gases to check the existence of an intensive thermodynamic variable which could determine "equilibration" between two driven lattice-gas systems being brought into contact [a part of the detailed results discussed here have appeared in Phys. Rev. Lett. **105**, 150601 (2010)]. We consider driven interacting particle systems where the microscopic interaction strengths and driving fields may be different in each of the systems. Two such systems in contact can exchange particles through the contact area with the total number of particles conserved. The contact area consists of a small number of sites ("weak contact") or a large number of sites ("strong contact"). Interestingly, we find that, to a very good approximation, there is an intensive variable, like equilibrium chemical potential, which determines the final steady state of two driven lattice gases in contact. Moreover, in the weak contact limit, a fluctuation-response relation between the fluctuations in particle-number and the corresponding susceptibility is also well satisfied. We also discuss the observable violations to these simple thermodynamic laws. We study in detail how the densities and the fluctuations in a driven system in contact with a particle reservoir depend on the driving field, size and shape of the system, size and shape of the contact area as well as the properties of the reservoir.

DY 10.2 Mon 17:00 P4

Time-dependent density functional theory for driven lattice gas systems with interactions — •Marcel Dierl[1,2], Philipp Maass[2], and Mario Einax[1,2] — [1]Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau, Germany — [2]Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück, Germany

Driven lattice gases are widely used model systems to study non-equilibrium processes in physics, biology and chemistry. So far most studies were carried for lattice systems with only hard-core exclusions. Here we present a new method to describe the kinetics of driven lattice gases with particle-particle interactions beyond hard-core exclusions. The method is based on the time-dependent density functional theory for lattice systems and allows one to set up closed evolution equations for mean site occupation numbers in a systematic manner. Application of the method to a totally asymmetric site exclusion process with nearest-neighbor interactions yields predictions for the current-density relation in the bulk, the phase diagram of non-equilibrium steady states and the time evolution of density profiles that are in good agreement with results from kinetic Monte Carlo simulations.

DY 10.3 Mon 17:00 P4

Migration of semiflexible polymers in a pressure driven flow — •Sebastian Reddig and Holger Stark — Institut für Theoretische Physik, TU-Berlin

Experiments on single α-actin filaments in microchannels showed that the steady state center-of-mass probability density is nonuniformly distributed across the channel under the influence of a Poiseuille flow[1]. Depletion layers near the walls and in the centerline were observed. Hydrodynamic interactions between the polymer and the walls lead to migration away from the walls, while a spatially varying diffusion coefficient resulting from a locally varying polymer conformation drives the polymer away from the centerline. These competing mechanisms give the observed bimodal distribution.

We introduce a model for a semiflexible polymer under the influence of a pressure driven flow, which is confined between two parallel planar walls. The polymer is modelled by a bead-spring chain including a bending potential. We describe hydrodynamic interactions between the beads with the two-wall Green tensor. It was derived by R.B. Jones[2] and takes into account the no-slip boundary condition at the walls.

Brownian dynamics simulations for our model reproduce the same behavior as in experiments, in particular, the bimodal distribution. We demonstrate how velocity of the Poiseuille flow and bending rigidity influence this distribution and also study end-to-end distance and the orientation of the polymer in the microchannel.

[1] D. Steinhauser, S. Köster, H. Stark, and T. Pfohl, submitted.
[2] R.B. Jones, J. Chem. Phys, **121**, 483 (2004).

DY 10.4 Mon 17:00 P4

Folding and unfolding of a triple-branch DNA molecule with four conformational states — •Sandra Engel[1], Anna Alemany[2,3], Nuria Forns[2,3], Philipp Maass[1], and Felix Ritort[2,3] — [1]Fachbereich Physik, Universität Osnabrück, Germany — [2]Departament de Física Fonamental, Universitat de Barcelona, Spain — [3]CIBER-BBN Networking center on Bioengineering, Biomaterials and Nanomedicine, Spain

Single-molecule experiments provide new insights into biological processes hitherto not accessible by measurements performed on bulk systems. We report on a study of the kinetics of a triple-branch DNA molecule with four conformational states by pulling experiments with optical tweezers and theoretical modelling. Three distinct force rips associated with different transitions between the conformational states are observed in the folding and unfolding trajectories. By applying transition rate theory to a free energy model of the molecule, probability distributions for the first rupture forces of the different transitions are calculated. Good agreement of the theoretical predictions with the experimental findings is achieved. Furthermore, due to our specific design of the molecule, we found a useful method to identify permanently frayed molecules by estimating the number of opened basepairs from the measured force jump values.

DY 10.5 Mon 17:00 P4

Cycle-Flux Decompositions of Non-Equilibrium Steady States — •Bernhard Altaner, Jürgen Vollmer, Stephan Herminghaus, and Marc Timme — Max Planck Institute for Dynamics and Self-Organization, 37073 Göttingen

It hat been proposed recently [1] that the currents provide a natural classification of non-equilibrium steady states of Markov processes. This approach does not allow, however, to deal with the entropy (or heat) production rate, which is of considerable interest in biological systems [2]. For this type of questions one can rather consider individual fluxes between adjacent nodes, and decompose the steady state in terms of closed flux cycles. We demonstrate the application of this novel approach using a simple biological membrane model.
[1] R.K.P. Zia & B. Schmittmann, *J Stat Mech: Theo and Exp* **2007** (2007) P07012.
[2] C. Jarzynski, *Eur Phys J B* **64** (2008) 331-340 [Proceedings of StatPhys23].

DY 10.6 Mon 17:00 P4

The impact of a memory trace on the long term routing in complete graphs — •Andre Schuelein, Dimitrije Markovic, and Claudius Gros — Institute for Theoretical Physics, Johann Wolfgang Goethe University, Frankfurt am Main, Germany

Vertex routing models are a recently introduced class of models describing the flow of information within networks via routing processes. The long term information flow in a network given a static routing table is governed by the properties of the existing cyclic attractors. In this poster we investigate the behavior of the cycle length distribution of complete graphs in the case of a memory trace and present analytic mean field approximations for them. Further we show that the cycle length distribution with a memory trace of a complete graph with size N, is very similar to the cycle length distribution without memory trace of a complete graph with size N^2. As a possibility to evaluate the cycle length distribution of bigger graphs we introduce the method of routing on the fly in contrast to the use of static routing tables and highlight their relation. We find a linear mean and median of the cycle length distribution in the case of routing on the fly, in the case of static routing tables the mean and median follow a power law.

DY 10.7 Mon 17:00 P4

Sparse Coding and Self-Sustained Dynamics with Leaky Integrators — •Mathias Linkerhand — Institut für Theoretische Physik der Johann Wolfgang Goethe-Universität, Frankfurt am Main, Germany

Extending the Winner-takes-all paradigm to clique encoding and sparse coding. Considering fully connected random graphs with ex-

hibitory and inhibitory synaptic strengths and changing the intrinsic plasticity to achieve special activity distributions using stochastic adaptation rules. The results will be shown in the poster...

DY 10.8 Mon 17:00 P4

Coherent-Potential approximation for noncrystalline structures — •Stephan Köhler[1] and Walter Schirmacher[1,2] — [1]Institut für Physik, Univ. Mainz — [2]Physik-Department E13, TU München

The Coherent Potential Approximation (CPA) has been used extensively in the past decades to calculate properties of disordered solids [1], although its derivation assumes an underlying lattice structure of the material. We present a general method to derive the CPA equations for an amorphous solid using techniques from Quantum field theory. The approach is applied to electrons moving in a spatially fluctuating potential and to diffusion in a material with random diffusion coefficient. The later problem is mathematically equivalent to scalar vibrational excitations (scalar phonons) in a solid with fluctuating sound velocity. The DC-AC crossover in the diffusive dynamics is equivalent to the boson peak anomaly in the vibrational spectrum [2]. Since the CPA equations do not specify the underlying probability distribution of the fluctuations it is possible to study characteristic quantities of disordered solids for different distributions and compare them to results obtained from the Self Consistent Born Approximation [3], which is the low-disorder limit of the CPA. [1] R. J. Elliot et al., Rev. Mod. Phys. 46, 465, (1974); [2] W. Schirmacher, M. Wagener, Philos. Mag. B65, 607 (1992); [3] C. Schirmacher et al., phys. stat. sol. (c) 5, 862 (2008)

DY 10.9 Mon 17:00 P4

Rayleigh scattering, long-time tails, and the harmonic spectrum of topologically disordered systems — •Walter Schirmacher[1,2], Carl Ganter[3], and Stephan Köhler[1] — [1]Institut für Physik, Univ. Mainz — [2]Physik-Department E13, TU München — [3]Institut für Radiologie, TU München

We show rigorously [1] that a topologically disordered system interacting harmonically via force constants, which have a sufficiently short-ranged site-distance dependence, exhibits Rayleigh scattering in the low-frequency limit, i.e. a sound attenuation constant, which is proportional to ω^{d+1}, where ω is the frequency and d the dimensionality. This had been questioned in the literature [2]. The corresponding non-analyticity in the spectrum is related to a long-time tail in the velocity autocorrelation function of the analogous diffusion problem, which varies with time t as $t^{-(d+2)/2}$. A self-consistent theory [1] for the spectrum is formulated, which has the correct analytical properties. [1] W. Schirmacher, C. Ganter, Phys. Rev. B 82, 094205 (2010); [2] T. S. Grigera et al. Nature 422, 289 (2003).

DY 10.10 Mon 17:00 P4

Glassy dynamics of orientation fluctuations in a stripe-forming system — •Christian Riesch., Günter Radons, and Robert Magerle — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz

We present numerical results indicating aging behavior in the orientation fluctuations of a stripe-forming system in the ordered state. We use a simple model which describes phase separation for a conserved order parameter with additional long-range interactions under the influence of thermal noise. It belongs to a class of models describing microdomain formation in block copolymers and other modulated phases, such as thin magnetic films with dipolar interactions. In our simulations, we focus on the dynamics which result from initial conditions of a defect-free ordered state, i.e. a set of parallel stripes. With increasing noise strength η, an order-disorder transition (ODT) occurs at a critical level η_c. Below the ODT, orientation correlation functions (OCF) computed from local stripe orientation depend on both, simulation time t and waiting time t_w. The OCF are found to scale as $C(t, tw) \sim t^{-\nu} \cdot f(t/t_w)$, where the scaling function $f(t/t_w)$ is well described by a stretched exponential.

DY 10.11 Mon 17:00 P4

Non-linear single-particle-response of glassforming systems to external fields — •David Winter[1], Jürgen Horbach[2], Peter Virnau[1], and Kurt Binder[1] — [1]Johannes Gutenberg-Universität, Mainz, Germany — [2]Deutsches Zentrum für Luft und Raumfahrt (DLR), Köln, Germany

Non-equilibrium molecular dynamics (NEMD) computer simulation are used to study the nonlinear response of single particles to external fields in glass-forming soft-sphere mixtures. Individual particles are pulled through the system by applying a constant force. If the force is strong enough, structural rearrangements as well as flow or plastic deformation in the host liquid or glass around the pulled particle will be induced. Force-velocity relations are compared to shear rate-stress relations from NEMD simulations where the non-linear response to macroscopic shear fields is probed. This allows to reveal to what extent the single-particle response to an external force probes the macro-rheological properties of a glass-forming system under shear.

DY 10.12 Mon 17:00 P4

How glassy are biological membranes? — •Sebastian Busch[1], Luis Carlos Pardo[2], and Tobias Unruh[3] — [1]Technische Universität München, Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) and Physik Department E13, 85748 Garching bei München, Germany — [2]Universitat Politècnica de Catalunya, Grup de Caracterització de Materials, 08028 Barcelona, Catalonia (Spain) — [3]Friedrich-Alexander-Universität Erlangen-Nürnberg, Lehrstuhl für Kristallographie und Strukturphysik, 91058 Erlangen, Germany

Biological membranes surround every cell and are important in pharmaceutical and food industry. Their dynamics is still rather poorly understood: The free volume theory was adapted to the membranes [1] and was a very successful description until it became clear from MD simulations that the molecules exhibit concerted flow-like motions rather than jump-like decaging events [2].

Measuring the self-correlation function of the molecules, the simulations could be supported with quasielastic neutron scattering measurements [3]. The flow-like motions bear a striking resemblance to the dynamical heterogeneities known from glassy dynamics [4].

Which concepts from glass physics can replace the free volume theory for the molecular description of phospholipid dynamics?

[1] W.L.C. Vaz et al., Biophys.J., 60(6):1553, 1991
[2] E. Falck et al., JACS 130(1):44, 2008
[3] S. Busch et al., JACS 132(10):3232, 2010
[4] S. Busch et al., BBA Biomembranes, in print, doi:10.1016/j.bbamem.2010.10.012

DY 10.13 Mon 17:00 P4

Pseudo-Rabi oscillations in dielectric absorption measurements on the glass BK7 at low temperatures — •Gudrun Fickenscher, Manfred von Schickfus, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Heidelberg University, Germany

The low temperature properties of glasses are to a large extent well described by the phenomenological standard tunnelling model. However, the behaviour of the dielectric function and the decay of the polarisation echo amplitude at temperatures below 50mK are not fully explained. To gain better understanding of the microscopic structure of tunnelling systems and the relaxation mechanisms in glasses, dielectric measurements at temperatures down to a few mK were performed with a Niobium microstrip $\lambda/2$ resonator ($f_{\mathrm{res}} \approx 1$GHz) structured onto a plate of BK7. We observe the saturation of the dielectric absorption due to resonant tunnelling systems. During the saturation process, we observe surprising low frequency oscillations ($f \approx 10$kHz) of the resonator transmission whose frequency is proportional to the electric field amplitude as would be expected for Rabi oscillations. They are clearly visible at temperatures from 10 to more than 500mK. However, we would not expect a coherent effect in glasses in this temperature and frequency range since it is known from earlier experiments that the phase relaxation time is below 1 μs at temperatures above 100mK. Experimental data of this phenomenon, which has never been observed in a glass before, will be shown and discussed.

DY 10.14 Mon 17:00 P4

Measurements of the low-frequency elastic properties of dielectric and metallic glasses with double paddle oscillators — •Marius Hempel, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, 69120 Heidelberg

Experimental results of both temperature and frequency dependence of the internal friction and of the change of sound velocity of glasses differ systematically from the predictions of the tunneling model which phenomenologically describes the low temperature properties of glasses. Mutual interaction of the tunneling states which is not incorporated in the tunneling model has been discussed as a possible explanation.

We investigated the elastic properties of the bulk metallic glass

$Zr_{55}Cu_{30}Al_{10}Ni_5$ and of the dielectric optical glass N-KZFS11. The dielectric glass and metallic glass in the superconducting state ought to yield a similar behaviour.

The samples are driven and read out capacitively. They are placed within a solenoid of superconducting niobium-titanium wire providing a magnetic field. The samples feature a double paddle oscillator geometry which exhibits very small background damping due to clamping compared to the vibrating reed method.

The sound velocity and the internal friction at frequencies between 0.5 and 7.5 kHz down to a temperature of 6 mK have been measured. We present experimental results of the different glasses and compare them to theoretical predictions.

DY 10.15 Mon 17:00 P4

Thermal Conductivity of Superconducting Bulk Metallic Glasses at Very Low Temperatures — •Daniel Rothfuss[1], Uta Kühn[2], Andreas Fleischmann[1], and Christian Enss[1] — [1]Kirchhoff-Institute for Physics, Heidelberg University, INF 227, 69120 Heidelberg — [2]IFW Dresden, Institute for Complex Materials, P.O. Box 270116, 01171 Dresden

As a new kind of vitreous material bulk metallic glasses offer several advantages for the investigation of glassy materials at very low temperatures. Particularly with superconducting bulk metallic glasses it is possible to probe not only the interaction between tunnelling systems and electrons, but also with phonons by switching between the normal and superconducting state with an external magnetic field. But until now only little is known about their properties down to milli-kelvin temperatures. The only existing measurements of thermal conductivity of bulk metallic glasses do not reach much below 1K or are performed on thin films down to 100mK. We present the thermal conductivity of bulk amorphous $Zr_{52,2}Ti_5Cu_{17,9}Ni_{14,6}Al_{10}$ in the superconducting state down to 6mK. Measurements were performed with a novel SQUID-based contact free technique because of its extremely small parasitic heating. Our results show that the thermal conductivity of the sample scales nearly quadratically with temperature. This suggests that sufficient below the critical temperature the thermal conductivity of this bulk metallic glass can be described well by the thermal diffusion of phonons and their resonant scattering at tunnelling systems.

DY 10.16 Mon 17:00 P4

Translational Granular Brownian Motor — •Chih-Wei Peng, Max Neudecker, Nabiha Saklayen, Johannes Blaschke, Jürgen Vollmer, and Matthias Schröter — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Germany

We construct a motor driven by the random motion of granular particles. In this setup, a wedge, which is allowed only translational freedom along one axis, is placed in granular gas. According to the idea of brownian motor, the time reversal symmetry-breaking due to the inelastic collisions between particles and wedge along with the symmetry breaking of rotational invariance implies that the wedge could have a preferred drift direction[1]. In addition, we also consider the effect due to the anisotropy of particle velocity distribution on different axes, which could largely change the drift velocity.

References

[1] Cleuren, B. and Van den Broeck, C. Europhys. Lett. 77, 50003 (2007).

DY 10.17 Mon 17:00 P4

Condensation time scale of a stochastic transport process with pair factorized steady states — •Hannes Nagel[1], Bartlomiej Waclaw[2], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Germany — [2]School of Physics & Astronomy, The University of Edinburgh, UK

Stochastic transport processes (such as [1]) can be tuned by their generating weight functions to exhibit a steady state with a condensate of particles that is separate from a fluid background phase. We study the dynamics of the relaxation into the steady state of such driven transport systems using numerical simulations to determine the condensation time scale and discuss the corresponding phenomenologic mechanisms. Despite the existence of short-range interactions in the studied system, the condensation behavior is found to be quite similar to that of the zero-range process on one- and two-dimensional lattices.

[1] M. R. Evans, T. Hanney, and S. N. Majumdar, *Interaction driven real-space condensation*, Phys. Rev. Lett. **97** (2006) 010602-1–4

[2] H. Nagel, *Mass Condensation in Stochastic Transport Processes and Complex Networks*, Diploma thesis, Leipzig (2010)

DY 10.18 Mon 17:00 P4

General relation between signal attenuation from gradient nuclear magnetic resonance and distribution of diffusivities from single-molecule tracking in diffusion processes — •Michael Bauer[1], Günter Radons[1], Rustem Valiullin[2], and Kärger Jörg[2] — [1]Chemnitz University of Technology, Germany — [2]University of Leipzig, Germany

Diffusion processes in heterogeneous environments appear in many physical and biological applications, for instance in ultra-thin liquid films. Liquid layering leads to a change of diffusion properties and induces heterogeneities in the observed motion of tracer molecules. In order to characterize processes observed by single-molecule tracking (SMT) we suggested to investigate the distribution of diffusivities and their dependence on observation time [1]. This technique provides advantages over conventional methods such as mean-squared displacements, which conceal the effects of inhomogeneities. In our contribution we extend the investigations to ensemble-based measurements obtained from pulsed field gradient nuclear magnetic resonance (PFG NMR). Our objective is to relate the signal attenuation of PFG NMR, which corresponds to the propagator in Fourier space, to the distribution of diffusivities [2]. We derive analytical expressions and illustrate the applicability of this approach by the well-established two-region exchange model known from PFG NMR studies. Furthermore, our method provides a promising approach to investigate ergodicity of such systems.

[1] M. Bauer et al., diffusion-fundamentals.org 11, 104 (2009)

[2] M. Bauer et al., J. Chem. Phys., submitted (2010)

DY 10.19 Mon 17:00 P4

1D Schrödinger equation with open boundaries for pumping potentials — •Niklas Rohling and Frank Grossmann — Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany

In order to generate a non-vanishing average current within the time-periodic Schrödinger equation the potential has to break parity and generalized parity. We therefore firstly consider the following potentials with position-dependence only in a central region and a non-static bias: a harmonically driven sawtooth potential (a) and a step-like potential (b). Secondly, we study a dipole field in the central region (c). The cases (b) and (c) contain driving by the fundamental and the second harmonic, so-called harmonic mixing [1]. To calculate the current, we use Floquet scattering theory as well as an open boundary wavefunction [2]. In case (c) we optimize the relative amplitude ratio between the fundamental and the second harmonic leading to a maximum in the pumping current.

[1] S. Kohler, J. Lehmann, and P. Hänggi, Phys. Rep. **406** 379-443 (2005)

[2] S. Kurth, G. Stefanucci, C.-O. Almbladh, A. Rubio, and E. K. U. Gross, Phys. Rev. B **72**, 035308 (2005)

DY 10.20 Mon 17:00 P4

Calculation of the diffusion coefficient of disordered systems by using the building block principle — •Arzu Bahar Yener and Stefanie Russ — Freie Universitaet Berlin

The self-diffusion coefficient D_s for linear diffusion on lattices and in pores in the Knudsen regime is calculated by the method of random walks for disordered systems, where the mean square displacement $\langle x(t) \rangle$ consists of the quadratic term and the correlation term. To this end, a building-block principle is applied that composes the system into substructures i ("building blocks") without cross correlations between them. We present different substructures for lattices whose correlation terms are calculated either analytically or numerically as simply as possible. For the latter, methods are revealed that allow to obtain the correlation terms of each substructure numerically with low costs. Finally, we show, how the correlation terms of the different substructures must be combined to find D_s of the total lattice. The results are verified numerically for lattices as well as for realistic pores.

DY 10.21 Mon 17:00 P4

Molecular dynamics simulation of hot Brownian motion — •Dipanjan Chakraborty[1,2], Daniel Rings[1], Frank Cichos[2], and Klaus Kroy[1] — [1]ITP, University of Leipzig, Germany — [2]EXP-I, University of Leipzig, Germany

We present a molecular dynamics (MD) study of "hot Brownian motion", a scenario in which a nanoparticle is kept at an elevated temperature with respect to the ambient fluid. This situation is experi-

mentally realized when a light-absorbing tracer particle diffuses in the focus of a laser. Because of the separation of time scales between heat propagation and Brownian motion, a steady temperature profile develops around the nanoparticle, which can be detected by a second laser [1]. Our MD simulations are used to investigate various microscopic phenomena associated with "hot Brownian motion", including effective temperatures and non-equilibrium hydrodynamic boundary conditions. The results are compared to recent analytical predictions obtained from fluctuating hydrodynamics [2].

[1] R. Radünz, D. Rings, K. Kroy, and F. Cichos, J. Phys. Chem. A 113 (9), 1674-1677 (2009)

[2] D. Rings, R. Schachoff, M. Selmke, F. Cichos, and K. Kroy, Phys. Rev. Lett., 105 (9), 090604 (2010)

DY 10.22 Mon 17:00 P4

Anomalous diffusion of Brownian particals in potential traps exposed to shear flow — •Johannes Greber, Diego Kienle, Jochen Bammert, and Walter Zimmermann — Universität Bayreuth, LS für theoreitsche Physik I, 95440 Bayreuth

The Brownian motion of particles in various potential shapes is investigated. Depending on the local curvature of potentials with a single minimum, we find either sub- or super-diffusive particle dynamics. The dependence of the anomalous exponent of the mean square displacement on the on the potential shape is explored. In addition, we study also the impact of shear flow on the diffusive behavior of particles in potentials, as recently investigated for small excursions in Ref. [1]. In addition , we study the dynamics of particles in a double well-potential well, where the particles are exposed to shear flow. As well, we find a nonlinear shear rate dependence of the probability current across the potential.

[1] A. Ziehl et al., Phys. Rev. Lett. 103, 230602 (2009)

DY 10.23 Mon 17:00 P4

Anomalous diffusion in crowded fluids revealed by a novel single-particle tracking technique — •Dominique Ernst[1], Marcel Hellmann[3], Matthias Weiss[2], and Jürgen Köhler[1] — [1]Experimental Physics IV, University of Bayreuth, 95440 Bayreuth, Germany — [2]Experimental Physics I, University of Bayreuth, 95440 Bayreuth, Germany — [3]Cellular Biophysics Group, German Cancer Research Center, 69120 Heidelberg, Germany

A versatile setup for automated single particle tracking in two dimensions is used to analyse anomalous diffusion processes in crowded fluids with a high spatio-temporal resolution. The ingenious tracking technique allows us to record trajectories of a single fluorescent nanoparticle (20 nm) for more than 15 minutes with a temporal resolution of 4 ms and a dynamic position accuracy of about 25 nm. We create a light orbit with a focussed laser beam and project that light orbit with a homebuilt fluorescence microscope into the sample plane. At the beginning of the tracking procedure, the nanoparticle has to be located in the center of the orbit. Subsequently, we detect the modulation of the emission intensity due to the movement of the particle out of the center of the light orbit, calculate the new position of the particle from the modulation parameters, and compensate for the movement of the particle with the aid of a piezostage. From that feedback we reconstruct the trajectory of the particle and determine the mean square displacement. Here we present the method and as an example its application to diffusion in crowded fluids like dextran as a model system for the cytoplasm of a cell.

DY 10.24 Mon 17:00 P4

Analyzing anomalous diffusion processes: the distribution of generalized diffusivities — •Tony Albers and Günter Radons — Chemnitz University of Technology, Germany

We propose a new tool for analyzing data from normal or anomalous diffusion processes: The distribution of generalized diffusivities $p_\alpha(D,\tau)$ is defined as the probability density of finding a squared displacement of duration τ, rescaled by its asymptotic time dependence τ^α. It describes the fluctuations appearing during the diffusion process around the mean anomalous diffusion coefficient, which can be obtained from the asymptotic behavior of the mean squared displacement (MSD) and is also equal to the first moment of the distribution $p_\alpha(D,\tau)$ for large τ. In comparison with the MSD we therefore obtain more information from the numerically or experimentally determined data. In this contribution we analyze with this new tool the diffusive transport in low and higher dimensional Hamiltonian systems and show with the help of modified continuous time random walks how the structures in phase space are reflected in the distribution of generalized diffusivities.

DY 10.25 Mon 17:00 P4

Diffusion in komplementären Strukturen — •Thorsten Emmerich[1] und Armin Bunde[2] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität 35392 Giessen — [2]Institut für Theoretische Physik, Justus-Liebig-Universität 35392 Giessen

Wir untersuchen mit Hilfe der Monte Carlo Simulation Diffusion in komplementären Räumen. Ziel ist es, herauszufinden, in wie weit man von der Diffusion in einem nanoporösen System auf die Diffusion im komplementären Porensystem schließen kann. Um experimentell relevante Porenstrukturen zu erzeugen, verwenden wir das Isingmodell mit Kawasaki-Spinaustausch. Um die gewünschte Porenstruktur zu erzeugen, wird bei vorgegebener Spin-up-Konzentration p das System auf eine Temperatur $T < T_c$ abgekühlt. Dabei bilden sich Domänen mit gleicher Spinausrichtung (Cluster). Die Porengröße der Cluster kann durch unterschiedliche Relaxationszeiten τ verändert, und durch die räumliche Spin-Spin Korrelationsfunktion quantifiziert werden. Wir bestimmen mit Hilfe von Monte Carlo Simulationen die Diffusionseigenschaften (mittleres Verschiebungsquadrat als Funktion der Zeit) des Systems und des komplementären Systems, sowohl in der Nähe als auch fern der Perkolationsschelle p_c. Ausser Volumendiffusion betrachten wir auch reine Grenzflächendiffusion, wo sich die diffundierenden Teilchen nur auf der Grenzfläche des jeweiligen Systems bewegen können. Wir diskutieren die Bedingungen unter denen die Diffusionseigenschaften in den komplementären Räumen einander ähnlich sind.

DY 10.26 Mon 17:00 P4

Are superdiffusive jumps in molecular diffusion triggered or destroyed by the chaotic dynamics of the molecule's internal degrees of freedom? — •Sarah Hallerberg[1] and Astrid S. de Wijn[2] — [1]Chemnitz University of Technology — [2]Radboud University Nijmegen

Long jumps in surface diffusion of organic molecules and nanoscale clusters have been observed experimentally, and were also found in numerical simulations. Recent studies[1] highlight the existence of a relation between the diffusion of molecules and the dynamics of their internal degrees of freedom. These internal chaotic dynamics lead to normal diffusion, even in the absence of thermal noise. Our contribution aims at determining the physical mechanism which trigger long superdiffusive jumps. Benzene on graphite is a prototype system and serves us to investigate these long jumps by postprocessing the output of atomistic simulations[1]. In more detail, we search for precursors[2] in the internal degrees of freedom by considering the energy in the vibrational modes of the linearised system and show that relevant precursors appear particularly in the torsional vibrations. Our results suggest a strong connection between lack of torsion of the molecule and long superdiffusive jumps.

[1] A. S. de Wijn and A. Fasolino. Journal of Physics: Condensed Matter, 21:264002, 2009. [2] S. Hallerberg, E. G. Altmann, D. Holstein, H. Kantz, Phys Rev. E, 2007, 75, 016706.

DY 10.27 Mon 17:00 P4

Anomalous magnetoresistance in a 2D Lorentz-Gas — •Benedikt Fuchs[1], Teresa Bauer[1], Felix Höfling[2], and Thomas Franosch[3] — [1]ASC and CeNS, Fakultät für Physik, Ludwig-Maximilians-Universität München, Germany — [2]Max-Planck-Institut für Metallforschung, Stuttgart, and Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany — [3]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

We simulate the transport of electrons through a two-dimensional random array of obstacles under the influence of a perpendicular magnetic field. At low density, a percolation transition arises, at which transport sets in. It can be rationalized as follows: For fixed magnetic field, the electrons circle around few obstacles and stay near their starting point at very low density, while they proceed from one obstacle to the next at intermediate density, traversing the whole system for sufficiently dense obstacles. This transition and the dependence of the critical density on the magnetic field have been anticipated before [1], but have yet never been verified in a simulation. We examplify the transition at several points, corrobating the predicted behavior. Anomalous transport is observed at these points for more than six orders of magnitude in time by both power-law behaviour of the MSD and power-law decay of the diffusion coefficient.

[1] A. Kuzmany and H. Spohn, Phys. Rev. E 57(5), 5544 (1998)

DY 10.28 Mon 17:00 P4

Determination of the attractor dimension at the synchronization transition of a delayed chaotic system — •Steffen Zeeb and Wolfgang Kinzel — Institut für Theoretische Physik, Universität Würzburg

A network of nonlinear units interacting by time-delayed couplings can sychronize to a common chaotic trajectory. Although the transmission time may be very long the units are completely synchronized without time shift.

We investigate the transition to synchronization. In particular, for networks of iterated maps we determine the Kaplan-Yorke dimension from the spectra of Lyapunov exponents which are calculated analytically for Bernoulli maps and numerically for tent maps. However, we argue that the Kaplan-Yorke conjecture cannot be true at the transition. For the synchronized state the Lyapunov exponents perpendicular to the synchronization manifold cannot contribute to the attractor dimension. Consequently, the attractor dimension has to jump discontinuously at the transition. We calculate the magnitude of this jump for different networks.

Finally, the Kaplan-Yorke dimension is compared to the information and correlation dimension, respectively, in order to check the discontinuous behavior of the attractor dimension.

DY 10.29 Mon 17:00 P4

Emergence of coherent motion in flocks of deterministics walkers: a coupled maps evolving network perspective — Garcia Cantu Ros Anselmo[1], Basios Vasileos[2], and •Antonopoulos Christos[2] — [1]Potstdam Institute for Climate Impact Research PIK, Potsdam, Germany — [2]Free University of Brussels ULB, Brussels, Belgium

The emergence of coherence in collective motion described by a system of interacting motiles is analyzed. By means of a nonlinear adaptative coupling, the system elements are able to swing along the route to chaos. Thereby, each motile can display different types of behavior, i.e. from ordered to fully erratic motion, accordingly with its surrounding conditions. The appearance of patterns of collective motion is shown to be related to the emergence of interparticle synchronization and the degree of coherence of motion is quantified by means of a network representation. It is shown that the highest degree of coherence of motion is attained when the system self-drives towards the border between order and chaos. The effect of both particles' density and of considering different weights for the interparticle distances is explored.

DY 10.30 Mon 17:00 P4

Information Spread during Building Evacuation Scenario with Long and Short-range Communication — •Mirko Kämpf and Jan W. Kantelhardt — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle/Saale, Germany

Based on extended lattice-gas simulations with additional short-range and long-range interactions we study the spread of information between human agents during a large-scale building evacuation scenario. Our evacuation simulation tool utilizes established algorithms for the emotional and intelligence driven motion of human beings in a building and includes direct (short-range) as well as communication technology enabled (long-distance) information spread between them. We compare our results with those from simulations in an unrestricted geometry (free space) and for varying prevalence of long-distance communication. This way we study the impact of futures communication technologies on effective exit strategies during emergency evacuation. To detect phases (steady flow, panic, jam, etc.) and phase transitions in the system we apply detrended fluctuation analysis and return interval statistics to the simulation data. The results help us to define basic functional requirements for the underlying communication and network topology as well as to needed sensors.

DY 10.31 Mon 17:00 P4

Synchronization of chaotic networks and the spectral gap of stochastic matrices — •Martin Paulig and Wolfgang Kinzel — Institute for Theoretical Physics, University Würzburg, Am Hubland, 97074 Würzburg, Germany

A network of coupled nonlinear units can synchronize to a common chaotic trajectory. Although the coupling may have a long time delay, synchronization occurs without any time shift. In the limit of very large delay time, the spectral gap of the coupling matrix determines the condition for a stable synchronization manifold. On the other side, the theory of stochastic matrices gives conditions for a nonzero spectral gap. From this relation, we calculate the parameter regions of stable synchronization for various networks with uni- and bi-directional couplings.

DY 10.32 Mon 17:00 P4

Master stability function for time-delayed networks of chaotic semiconductor lasers — •Sven Heiligenthal, Anja Englert, Marco Winkler, and Wolfgang Kinzel — Julius-Maximilians-University, Würzburg, Germany

The master stability function allows to calculate the stability of the synchronization manifold of arbitrary networks. We use this method to numerically analyze the stability of several different networks of chaotic semiconductor lasers with time-delayed mutual couplings by simulating the Lang-Kobayashi equations.

We make predictions about the synchronizability of such networks by relating the modulus of the second largest eigenvalue of the network's adjacency matrix to the maximal Lyapunov exponent of the network dynamics. Our numerical simulations confirm these predictions for two examples of different network topologies.

Furthermore, we show symmetries of the master stability function for networks with two different delay times which were recently proven for networks of simple Bernoulli maps. Our numerical results for networks of chaotic semiconductor lasers show these symmetries, as well.

Finally, we show by using the master stability function that networks of chaotic semiconductor lasers in which the delay time of the mutual couplings is much larger than the internal time scales of the chaotic lasers cannot be synchronized if the local Lyapunov exponent is positive. We also make a proposal for an experimental method which can measure this local Lyapunov exponent.

DY 10.33 Mon 17:00 P4

A dynamical model of controlled nanochannel lattice formation utilizing prepatterned substrates — •Michael H. Köpf, Svetlana V. Gurevich, and Rudolf Friedrich — Institut für Theoretische Physik, Universität Münster

Self-organized processes in dewetting systems provide effective methods for the controlled fabrication of micro- and nanostructured surfaces. Lipid monolayers such as DPPC and DMPE are known to form regular stripe patterns upon Langmuir-Blodgett transfer onto solid substrates [1]. These patterns consist of alternating domains of different thermodynamic phases and result from phase transitions induced by a substrate-monolayer interaction. By incorporation of the monolayer thermodynamics into a hydrodynamic model of thin film flow, this process can be described in terms of two coupled nonlinear partial differential equations [2,3]. Here, we present a theoretical study of the effect of prepatterned substrates, focussing on periodic prestructures. These structures lead to a periodic forcing of the pattern formation at the meniscus. Synchronization with this forcing can be exploited to generate complex periodic structures in a controlled manner [4].

[1] M. Gleiche, L. F. Chi, H. Fuchs, *Nature*, **403** (2000) 173-175

[2] M. H. Köpf, S. V. Gurevich, R. Friedrich, *EPL (Europhysics Letters)*, **86** (2009) 66003 (6 pages)

[3] M. H. Köpf, S. V. Gurevich, R. Friedrich, L. F. Chi, *Langmuir*, **26** (2010) 10444-10447

[4] M. H. Köpf, S. V. Gurevich, R. Friedrich, *submitted to PRE*, arXiv:1011.1140v1 [nlin.PS] (2010)

DY 10.34 Mon 17:00 P4

Pattern deposition in driven lattices — •Benno Liebchen, Christoph Petri, Florian Lenz, and Peter Schmelcher — Zentrum für optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

The nonlinear dynamics of classical, noninteracting particles in a one-dimensional lattice of laterally driven square potentials is studied, by means of exact numerical simulation.

We demonstrate two different mechanisms for the creation of controllable pattern-like particle-localization. Apparently, this is not possible in a system of static barriers, since trapping would prohibit the coexistence of diffusion there. By instantly increasing the barrier-potential in a periodic lattice with nonlinear phase-gradients, we observe the development from a uniform particle-distribution to a pattern-like structure. The mechanism is explained by symmetry considerations. Within a lattice with spatially varying barrier-frequency, transient global patterns are created and frozen via an instant increase of the barrier-potential.

DY 10.35 Mon 17:00 P4

Plasticity in a Spiking Neural Network Model — •Cornelia

Petrovic and Rudolf Friedrich — Westfälische Wilhelms-Universität Münster, Institut für Theoretische Physik

We study the influence of spike-timing-dependent plasticity (STDP) in a spiking neuronal network which consists of pulse-coupled phase oscillators introduced by Haken as the lighthouse model [1]. It is a single neuron model that falls between spiking neuron models and firing rate descriptions and thus combines "best of both worlds". In the limit of slow synaptic interactions it can be reduced to the classic Wilson-Cowan and Amari type firing rate models [2,3,4]. For fast synaptic dynamics, it shows some of the complex properties of spiking neural networks.

[1] H. Haken, Brain Dynamics, Springer-Verlag, New York, Berlin, 2002.
[2] H.R. Wilson and J.D. Cowan, Biophys. J., 12 (1972), pp. 1-24.
[3] S. Amari, IEEE Trans. Systems Man Cybernet., 2 (1972), pp. 643-657.
[4] C.C. Chow and S. Coombes, SIAM J.Appl. Dyn. Syst., 5 (4) (2006), pp. 552-574.

DY 10.36 Mon 17:00 P4

Where can one observe non-hyperbolicity? — •Jian Wang, Hongliu Yang, and Günter Radons — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

Hyperbolicity is an important property of dynamical systems. Many physically relevant dynamical systems are not hyperbolic, and many of the available theoretical results have been derived under the assumption of strict hyperbolicity. Recently, a new method for determining the so-called covariant Lyapunov vectors (CLV) was introduced by F. Ginelli et al. With CLV the degree of hyperbolicity of the dynamics can be quantified. Since in a non-hyperbolical system the violation of hyperbolicity occurs only at certain locations in state space, the determination of these locations is of much interest. In this study we investigate the relationship between hyperbolicity and the covariant Lyapunov analysis along the trajectory. Our main focus lies on the relation of angles between different local CLV to the variation of local Lyapunov exponents. The positions, where non-hyperbolictiy arises, are shown.

DY 10.37 Mon 17:00 P4

Continuous path-based measures for ε-recurrence networks — •Jonathan F. Donges[1,2], Jobst Heitzig[1], Reik V. Donner[1], and Jürgen Kurths[1,2] — [1]Potsdam Institute for Climate Impact Research, P.O.Box 60 12 03, 14412 Potsdam, Germany — [2]Department of Physics, Humboldt University of Berlin, Newtonstr. 15, 12489 Berlin, Germany

Continuous versions of various path-based graph-theoretical measures are defined for ε-recurrence networks, which have recently been successfully used in various applications of dynamical systems theory and time series analysis. We derive closed form expressions for two well-known one-dimensional maps as well as for the hypersphere and hypercube in various dimensions m. The latter problems are found to be closely linked to current research in probabilistic geometry and applied mathematics. Some comparison of the rigorous results to numerical estimates from ε-recurrence networks of finite length time series is also made. We argue that the proposed theory of path-based ε-recurrence network measures contributes substantially to a deeper understanding of the method of ε-recurrence network based time series analysis, which has already been utilized successfully in several distinct applications. Some geometrical applications of these measures, e.g., to define well-behaved measures of the convexity of a set, are also suggested.

DY 10.38 Mon 17:00 P4

State switching in a conductance-based cortical model: phase diagram and pulse stimulation — •Arne Weigenand, Thomas Martinetz, and Jens Christian Claussen — Neuro- and Bioinformatik, Universität zu Lübeck

A recent experiment [1] investigated the on- and off switching of bursting activity in ferret brain slices. This experiment is seen as a paradigmatic system towards the understanding of the emergence of cortical slow waves. The basic dynamics can be modeled by a simplified discretized integrate - and - fire model having intrinsic inhibitory currents but lacking inhibitory connections [2]. Here we use a conductance-based model to reproduce the spike-burst dynamics and the triggering of Up states as observed in [1]. Finally we investigate the phase diagram of the qualitatively different network states depending on the coupling strength and network noise intensity [3].

[1] Y. Shu, A. Hasenstaub, and D. A. McCormick, Nature 423, 288 (2003). [2] H. V. Ngo, J. Köhler, J. Mayer, J. C. Claussen, and H. G. Schuster, EPL 89, 68002 (2010) [3] A. Weigenand et al., in preparation

DY 10.39 Mon 17:00 P4

Spiral Defect Chaos in Rayleigh Benard Systems — •Hira Affan and Rudolf Friedrich — Westfälische Wilhelms Universität Münster

The importance of mean flow is addressed in a system of Rayleigh Benard Convection. A numerical study is carried out to investigate the model equations so that it can be argued that mean flow is important for the spiral defect chaos.

DY 10.40 Mon 17:00 P4

Synchronisation in networks of delay-coupled type-I excitable systems — Andrew Keane, •Thomas Dahms, Judith Lehnert, Philipp Hövel, and Eckehard Schöll — Institut f. Theo. Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We use a generic model for type-I excitability (known as the SNIPER or SNIC model) to describe the local dynamics of nodes within a network and apply time-delayed coupling as a means of control to stabilise the synchronised dynamics. Utilising the method of the master stability function, we investigate the stability of the synchronised dynamics (i.e. the success of the control) and its dependence on the two coupling parameters, namely the coupling strength and delay time. The results are compared to numerical simulations for exemplary cases (including random networks and small-world networks). It is shown that for particular parameter ranges the results are comparable to previous work with the FitzHugh-Nagumo model (a model for type-II excitability), while for other parameter values the stability of synchronisation will depend on the coupling strength and delay time.

DY 10.41 Mon 17:00 P4

Spatial instability in diffusive system with variable delay — •Jian Wang and Günter Radons — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

In ubiquitous natural and laboratory situations the action of time delayed signals is a crucial ingredient to understand the dynamical behavior of these systems. A frequently encountered situation is that the length of the delay time changes with time. With the introduction of varying delay, a simple system can exhibit complicated behavior. In this study we investigate spatial diffusive system with variable delay and show that the spatial instability increases with the introduction of varying delay. Lyapunov exponents and dynamic structure factor are calculated. Special space-time structures, such as travelling wave, are investigated in some detail.

DY 10.42 Mon 17:00 P4

Diffusive Coupling Can Discriminate Between Similar Reaction Mechanisms in an Allosteric Enzyme System — •Ronny Straube[1] and Ernesto M. Nicola[2] — [1]Systems Biology Group, Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany — [2]Institute for Cross-Disciplinary Physics and Complex Systems, Campus UIB, Palma de Mallorca, Spain

Recently, inward rotating spiral waves (anti-spirals) have been observed in cell free yeast extracts [1]. Such anti-spirals were, so far, only observed in purely chemical systems. To elucidate the molecular mechanism leading to this unusual wave dynamics we compare two mechanisms of product activation for the allosteric enzyme phosphofructokinase. We find that a sequential activation mechanism as in the Monod-Wyman-Changeux (WMC) model is able to generate inward propagating waves while a simple Hill function as employed in the Selkov model is not [2]. The occurrence of inward propagating waves is related to the sensitivity of the enzyme cooperativity with respect to the activator concentration, and we show that the waves generated by the MWC mechanism are more stable against long wave length perturbations. These results explicitly show how the type and the stability of macroscopically observable wave patterns depend on the underlying molecular reaction mechanism in a simple allosteric enzyme system.

[1] R. Straube, S. Vermeer, E. M. Nicola, T. Mair, *Biophys. J.* **99**, L4-L6 (2010). [2] R. Straube, E. M. Nicola, *BMC Systems Biology* **4**:165 (2010).

DY 10.43 Mon 17:00 P4

Evolution of a scroll ring in an oscillatory medium close to

a Neumann boundary — •Fabian Paul and Harald Engel — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany

It is shown that scroll ring solutions of the complex Ginzburg-Landau equation can be stabilized by the interaction with a Neumann boundary. Two antagonistic tendencies govern the dynamics of the scroll ring: Boundary-induced expansion and contraction caused by positive filament tension. Depending on the initial conditions and the chosen parameters, due to the interaction with the Neumann boundary the contraction of the scroll ring is slowed down or even terminated at a finite radius. For certain parameter values numerical simulations suggest a limit cycle regime with alternating phases of contraction and expansion of the scroll ring. This object reminds of an autonomous pacemaker in an active medium close to the transition between excitable and oscillatory kinetics.

DY 10.44 Mon 17:00 P4

Predicting Outliers in Ensemble Forecasts — •Stefan Siegert, Jochen Bröcker, and Holger Kantz — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

An ensemble forecast is a collection of runs of a numerical dynamical model, initialized with perturbed initial conditions. In modern weather prediction for example, ensembles are used to retrieve probabilistic information about future weather conditions. In this contribution, we are concerned with ensemble forecasts of a scalar quantity (say, the temperature at a specific location), and their relation to the verification (i. e. the actual observation of that quantity). We consider the event that the verification is smaller than the smallest or larger than the largest ensemble member. We call these events *outliers*. If a K-member ensemble accurately reflects the variability of the verification, outliers should occur with a relative frequency of $2/(K+1)$. In operational forecast ensembles though this frequency is often found to be higher. We study the predictability of outliers and find that, exploiting information available from the ensemble, forecast probabilities for outlier events can be calculated which are more skillful than the unconditional relative frequency. In other words, using ensemble information, more accurate forecasts of impending outliers are possible than just stating their relative frequency. We show this analytically for statistically consistent ensembles and empirically for an operational ensemble using methods of model output statistics. Our results are relevant for evaluating and post-processing ensemble forecasts.

DY 10.45 Mon 17:00 P4

Drawing energy landscapes of spin glasses — •Karsten Looschen and Alexander Hartmann — Carl von Ossietzky Universität Oldenburg, Institut für Physik, D-26111 Oldenburg

The rough energy landscape of a spin glass is regarded as one of its main features, but how does it look like? Often a schematical sketch with a one dimensional arrangement of states is drawn, however for a spin glass of N Ising spins the energy landscape consists of 2^N states in a N-dimensional space. We propose different algorithms to systematically retrieve a meaningful arrangement of states.

Since enumeration of all states is impossible for all but very small systems, some (10^3 - 10^5) states are statistically sampled. Efficient hierarchical clustering algorithms based on a similarity measure for the sampled states can be used to alleviate the problem of high dimensionality. Leafs which are near each other in the resulting tree represent states with high similarity. This feature of the tree enables a simple plot of the energy landscape with a one dimensional arrangement of states.

The three dimensional Edwards-Anderson $\pm J$ spin glass with bond strengths $-J$ (probability p) and $+J$ (probability $1-p$) is examined. This system is a spin glass if $0.23 < p < 0.77$ and a ferromagnet else. Graphical representations of its energy landscape are retrieved and the "roughness" is characterized as a function of p.

DY 10.46 Mon 17:00 P4

Large-scale transitions in Plio-Pleistocene African dust flux dynamics identified by recurrence network analysis — Jonathan F. Donges[1,2], •Reik V. Donner[1], Martin H. Trauth[3], Norbert Marwan[1], and Jürgen Kurths[1,2] — [1]Potsdam Institute for Climate Impact Research, Potsdam, Germany — [2]Department of Physics, Humboldt University of Berlin, Germany — [3]Department of Earth and Environmental Sciences, University of Potsdam, Germany

These days, long-term environmental changes are believed to have acted as a key factor in the evolutionary history of the human race. For the Plio-Pleistocene climate history of East Africa (the "cradle of mankind"), recent studies on terrestrial as well as marine paleoclimate archives suggested different possible climatic forcing mechanisms. Here, we apply recurrence network analysis, a novel nonlinear statistical technique, to three distinct marine records of terrigeneous dust flux. Our method identifies subtle, but robust transitions between qualitatively different types of dust flux dynamics at about (i) 3.45-3.05, (ii) 2.1-1.7, and (iii) 1.2-0.7 Myr BP, which reflect changes in the variability of environmental conditions in North and East Africa. The timing of the identified transition periods reveals both low- and high-latitude climatic changes as possible dynamic origins of the observed regime shifts, the sources of which are identified and critically discussed.

DY 10.47 Mon 17:00 P4

Towards first-passage-time prediction for temperature data — •Anja Garber, Nicholas Moloney, and Holger Kantz — Max-Planck-Institut für Physik komplexer Systeme, Dresden

In the operational short term weather prognoses, detailed models are run only for a lead time of ten days, preventing predictions further into the future. However, in the more medium range exceeding the lead time of model runs where detailed predictions are currently unavailable, already the first passage time until a threshold crossing can be of significant interest, e.g. the expected time until first frost.

In order to develop methods towards a suitable approximation and prediction of these first passage times from the existing model runs, we study the first passage time distribution both for an autoregressive model process and actual temperature data.

DY 11: Focus Session: Thermodynamics and Statistical Physics of Small Systems

Time: Tuesday 10:00–13:15 Location: HÜL 186

Invited Talk DY 11.1 Tue 10:00 HÜL 186

Doing small systems: Concepts, Role of Ensembles, Thermalization and Fluctuation Theorems — •Peter Hänggi — Universität Augsburg, Institut für Physik, Universitätsstr. 1, 86135 Augsburg

This symposium is aimed at highlighting issues that relate of doing thermodynamics and statistical physics of finite size systems. This theme gained considerable importance in view of fascinating advances in nanotechnology and system biology. While the fathers of thermodynamics developed the famous Laws having in mind macroscopic systems these grand concepts need to be inspected anew in view of the fact that the fluctuations grow with decreasing size to a level where they even may play the dominant role.– The symposium touches upon several timely issues in designing, measuring and operating systems at the submicron scale, both IN and also FAR AWAY from thermal equilibrium. With this introduction I discuss subtleties related to thermodynamics of small systems, such as (i) the role of finite size for quantities such as (in some cases negative-valued) heat capacitance [1], (ii) the role of entropy and temperature in these small systems, or (iii) the issue of thermalization. Moreover, a key role in doing statistical physics of submicron systems relates to (iv) the choice of the ensemble description and the inter-relationships between the sizable fluctuations of measures like work, heat & heat flow and thermodynamic equilibrium quantifiers such as free energy changes or changes of entropy. [1] P. Hänggi, et al., Finite quantum dissipation: the challenge of obtaining specific heat, New J. Phys. 10, 115008 (2008); in addition see also: G. Ingold, et al., Phys. Rev. E 79, 061105 (2009) .

Invited Talk DY 11.2 Tue 10:30 HÜL 186

Microcanonical singularities in finite systems — •Jörn Dunkel[1] and Stefan Hilbert[2] — [1]Department of Applied Mathematics and Theoretical Physics, Centre for Mathematical Sciences, University of Cambridge, Wilberforce Road, Cambridge CB3 0WA, UK — [2]Instititut für Astronomie, Universität Bonn, Auf dem Hügel 71, 53121 Bonn, Germany

The microcanonical equations of state of a finite isolated system can exhibit a substantially more complex structure than their canonical counterparts [1,2]. Prominent examples are singularities and oscillations in the caloric temperature curves, corresponding to regions of negative specific heat, which reflect structural changes in the microscopic properties of the underlying Hamiltonian system as the energy control parameter is varied. After taking a brief look at the virtues and drawbacks of competing microcanonical entropy definitions, we will illustrate the aforementioned phenomena by means of an exactly solvable 1D dissociation model [1]. Although the model is relatively simple, it suggests an interesting general connection between the microscopic temperature oscillations in a finite microcanonical system and macroscopic canonical phase transitions in the corresponding infinite system.

[1] S. Hilbert and J. Dunkel, Phys. Rev. E 74: 011120, 2006
[2] J. Dunkel and S. Hilbert, Physica A 370(2): 390, 2006

Invited Talk DY 11.3 Tue 11:00 HÜL 186

Recent progress in fluctuation theorems and free energy recovery — •Felix Ritort — Departament de Fisica Fonamental, Facultat de Fisica, Universitat de Barcelona, Diagonal 647, 08028 Barcelona (Spain)

Recent developments in micro and nanotechnologies enable the manipulation of single molecules one at a time. Single molecule experiments make possible to resolve energy processes with unprecedented detail at the level of 1 kT, the typical energy scale of Brownian fluctuations.* Fluctuation theorems establish relations governing energy exchange processes at this level and provide a new methodology to obtain equilibrium information from non-equilibrium experiments. In this talk I will show applications to free energy recovery* in single molecule experiments obtained in our laboratory (Small biosystems lab, Barcelona, Spain) in unzipping experiments carried out on DNA, RNA and proteins. The range of applications covers free energy recovery of molecular native states, intermediate states and misfolded states. I will also show how fluctuation relations can be applied to recover base pairing free energies in RNA, essential to improve free energy prediction of RNA secondary structures.

15 min. break

Invited Talk DY 11.4 Tue 11:45 HÜL 186

Efficiencies and fluctuations in small out-of-equilibrium devices — •Massimiliano Esposito — Center for Nonlinear Phenomena and Complex Systems, Université Libre de Bruxelles, Campus Plaine CP 231, Brussels B-1050, Belgium.

Small systems undergo strong fluctuations and can easily be driven far from their thermodynamic equilibrium. A stochastic description of their dynamics combined with very few physical assumptions and the correct identification of entropy production provide a consistent nonequilibrium thermodynamic description of these small systems. I will show that such description enables the study of finite-time efficiencies and nonequilibrium fluctuations in various small devices such as thermoelectric quantum dots and photoelectric cells.

Invited Talk DY 11.5 Tue 12:15 HÜL 186

Quantum Fluctuation Theorems — •Michele Campisi — Pisa, Italy — Institute for Physics, University of Augsburg, Germany

The second law of thermodynamics poses a stringent constraint on the direction that physical processes may take in macroscopic systems. As their size shrinks, processes taking the opposite direction, apparently defying the second law, become possible and the fluctuation theorems quantify the likelihood of their occurrence. We will address the following issues concerning quantum fluctuation theorems i) the problem of gauge freedom affecting the definitions of work and free energy, ii) the notions of inclusive, exclusive and dissipated work [1], iii) the absence of a work operator in quantum mechanics and the notion of two-point quantum observable iv) the difficulties related to the experimental verification of quantum fluctuation theorems and the possibility to overcome them [2].

[1] M. Campisi et al. "Quantum Bochkov-Kuzovlev work fluctuation theorem" arXiv:1003.1052.
[2] M. Campisi, et al. "Fluctuation theorems for continuously monitored quantum fluxes" Phys. Rev. Lett. 105, 104601 (2010)

Invited Talk DY 11.6 Tue 12:45 HÜL 186

Time-reversal symmetry relations: From the multibaker map to open quantum systems — •Pierre Gaspard — Université Libre de Bruxelles, Brussels, Belgium

On the basis of microreversibility, symmetry relations have been established for the counting statistics of different currents flowing through classical, stochastic, or quantum systems sustaining nonequilibrium steady states in the absence or presence of an external magnetic field. Recently, it has been shown that these relations have consequences on the nonlinear-response properties of the system, extending linear-response Onsager reciprocity relations. These results apply to nonequilibrium processes such as chemical reactions, molecular motors, or electron transport in quantum dots.

References:

- S. Tasaki and P. Gaspard, Fick's Law and Fractality of Nonequilibrium Stationary States in a Reversible Multibaker Map, J. Stat. Phys. 81 (1995) 935.
- P. Gaspard, Fluctuation theorem for nonequilibrium reactions, J. Chem. Phys. 120 (2004) 8898.
- D. Andrieux and P. Gaspard, Fluctuation theorem and Onsager reciprocity relations, J. Chem. Phys. 121 (2004) 6167.
- D. Andrieux and P. Gaspard, A fluctuation theorem for currents and non-linear response coefficients, J. Stat. Mech. (2007) P02006.
- D. Andrieux, P. Gaspard, T. Monnai, and S. Tasaki, The fluctuation theorem for currents in open quantum systems, New J. Phys. 11 (2009) 043014.

DY 12: Quantum Dynamics, Decoherence, and Quantum Information II

Time: Tuesday 10:15–13:15 Location: ZEU 255

DY 12.1 Tue 10:15 ZEU 255

Hamiltonian of mean force for a damped quantum oscillator — •Stefanie Hilt, Benedikt Thomas, and Eric Lutz — Department of Physics, University of Augsburg, 86135 Augsburg, Germany

We consider a quantum harmonic oscillator linearly coupled to a reservoir of harmonic oscillators. For a finite coupling strength the stationary distribution of the damped oscillator is not of the Gibbs form, in contrast to standard thermodynamics. We quantify this deviation by evaluating the quantum Hamiltonian of mean force exactly and discuss its connection with the initial coupling process between system and reservoir.

DY 12.2 Tue 10:30 ZEU 255

Energy-time uncertainty for driven quantum systems — Sebastian Deffner and •Eric Lutz — Department of Physics, University of Augsburg, D-86135 Augsburg

We derive a generalization of the energy-time uncertainty relation for driven quantum systems based on the Bures geometric distance in Hilbert space and the concept of quantum speed limit. This relation is valid for arbitrary driving protocol and arbitrary distance between initial and final state.

DY 12.3 Tue 10:45 ZEU 255

Asymmetric Bethe-Salpeter equation for pairing and condensation — •Klaus Morawetz — University of Applied Science Münster, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP), Universidade Federal do Rio grande do Norte - UFRN, Brazil

The Martin-Schwinger hierarchy of correlations are reexamined and the three-particle correlations are investigated under various partial summations. Besides the known approximations of screened, ladder and maximally crossed diagrams the pair-pair correlations are considered. It is shown that the recently proposed asymmetric Bethe-Salpeter equation to avoid unphysical repeated collisions is derived as a result of the hierarchical dependencies of correlations. Exceeding the parquet approximation we show that an asymmetry appears in the selfconsistent propagators. This form is superior over the symmetric selfconsistent one since it provides the Nambu-Gorkov equations and

gap equation for fermions and the Beliaev equations for bosons while from the symmetric form no gap equation results. The selfenergy diagrams which account for the subtraction of unphysical repeated collisions are derived from the pair-pair correlation in the three-particle Greenfunction. It is suggested to distinguish between two types of selfconsistency, the channel-dressed propagators and the completely dressed propagators, with the help of which the asymmetric expansion completes the Ward identity and is Φ-derivable.

arXiv:1006.4695

DY 12.4 Tue 11:00 ZEU 255

Modular Entanglement — •Giulia Gualdi[1,2], Salvatore Marco Giampaolo[2], and Fabrizio Illuminati[2] — [1]Universiät Kassel Fachbereich 10 - Mathematik und Naturwissenschaften Institut für Physik Heinrich-Plett-Str. 40 D-34132 Kassel — [2]Dipartimento di Matematica e Informatica, Università degli Studi di Salerno, Via Ponte don Melillo, I-84084 Fisciano (SA), Italy; CNR-SPIN, and INFN Sezione di Napoli, Gruppo collegato di Salerno, I-84084 Fisciano (SA), Italy

We introduce and discuss the concept of modular entanglement. This is the entanglement that is established between the end points of modular systems composed by sets of interacting moduli of arbitrarily fixed size. We show that end-to-end modular entanglement scales in the thermodynamic limit and rapidly saturates with the number of constituent moduli. We clarify the mechanisms underlying the onset of entanglement between distant and non-interacting quantum systems and its optimization for applications to quantum repeaters and entanglement distribution and sharing.

DY 12.5 Tue 11:15 ZEU 255

Dynamics of quantum phase transitions using ensembles of classical trajectories — •Alexander Itin[1,2] and Peter Schmelcher[1] — [1]Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Space Research Institute, Profsoyuznaya str. 84/32, Moscow 117997, Russia

Recently, Truncated Wigner Approximation was applied to study dynamics of quantum phase transitions (QPT) in infinitely-coordinated models such as the Dicke and Lipkin-Meshkov-Glick models [1,2,3]. The initial quantum state is represented by an ensemble of classical trajectories, with quantum observables being obtained by averaging over the classical ensemble. As an external parameter is changed, the quantum system experiences a passage through a QPT, while trajectories from the classical ensemble undergo a passage through a bifurcation. Non-adiabaticity of the ensemble of classical trajectories can be described by mapping to Painleve equations, as shown recently in [2,3]. After overviewing recent results in this field, we present the application of the method to the dynamics of splitting and merging of multiple Bose-Einstein condensates [4,5].

[1] A. Altland et al., Phys.Rev,A 79, 042703 (2009).
[2] A.P. Itin and P. Törmä, Phys. Rev. A 79, 055602 (2009).
[3] A.P. Itin and P. Törmä, arXiv:0901.4778.
[4] J. Dziarmaga et al., Phys. Rev. Lett. 101, 115701 (2008)
[5] R. Schützhold et al., Phys. Rev. Lett. 97, 200601 (2006)

DY 12.6 Tue 11:30 ZEU 255

Quantum dynamics of the time-dependent elliptical billiard — •Florian Lenz[1], Fotis K. Diakonos[2], and Peter Schmelcher[1] — [1]Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg — [2]Department of Physics, University of Athens, GR-15771 Athens, Greece

We analyze the quantum dynamics of the time-dependent elliptical billiard. Since there are no standard methods available to tackle this problem, a numerical procedure for the time-propagation of an arbitrary initial state is developed. To circumvent the time-dependent Dirichlet boundary conditions, a series of transformations is applied, yielding a Hamiltonian with static boundary conditions but in turn time-dependent masses and additional time-dependent potential terms. By means of an expansion ansatz, this eventually yields a large system of coupled ordinary differential equations, which can be solved by standard techniques. While for low driving frequencies the evolution of the energy is purely adiabatic, with increasing frequency more and more higher excited states with the same symmetry properties as the initial state get populated. The time-evolution of the population coefficients of the instantaneous eigenstates exhibit characteristic periods, which are much larger than the period of the external driving. These periods depend sensitively on the driving frequency and display a resonance like structure. We employ a Rabi-like coupled, driven few level model to trace the origin of the large periods of the population coefficients and find excellent agreement with the full numerical simulations.

15 min. break.

DY 12.7 Tue 12:00 ZEU 255

Probing quantum coherence in arrays of superconducting qubits — •Alexandra Liguori, Angel Rivas, Susana Huelga, and Martin Plenio — Institut f\"ur Theoretische Physik, Universit\"at Ulm, D-89069 Ulm, Germany

In the mid-80's the so-called phenomenon of dynamic localization was shown for a charged particle moving under the influence of a sinusoidally-varying time-dependent electric field, and more recently similar resonances in the conduction were found to be present also in ion channels. In this work we study the conditions under which this dynamic localization can be found in arrays of superconducting qubits. This phenomenon can serve as a signature of quantum coherence in such systems and moreover could be checked experimentally by various groups constructing arrays of superconducting flux qubits.

DY 12.8 Tue 12:15 ZEU 255

Dissipative quantum mechanics: Taming the sign problem — •Jürgen T. Stockburger — Universität Ulm, Institut für Theoretische Physik, 89069 Ulm

Influence functionals are a straightforward non-perturbative approach to open quantum systems in the path integral formalism. Numerical work based on this approach suffers from the dynamical sign problem, a severe degradation of sampling statistics for long time intervals. However, influence functionals can be formally re-interpreted as generating functionals of c-number-valued quantum noise. This immediately leads to an equivalent non-Markovian stochastic dynamics in terms of pure or mixed quantum states, allowing numerical simulation in the Schrödinger picture. Since the noise forces are complex-valued, a new (typically milder) sign problem arises from the non-unitary propagation of stochastic samples. For friction kernels with finite effective support, this simulation method is modified such that stochastic variances remain bounded in the long-time limit, thus curing the sign problem. Hybrid stochastic approaches which preserve hermiticity of individual samples are also discussed.

DY 12.9 Tue 12:30 ZEU 255

Generating particle-like scattering states in wave transport — •Stefan Rotter, Philipp Ambichl, and Florian Libisch — Institute for Theoretical Physics, TU Vienna, Austria

We introduce a class of scattering states which display trajectory-like wave function patterns in coherent transport through complex scatterers. These deterministic scattering states feature the dual property of being eigenstates to the Wigner-Smith time-delay matrix and to the transmission matrix with classical transmission eigenvalues close to 0 or 1. An operational protocol for generating these states based on the scattering matrix is put forward and successfully tested numerically for regular, chaotic and disordered scattering systems. These results pave the way for the experimental realization of particle-like wave fronts in transport through complex media with possible applications like secure and low-power communication.

Preprint available at: arXiv:1008.3132

Topical Talk DY 12.10 Tue 12:45 ZEU 255

Non-equilibrium quantum relaxation, thermalization and boundary effects — •Heiko Rieger[1] and Ferenc Iglói[2] — [1]Theoretical Physics, Saarland University, D-66041 Saarbrücken, Germany — [2]Research Institute for Solid State Physics and Optics, H-1525 Budapest, Hungary

The quantum dynamical evolution of an interacting many-body system prepared in a specific state that is not an eigenstate of the Hamiltonian is an interesting and theoretically challenging problem. Experimentally achieved for instance by fast quenches of external parameters fundamental questions concern the nature of the stationary (i.e. time-translational invariant) state of this non-equilibrium quantum relaxation including the issue of thermalization and potential descriptions by Gibbs ensembles. In this talk we focus on two issues that we address within the context of an integrable model, the transverse Ising chain. The first concerns the characterization of the non-stationary quantum relaxation following a quench: How is thermalization achieved during the time-evolution? How do correlations develop in time towards the

stationary state, is there a time dependent correlation length, etc.? The second addresses quantum relaxation and potential thermalization in the presence of boundaries. Obviously an interesting question is whether the time and length scales characterizing the stationary relaxation in the bulk is altered in the vicinity of the boundary, and whether thermalization is achieved there and if yes, how?

DY 13: Fluid Dynamics and Turbulence I

Time: Tuesday 10:15–12:45 Location: ZEU 118

Topical Talk DY 13.1 Tue 10:15 ZEU 118

Aggregation and Fragmentation of fractal-like particles in synthetic turbulent flows — •Ulrike Feudel, Jens Zahnow, and Joeran Maerz — ICBM, Carl von Ossietzky University Oldenburg

Inertial particles in fluid flows are of increasing interest in different disciplines of science such as dynamical systems theory, atmospheric and marine science as well as engineering. In many cases particles are not only transported passively by advection but exhibit a dynamics of their own as they can form larger particles upon collision or can break up. Examples of particle dynamics are raindrop formation in clouds, sedimentation of particles in lakes and the ocean or flocculation of marine aggregates and cells. We present a coupled model for advection, aggregation and fragmentation that is based on the dynamics of individual, spherical and fractal-like inertial particles in synthetic turbulent flows. Due to the particle inertia advection leads to the preferential concentrations of the particles in certain spatial regions. The collision of the particles leads to aggregation and larger aggregates are formed. These can in turn fragment due to shear forces in the flow. We find that the combination of aggregation and fragmentation leads to an asymptotic steady state for the size distribution of the aggregates which depends crucially on the considered mechanism of fragmentation. We discuss the dependence of the final size distributions on the properties of the aggregates as well as of the flow.

DY 13.2 Tue 10:45 ZEU 118

Travelling wave solutions for multiphase flow in porous media — •Oliver Hönig[1] and Rudolf Hilfer[1,2] — [1]Institut für Computerphysik, Universität Stuttgart, 70569 Stuttgart, Deutschland — [2]Institut für Physik, Universität Mainz, 55099 Mainz, Deutschland

We study travelling wave solutions of multiphase flow in one-dimensional porous media on a macroscopic scale. Therefore, fractional flow formulations with coupled flow functions and capillary diffusion are employed to formulate a dynamical system. This system is discussed with analytical and numerical methods.

DY 13.3 Tue 11:00 ZEU 118

Generation and quantitative analysis of thickness modulations on micron sized liquid sheets — •Paul Steffen and Stephan Herminghaus — MPI for Dynamics and Self-Organization, Göttingen

The destabilization of liquids and liquid sheets by surface deformations is a major mechanism for the production of micron sized droplets. We investigate periodic thickness modulations on moving liquid sheets of different viscosities, at thicknesses below 100 microns and surrounded by air. The excitation of the thickness modulations is obtained by piezo driven velocity oscillations at the outlet of an annular nozzle. The analysis of the modulations is performed by direct observation of the liquid/air-interface and by employing the diffraction effects of the sheet on a transmitted laser beam. Quantitative measurements of the amplitude and wave length of the thickness modulations as a function of the frequency and strength of the excitation are presented. For thickness modulation depths up to 30% of the sheet thickness we mainly excite thickness oscillations and interference between the resulting capillary waves. The modulation wave length is as expected. For larger amplitudes up to the break up of the sheet we observed lateral structures as well. Their interpretation is still under investigation.

DY 13.4 Tue 11:15 ZEU 118

Nematic electroconvection under time-reversed excitation — •Dirk Pietschmann, Thomas John, and Ralf Stannarius — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg

We investigate experimentally nematic electrohydrodynamic convection (EHC) as a paradigm for a dissipative pattern formation system. We construct periodical waveforms which are reversed in time (forward and backward) to the same control parameter amplitudes. The standard model of EHC is described by a set of two linear differential equations (Carr-Helfrich mechanism). Because of additional symmetries in the equations, EHC belongs to the special class of dynamical systems, in which no differences in the threshold voltages for forward and backward excitation are expected. But our experimental investigations shows in certain parameter regions different threshold voltages for forward and backward excitations. This can not be explained with the standard model for electrohydrodynamic convection. Traveling rolls and localized structures (worms) are observed in the transition regime between the thresholds.

D. Pietschmann, Th. John and R. Stannarius, Phys. Rev. E 82, 046215 (2010).

DY 13.5 Tue 11:30 ZEU 118

Artificial Microfluidic Squirmers — •Shashi Thutupalli[1], Ralf Seemann[1,2], and Stephan Herminghaus[1] — [1]MPI for Dynamics and Self-organisation, Göttingen — [2]Physik Fakultät, University des Saarlandes, Saarbrücken

While there is a growing consensus on the propulsion mechanisms of swimmers at low Reynolds' numbers, many questions remain open regarding the hydrodynamic effects on such swimmers, in particular the coupling between swimmers. Here we present experiments on artificial swimmers, where hydrodynamics is seen to be responsible for a wide range of collective behavior and interactions. Using droplet microfluidics with a surfactant laden continuous oil phase, we create monodisperse aqueous droplets containing chemicals that produce a steady source of Bromine ions. The surfactant (mono-olein) reacts at the droplet interface with the Bromine produced within the droplets, and a dynamic instability leads to gradients of interfacial tension at the droplet interface. These gradients set up Marangoni flows propelling the droplets, in a manner similar to the classical squirmer model of swimming. The flow around the swimmers as well as its effect on the droplet motion are measured using particle image velocimetry (PIV). The PIV analysis reveals the far field flows generated by the swimmers in the surrounding liquid, leading to the emergence of bound states and oriented clusters. We discuss the interaction mechanisms and compare it to previous theoretical work and simulations.

DY 13.6 Tue 11:45 ZEU 118

Numerical study of inertial microfluidics using stochastic rotation dynamics — •Michael Gierlak and Holger Stark — Technische Universität Berlin

The method of stochastic rotation dynamics is an efficient solver for the Navier-Stokes equations which captures hydrodynamic interactions between objects suspended in a viscous fluid as well as thermal fluctuations. It is therefore particularly suited to study microfluidic systems. Recently, inertial microfluidics has been established where colloidal suspensions at non-zero Reynolds number are studied with applications for particle sorting and filtering [1].

We present numerical results for colloid flow through a cylindrical microchannel at moderate Reynolds numbers (1-90), where inertial effects become important. In this range, inertial focusing is observed, where a uniform colloid concentration turns into an annular concentration profile with a peak situated between the channel axis and wall[2].

We investigate the formation of these concentration profiles as a function of flow velocity and colloid size. Due to this inertial focusing, colloids migrate away from the channel axis. Using feedback control with external fields, we try to revert this effect and stabilize the colloids near the channel center.

[1] D. Di Carlo, J. F. Edd, K. J. Humphry, H. A. Stone, and M. Toner, Particle segregation and dynamics in confined flows, Phys. Rev. Lett. 102, 094503 (2009)

[2] Segre G, Silberberg A, Nature 189:209*210.(1962)

DY 13.7 Tue 12:00 ZEU 118

Magnetic spatial forcing of a ferrofluid layer — •Thomas Friedrich, Ingo Rehberg, and Reinhard Richter — Experimen-

talphysik 5, Universität Bayreuth

Historically, spatial forcing of a pattern forming system was first studied experimentally in electroconvection [1]. More recently, inclined layer convection was measured under the influence of lamellar surface corrugations [2]. In both cases, stripes are the first convection pattern beyond a threshold.

The Rosensweig instability in a layer of ferrofluid can provide a primary instability to hexagons if a homogeneous magnetic field normal to the flat surface is applied [3,4]. In case of a tilted magnetic field, a primary instability to stripes can be observed [5]. As a consequence, switching between these two basic types is possible in one single system. We explore how both configurations respond to a stripe like modulation of the magnetic induction. To detect the fluid's response to the different configurations of magnetic fields, x-ray imaging technique [6] is used.

[1]M. Lowe et al, Phys. Rev. Lett., **51**(9):786–789, 1983
[2]G. Seiden et al, Phys. Rev. Lett., **101**(21):214503, 2008.
[3]M. D. Cowley and R. E. Rosensweig, J. Fluid Mech.,**30**:671, 1967.
[4]R. Richter, Physik Journal, **7**:39–44, 2008.
[5]B. Reimann et al, Phys. Rev. E, **71**:055202(R), 2005.
[6]R. Richter, J. Bläsing, Rev. Sci. Instrum. **72**:1729-1733 (2001)

DY 13.8 Tue 12:15 ZEU 118

Measuring the onset of the Rayleigh-Taylor instability in a rotating magnetic field — •Andreas Pöhlmann, Ingo Rehberg, and Reinhard Richter — Experimentalphyisk V, Universität Bayreuth, Germany

If a dense fluid is supported by a less dense fluid, the flat interface separating them is subject to the Rayleigh-Taylor instability. The interface tension between the fluids suppresses the growth of all unstable modes with wavenumbers greater than the critical wavenumber. This gives rise to a maximum experimental interface diameter (size of boundary) at which the flat interface is stable.

In the case of one of the fluids being magnetic, an azimuthally rotating magnetic field can be used to stabilize modes with wavenumbers smaller than the critical wavenumber [1]. This allows for the preparation of the flat interface with greater interface diameters. When switching off the field, all unstable modes, which are not suppressed by the size limitation of the experiment, start to grow. Consequently, a precise study of the Rayleigh-Taylor instability should be possible.

In our experiment a magnetic fluid is covered by a more dense transparent one. The flat interface is stabilized by a rotating magnetic field. The interface size is restricted to a circular shape. For different diameters the field strength is lowered to a threshold level, so that the stability boundaries can be observed. They are compared with the predictions of Ref.[1].

[1] D. Rannacher and A. Engel, Phys. Rev. E, **75**, 016311 (2007).

DY 13.9 Tue 12:30 ZEU 118

Magnetization model for magnetorheological fluids — •Hanna Lagger, Joël Peguiron, Claas Bierwisch, and Michael Moseler — Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

Typical magneto-rheological fluids (MRF) consist of micron-sized magnetically permeable particles (mostly iron) dispersed in carrier oil. MRF are increasingly being considered in variety of devices such as dampers, vibration insulators, brakes or clutches. The activation of an external magnetic field causes a fast and dramatic change in the viscosity of the MRF. Chains of magnetized particles are formed within a few milliseconds. The flow properties of the MRF change from liquid to solid.

A magneto-rheological clutch can be built by placing the MRF between the two inner surfaces of the clutch. In the solidified state of the MRF large torque transmission is possible, which makes it interesting for the application in automotive clutches.

In this study, numerical simulations based on the Discrete-Element-Method (DEM) are used to model magneto-rheological fluids.

To accurately treat the magnetic interaction between particles, an appropriate anhysteretic magnetization model for the particles is implemented. DEM-simulations of the MRF with different volume fractions are carried out and the resulting magnetization curves are compared with experimentally measured data. From simulations with different sets of parameters we get useful insights for the optimization of the MRF with regard to high torque transmission.

DY 14: Delay Dynamics

Time: Tuesday 14:00–15:15 Location: ZEU 255

DY 14.1 Tue 14:00 ZEU 255

Dimension of linear delay differential equations with time-varying delay — •Andreas Otto and Günter Radons — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

It is well known, that delay differential equations (DDE) with constant delay constitute an infinite dimensional dynamical system. On the other hand, the phase space of DDE with time-varying delay can be also finite dimensional.

In this contribution we investigate the dimension of DDE with time-varying delay. Depending on the structure of the deviating argument the the asymptotic dimension of the solution space can be infinite or finite. Furthermore, it is possible that the dimension of the solution space is only an infinite dimensional subspace of the domain of the initial function.

We present a method to calculate the dimension of DDE with time-varying delay. The iterated map of the stepwise retarded access by the deviating argument up to values of the initial function can characterize the dimensional behavior of the solution of DDE with time-varying delay. The results of the presented method are verified by the Lyapunov spectrum of the discretized DDE.

DY 14.2 Tue 14:15 ZEU 255

Destabilization of localized structures induced by delayed feedback — •Svetlana Gurevich and Rudolf Friedrich — Institut for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, D-48149

We study the properties of one- and two-dimensional localized structures in reaction-diffusion systems and in the Swift-Hohenberg equation subjected to a delayed feedback. We compare the spectral properties of both models and show that for reaction-diffusion systems the delay can induce complex behavior of the localized structures, including, e.g., spontaneous motion and breathing of the objects.

DY 14.3 Tue 14:30 ZEU 255

Synchronizing distant nodes: a universal classification of networks — •Valentin Flunkert[1], Serhiy Yanchuk[2], Thomas Dahms[1], and Eckehard Schöll[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Institut für Mathematik, Humboldt Universität Berlin, Unter den Linden 6, 10099 Berlin, Germany

Stability of synchronization in delay-coupled networks of identical units generally depends in a complicated way on the coupling topology. We show that for large coupling delays synchronizability relates in a simple way to the spectral properties of the network topology [1]. The master stability function used to determine stability of synchronous solutions has a universal structure in the limit of large delay: it is rotationally symmetric around the origin and increases monotonically with the radius in the complex plane. This allows a universal classification of networks with respect to their synchronization properties and solves the problem of complete synchronization in networks with strongly delayed coupling.

[1] V. Flunkert, S. Yanchuk, T. Dahms, and E. Schöll, Phys. Rev. Lett. (2010) in print.

DY 14.4 Tue 14:45 ZEU 255

Effect of distributed delays on synchronization dynamics — •Lucas Wetzel[1], Saul Ares[1], Luis G. Morelli[2], Andrew C. Oates[2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden

We study systems of identical coupled phase oscillators, introducing a delay distribution that weights the contributions to the coupling arising from different past times. We have previously shown that for an

arbitrary coupling topology with equal number of neighbors for each oscillator, the frequency and stability of the fully synchronized states only depend on the first moment of the delay distribution.

In this contribution we will explore the dynamics of systems approaching full synchronization. We find analytical expressions, confirmed through numerical simulations, for the exponential decay of small perturbations and the dependence of this decay on the delay distribution. We conclude that distributed delays can change the transient behavior for systems with nearest neighbor coupling, but not in the case of mean field. This result may be relevant to biological systems, where fluctuations in the frequency of individual oscillators keep the system away from the synchronized state, and coupling is required to counteract such fluctuations.

DY 14.5 Tue 15:00 ZEU 255

Global bifurcations in delay differential equations with multiple feedback loops — •Ernesto M. Nicola[1], Saul Ares[2], and Luis G. Morelli[3] — [1]IFISC, Institute for Cross-Disciplinary Physics and Complex Systems (CSIC-UIB), Campus Universitat Illes Balears, E-07122 Palma de Mallorca, Spain. — [2]Max-Planck Institute for the Physics of Complex Systems, Noethnitzer Strasse 38, 01187 Dresden, Germany. — [3]Max-Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstrasse 108, 01307 Dresden, Germany.

Feedback loops are ubiquitous in dynamical systems. In particular those systems which are capable of showing oscillations are typically based on a negative feedback loop whose effect is not instantaneous but delayed in time. This delayed feedback is usually described by intermediate variables which relay the information and induce an implicit time delay. Added to this delayed negative feedback, systems with realistic applications typically include extra feedback mechanisms. In this contribution we analyze the effect of this extra feedback loops in simple models showing oscillatory behavior. We include explicit time delays in our models to minimize the number of variables and parameters while keeping the richest possible phenomenology in the models. A thorough bifurcation analysis shows that the addition of extra feedback loops results in a number of global bifurcations appearing. These global bifurcations greatly enrich the dynamics of the oscillators under consideration and offer mechanisms to control the oscillatory behavior of the system.

DY 15: ISPS Intersectional Poster Session

Time: Tuesday 18:00–20:00 Location: P1

DY 15.1 Tue 18:00 P1

Wave packet spreading in strongly disordered nonlinear lattices — Mikhail Ivanchenko[1,2], •Tetyana Laptyeva[2], and Sergej Flach[2] — [1]Theory of Oscillations Department, University of Nizhniy Novgorod, Russia — [2]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany

Localization of eigenmodes and halt of wave propagation in linear lattices by disorder, the famous Anderson localization, underpins a set of fundamental physical phenomena. To mention are electrical and thermal conductivities, localization of light and matter waves in optical lattices. Nonlinearity induces interaction between eigenmodes and the question of whether it destroys Anderson localization or not is under hot debate in the fields of nonlinear science and condensed matter.

We achieve a progress there by studying analytically and computationally the limit of strongly disordered nonlinear lattices characterized by compactly localized eigenmodes. Employing perturbation theory techniques we demonstrate that even in this case there is always a finite probability for a wave packet to spread that decreases linearly with the energy. Moreover, we show that the same holds in the limit of infinitely small energy density too, the full energy being the only control parameter. Above a certain threshold in energy finite-size excitations will spread with probability 1. Infinitely small energy density limit gives an exponentially small probability of localization in this case. Numerics confirm the predictions above, revealing, in addition, intermittent and not diffusive type of spreading in this strong disorder limit.

DY 15.2 Tue 18:00 P1

Interaction-induced fractional Bloch and tunneling oscillations — •Dmitry Krimer[1,2], Ramaz Khomeriki[1,3], Masudul Haque[1], and Sergej Flach[1] — [1]Max Planck Institute for the Physics of Complex Systems, 01189 Dresden, Germany — [2]Institute for Theoretical Physics, University of Tuebingen, 72076 Tübingen — [3]Physics Department, Tbilisi State University, 0128 Tbilisi, Georgia

We study the dynamics of few interacting bosons in a one-dimensional lattice with dc bias in the framework of Bose-Hubbard model [1]. The resulting dynamics turned out to be substantially different than that obtained within the mean-field approximation valid for the description of Bose-Einstein condensates [2]. In particular, for strong interaction the Bloch oscillation regime reemerges with fractional Bloch periods, which are inversely proportional to the number of bosons clustered into a bound state. The interaction strength is affecting the oscillation amplitude. Excellent agreement is found between numerical data and a composite particle dynamics approach. For specific values of the interaction strength a particle tunnels from the interacting cloud to a well defined distant lattice location. This is in contrast to the case of the mean-field approach, where any nonlinearity destroys integrability, introduces chaos, and ultimately leads to a destruction of localization [2].

[1] R. Khomeriki, D.O. Krimer, M. Haque, S. Flach, Phys. Rev. A 81, 065601 (2010)

[2] D.O. Krimer, R. Khomeriki, S. Flach, Phys. Rev. E 80, 036201 (2009)

DY 15.3 Tue 18:00 P1

Juggling with geological time scales! — •Philipp Aurin[1], Cornelius Fischer[1], Julie Murison[2], and Matthias Schröter[2] — [1]Department of Geoscience, Georg-August-University, Göttingen, DE — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, DE

The investigation of fluid flow through porous media is of great interest to, among others, the petroleum industry. We want to create a model sandstone with selectable but well controlled fluid flow parameters such as porosity and permeability. In this way we can monitor the main steps of diagenesis, compaction and cementation, allowing systematic testing and characterisation of parameters with reduced complexity, all on laboratory time scales.

Compaction - the physical process by which sediments are compressed - is obtained by using water flow pulses and by vertical shaking. Both methods result in the reduction of pore space as grains (soda-lime glass beads) are packed closer together.

The second phase of our experimental protocol consists of calcium carbonate precipitation, which acts as cement between the compacted grains. In-situ observation of the cementation process is obtained using x-ray radiograms. After cementation thin sections of the sample are prepared and lithification quantified using polarizing petrographic microscopy.

DY 15.4 Tue 18:00 P1

Influence of Superconductivity on the Phonon in $BaFe_{1.8}Co_{0.2}As_2$ — •Daniel Lamago[1,2], Lothar Pintschovius[1], Dmitry Reznik[3], Rolf Heid[1], and Thomas Wolf[1] — [1]Karslruhe Institut für Technologie (KIT), Institut fuer Festkoerperphysik, P.O.B. 3640, 76021 Karlsruhe, Germany — [2]Laboratoire Leon Brillouin, CEA Saclay, 91191 Gif sur Yvette Cedex, France — [3]Department of Physics, University of Colorado-Boulder, CO 80309 Boulder, USA

We used inelastic neutron scattering technique to investigate the role of electron-phonon coupling in the mechanism of high-Tc superconductivity in the iron arsenides. Density functional theory predicts only a weak electron-phonon coupling but theory might underestimate the coupling strength. One way to obtain experimantally information on the electron-phonon coupling strength is to measure superconductivity-induced phonon frequency shifts. Such shifts have been observed not only in conventional superconductors but also in cuprates, i.e. in compounds in which electron-phonon coupling is probably not the main driving mechanism for superconductivity. We have measured phonon modes with an energy close to the superconducting energy gap, because it is known from theory that such phonons will respond most strongly to the opening of the superconducting gap. The gap energy

was estimated to be about 6 meV for the overdoped sample and about 8 meV for the optimally doped one. We could not detect any influence of superconductivity on the phonons, neither on the linewidth nor on the frequencies.

DY 15.5 Tue 18:00 P1

Extreme value statistics in the solar wind: an application to correlated Levy processes — •Nicholas Moloney — Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany

We analyze the block maxima of solar wind power bursts during 2000 – 2007. Extreme values over time windows of about 18 hours and longer can be accurately described by parametric generalized extreme value statistics. These models predict that significantly larger values can be expected during any 50-year period than observed to date.

DY 15.6 Tue 18:00 P1

Stochastically driven Preisach models of hysteresis — •Sven Schubert and Günter Radons — Chemnitz University of Technology, 09107 Chemnitz, Germany

Hysteresis is a ubiquitous phenomenon. It is observed in physics (ferromagnetic materials), chemistry (catalysis), and mechanics (friction), to name same branches of science and examples therein. The most prominent and often successfully applied model is the so-called Preisach model of hysteresis. Its phenomenological character allows the simulation of the response of hysteretic systems from different scientific fields to external driving. We consider stochastic external driving fields and derive properties of the system's response using rigorous methods and simulations.

The development of a hysteresis memory is reflected in the possibility of long-time tails in the autocorrelation of the system's response even for uncorrelated external driving fields. Hence hysteresis is a mechanism for the generation of $1/f$-noise [1]. These rigorous results are extended by simulations to driving fields showing long-term correlations themselves. One observes that the autocorrelation of the response does not decay faster than the autocorrelation of the external driving. But the picture is more complicated; there is a possibility that long-term memory in the hysteretic response is more pronounced in the case of uncorrelated driving than for correlated driving.

[1] G. Radons, Phys. Rev. Lett. **100**, 240602 (2008).

DY 15.7 Tue 18:00 P1

Monte Carlo study of the evaporation/condensation transition of Ising droplets — •Micha Wiedenmann, Andreas Nussbaumer, Elmar Bittner, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100920, 04009 Leipzig

This work builds on recent work of A. Nußbaumer *et al.* [*Europhys. Lett.* **75** (2006) 716] and studies the evaporation/condensation transition of Ising droplets in three dimensions. We performed Monte Carlo simulations of the Ising model with nearest-neighbor couplings on a simple cubic lattice with periodic boundary conditions at a fixed magnetization, corresponding to a certain amount v_L of overturned spins. The volume v_d of the largest droplet was measured at constant magnetization employing a flood-fill algorithm. For values of the magnetization $m < m_c$ there exists no droplet in the system and the fraction of overturned spins above the equilibrium magnetization m_0 in the largest droplet $\lambda = v_d/v_L$ is zero. At $m = m_c$ one half of the overturned spins form a droplet which grows for larger values of the magnetization. This behavior can be compared to analytical results given by Biskup *et al.* [*Europhys. Lett.* **60** (2002) 21]. In order to do so we measured the spontaneous magnetization m_0, the magnetic susceptibility χ and the planar surface tension τ (which is a good approximation of a Wulff shaped droplet). Rescaling the magnetization to a dimensionless parameter $\Delta = \Delta(m, \chi, \tau, m_0)$, our measured results are in good agreement with the theoretical predictions.

DY 15.8 Tue 18:00 P1

Structure of the Tip4p water model in the ice I_h phase — •Johannes Zierenberg[1], Bernd A. Berg[2], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Germany — [2]Dept. of Physics, Florida State University, Tallahassee, USA

Potential water models have been widely used throughout the last decades in a variety of computer simulations. Especially in the simulations of processes where water is used as a solvent, the influence of the model is easily underestimated and can provide a large source of error. We investigated the behavior of the Tip4p model with different parametrizations in the hexagonal, ordinary ice phase. To this end random spherical nanosized water clusters were arranged in the experimentally determined tetrahedral structure. These configurations were minimized in energy with a semi-dynamic technique, resulting in local energy minimium configurations of the specific water model. Important to notice is the necessity to correctly consider the involved long-range interactions, especially the electrostatic one which cannot be handled trivially by a cutoff. This process revealed insight into the properties of the model near and in the ice phase, confirming the stability of the hexagonal structure with multiple local minima, with almost identical energies. That way the principle structure of the unit cell was obtained and compared for the different parameterizations.

DY 15.9 Tue 18:00 P1

Rounding Effects Influencing the Quality of Heuristic Optimization Algorithms — •Martin Ransberger[1], Ingo Morgenstern[1], and Johannes Josef Schneider[2] — [1]Faculty of Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, Mathematics, and Computer Science, Johannes Gutenberg University of Mainz, Staudinger Weg 7, 55099 Mainz, Germany

Search space smoothing and related heuristic optimization algorithms provide an alternative approach to simulated annealing and its variants: while simulated annealing overcomes barriers in the energy landscape at finite temperatures, search space smoothing intends to remove these barriers, such that a greedy algorithm is sufficient to find the global minimum. Several formulas for smoothing the energy landscape have already been applied, one of them making use of the finite numerical precision on a computer. In this presentation, we thoroughly investigate the effect rounding errors have on the quality of results achieved with heuristic optimization algorithms. We present computational results for the traveling salesman problem.

DY 15.10 Tue 18:00 P1

Magic Squares in a Heatbath — •Christoph Schuster and Johannes Josef Schneider — Department of Physics, Mathematics, and Computer Science, Johannes Gutenberg University of Mainz, Staudinger Weg 7, 55099 Mainz, Germany

Magic squares are fascinating objects with interesting properties. In this presentation, we demonstrate how simulated annealing is applied to the problem of ordering integer numbers on a square lattice in order to create a magic square. We show that the cooling process exhibits interesting properties including power laws and that the usage of simulated annealing allows a straightforward extension of this approach to magic squares with constraints, like the retaining water problem.

DY 15.11 Tue 18:00 P1

Investigation of a highly frustrated point packing problem — Frederic Alexander Stein[1], Sebiha Sahin[1], Andre Müller[1], Michael Kwasnicki[1], Tobias Preis[1], Elmar Schömer[1], Ingo Morgenstern[2], and •Johannes Josef Schneider[1] — [1]Department of Physics, Mathematics, and Computer Science, Johannes Gutenberg University of Mainz, Staudinger Weg 7, 55099 Mainz, Germany — [2]Faculty of Physics, University of Regensburg, 93040 Regensburg, Germany

We consider a highly frustrated point packing problem. The task of this problem is to place a proposed number of points on the nodes of a square lattice in the way that the radius of the circumcircle around the points is minimized and that each Euclidean distance value between each pair of points only occurs once. We show that this latter constraint leads to a large frustration effect by comparison with the corresponding un-frustrated system. We solve this problem by using simulated annealing, study the dynamics of the cooling process, and demonstrate that this problem exhibits interesting features, including scaling laws for the radius of the circumcircle and for the distribution of points [1].

[1] Frédéric Alexander Stein, Sebiha Sahin, André Müller, Michael Kwaśnicki, Tobias Preis, Elmar Schömer, Ingo Morgenstern, and Johannes Josef Schneider, *Investigation of a highly frustrated point packing problem*, submitted to Physical Review E, 2010.

DY 15.12 Tue 18:00 P1

Quantum properties of 4D area preserving maps — Arnd Bäcker, Roland Ketzmerick, and •Martin Richter — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

We investigate quantum mechanical properties of 4D area preserving maps in the presence of nonlinear resonances. The focus is on regular-to-chaotic tunneling rates for designed models. For maps without resonances a prediction using the fictitious integrable system approach developed for lower dimensional systems is given. Adding nonlinearities leads to prominent peaks in the tunneling rates γ vs. $1/h$ which can be explained qualitatively by an examination of the structure in the frequency plane. A visualization of these resonances is provided by sections through the 4D phase space which show complex regular regions interwoven with the chaotic sea. We present eigenfunctions concentrating in the chaotic sea in between resonance regions.

DY 15.13 Tue 18:00 P1

Is there universality in the quantum transport of partial barriers? — Arnd Bäcker[1,2], Roland Ketzmerick[1,2], and •Matthias Michler[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]MPI für Physik komplexer Systeme, 01187 Dresden

In generic Hamiltonian systems classical transport in the chaotic sea is limited by partial barriers, which allow a flux Φ given by the turnstile area. Quantum mechanically they are even more restrictive for Planck's constant $h \gg \Phi$, while for $h \ll \Phi$ classical transport is recovered. This transition is qualitatively well understood, however, many quantitative questions are still open.

We study the standard map and a designed kicked system, where both have two chaotic regions separated by one dominant partial barrier. We find scaling with the single parameter Φ/h, however with different functional dependence. The origin of the different scaling behavior is an open problem.

DY 15.14 Tue 18:00 P1

Power–Law Level–Statistics due to Dynamical Tunneling — Arnd Bäcker[1,2], Roland Ketzmerick[1,2], Steffen Löck[1], and •Normann Mertig[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden — [2]MPI für Physik komplexer Systeme, 01187 Dresden

For systems with a mixed phase space we demonstrate that dynamical tunneling universally leads to a fractional power-law of the nearest-neighbor level-spacing distribution $P(s)$ at small spacings s. Going beyond Berry-Robnik statistics, we take into account that dynamical tunneling rates between the regular and the chaotic region vary over many orders of magnitude. This results in a prediction of the level-spacing distribution which excellently describes the spectral data of the standard map. Moreover, we show that the fractional power-law exponent is proportional to the effective Planck constant h and discuss the emergence of Berry-Robnik statistics in the semiclassical limit $h \to 0$.

DY 15.15 Tue 18:00 P1

Integrable Approximation for Regular Islands in Billiards — Arnd Bäcker[1,2], Roland Ketzmerick[1,2], •Clemens Löbner[1], and Steffen Löck[1] — [1]Technische Universität Dresden, Institut für Theoretische Physik, 01062 Dresden — [2]MPI für Physik komplexer Systeme, 01187 Dresden

Our aim is to approximate the dynamics of a regular island in a non-integrable billiard by an integrable Hamiltonian. For this purpose we use canonical transformations and interpolation techniques in the 4D phase space such that the regular tori of both systems and their dynamics agree as closely as possible. The resulting integrable Hamiltonian describes a billiard with the same boundary, but a nontrivial time evolution. We present the application of this method for the cosine billiard. This provides a basis for the determination of regular-to-chaotic tunneling rates with the fictitious integrable system approach.

DY 15.16 Tue 18:00 P1

Singularities in the delay-time distribution of 2D scattering systems — •Stefan Majewsky[1] and Holger Schanz[2,3] — [1]Computational Physics Group, Technische Universität Dresden, Institut für Theoretische Physik, 01062 Dresden — [2]Institut für Maschinenbau, Hochschule Magdeburg-Stendal, 39114 Magdeburg — [3]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden

We investigate scattering systems where the probability distribution of the time delay shows logarithmic singularities and thus a clustering of delay times near some system-specific values. The effect can be understood as a generalization of caustics to the time domain. Its dynamical origin are saddle points in the time delay function. They arise either due to the details of the dynamics in the scattering region or, in some trivial cases, as a side-effect of a coordinate transformation. We use small clusters of non-overlapping potentials as model systems and study both, the classical and the quantum time delay.

DY 15.17 Tue 18:00 P1

Stability induced by chaos and disorder in the time reversal focalization — •Hernan L. Calvo[1,2] and Horacio M. Pastawski[1] — [1]Instituto de Fisica Enrique Gaviola and FaMAF UNC, 5000 Cordoba, Argentina — [2]Institut für Theoretische Physik A, RWTH Aachen University, D-52056 Aachen, Germany

The experimental procedure known as the time reversal mirror successfully achieves the focusing of a local excitation after its propagation through a chaotic or disordered medium. An initially localized pulse that becomes in a series of low amplitude reverberations is registered by a transducer that re-injects the signal in the reverse temporal order. This enables the focalization of the original pulse whose quality increases with the level of disorder in the system. We study the stability of this phenomenon against two irreversible processes: the escape in an open cavity, and a closed cavity under the effects of an external perturbation. Within a semiclassical approach in terms of time-dependent trajectories, the multiple reflections of the redundant registration yield a focalization signal that can be related with the Loschmidt echo amplitude. Both situations describe a Fermi Golden Rule regime, where the decay of the focalization is dominated by the perturbation strength. However, in the closed cavity this decay diminishes with the Lyapunov exponent of the system. This counter-intuitive result is a form of the quantum Zeno effect, which provides a new interpretation of the remarkable stability of the experiments.

DY 15.18 Tue 18:00 P1

Trace Formula for Three-dimensional Dielectric Resonators — •Stefan Bittner[1], Barbara Dietz[1], Maksim Miski-Oglu[1], and Achim Richter[1,2] — [1]Institut für Kernphysik Darmstadt — [2]ECT* Trento

Microlasers and dielectric microcavities have gained great interest due to possible applications in e.g. telecommunications and as a new type of wave-dynamical billiards. Especially the correspondence between ray and wave-optics is intensely studied for these systems. Trace formulas provide a connection between the density of states of the cavity and the periodic orbits of the corresponding billiard. A trace formula for two-dimensional dielectric resonators has been proposed [1] and successfully tested [2] in recent experiments. Typically microcavities, however, are three-dimensional flat disks which can only be approximated as two-dimensional objects with the help of a so-called effective index of refraction. We investigate 3d dielectric microwave resonators with the shape of circular flat disks. The experimental length spectra are analyzed with a combination of the trace formula for 2d dielectric resonators and the effective index of refraction model. The positions of the peaks in the length spectra can be successfully assigned to the lengths of periodic orbits when taking into account the dispersion of the effective index of refraction and the systematic inaccuracy of the effective index of refraction model. The work presented on this poster was supported by the DFG within SFB 634.

[1] Bogomolny *et al.*, Phys. Rev. E **78**, 056202 (2008).
[2] Bittner *et al.*, Phys. Rev. E **81**, 066215 (2010).

DY 15.19 Tue 18:00 P1

Equilibration of the harmonic oscillator from non-thermal initial states — •Daniel Pagel[1], Andreas Alvermann[2], and Holger Fehske[1] — [1]Institut für Physik, Universität Greifswald, Deutschland — [2]Cavendish Laboratory, University of Cambridge, United Kingdom

Quantum dissipation can be studied in a microscopic setting with the well known model of a central oscillator coupled linearly to a bath of harmonic oscillators. By making use of operator equations of motion we study the long time behaviour of the central oscillator density matrix. Applying general non-thermal initial states we show that only weak conditions on the initial preparation are necessary for the central oscillator to equilibrate. The stationary density matrix in the long time limit is then characterized by a parameter which can be identified as the 'temperature' of the central oscillator. We thus provide an example of how the thermodynamics of the canonical ensemble can be obtained from a purely microcanonical description.

DY 15.20 Tue 18:00 P1

Directed excitation transfer in non-equilibrium networks —

•Maximilian Bauer and Oliver Mülken — Physikalisches Institut, Albert-Ludwigs Universität Freiburg, Freiburg, Germany

In the framework of continuous-time quantum walks (CTQW), the coherent dynamics of excitations is usually studied on static networks. We consider a CTQW on a dynamically varying structure, namely a vibrating chain. By applying an external field and matching the field strength with the oscillation frequency of the chain it is possible to obtain an (average) transport of an initial Gaussian wave packet. We distinguish between a uniform oscillation of all nodes of the chain and the chain being in its lowest eigenmode. Both cases can lead to directed transport. Furthermore, the coupling of these systems to an environment by Lindblad operators and the generalization to interacting particles is investigated.

Reference: [1] O. Mülken and M. Bauer, submitted (2010)

DY 15.21 Tue 18:00 P1

Generalized Master Equation Approach to Excitation Transport and Trapping on Networks — •Benjamin Berger and Oliver Mülken — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Germany

Due to the recent interest in excitation dynamics in light-harvesting complexes, we present a Generalized Master Equation (GME) Model for coherent and incoherent transport on networks. For small networks, the focus is on the phenomenological incorporation of both, a heat bath causing decoherence and an exciton trap. Under certain conditions the solutions of the usual GME approaches become unphysical because of, say, negative probabilities. Here, we show how one can circumvent these difficulties.

DY 15.22 Tue 18:00 P1

Discrete Wigner function dynamics on rings — •Per Liebermann and Oliver Mülken — Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany

The Wigner function provides a representation of quantum mechanics in phase space in terms of a real-valued distribution function. Calculating the Wigner function for a continuous-time quantum walk on a discrete ring for different initial conditions analytically enables us to investigate the dynamics in phase space. Starting with a Gaussian distribution, the dynamics are similar to the case of a coherent state of the harmonic oscillator. Namely, we obtain revivals of the Wigner function at the initial position as well as at the opposite one, i.e. the wave packet oscillates back and forth.

DY 15.23 Tue 18:00 P1

Dissipative exciton dynamics on small networks — •Johannes Kohlberger and Oliver Mülken — Albert-Ludwigs-Universität Freiburg, Germany

Excitation transfer through networks coupled to an environment plays an important role in many areas of physics and biology. We would like to understand the fundamental transport phenomena of different kinds of networks like the Fenna-Matthews-Olson (FMO) complex. For this purpose we consider small networks like dimers and trimers and use different approaches of the Lindblad-Master equation to couple them to an environment. With this approach it is possible to connect the network to different kinds of reservoirs like a trap or a source to get a more realistic coupling from the FMO-complex to the chlorosomes and the reaction centre. The advantage of studying those small networks is, that it is partly possible to solve them analytically and therefore get some fundamental insights in such transport processes, which can be used to understand transport phenomena in larger networks.

DY 15.24 Tue 18:00 P1

Projection operator approach to spin diffusion in the anisotropic Heisenberg chain at high temperatures — •Robin Steinigeweg[1] and Roman Schnalle[2] — [1]Institut für theoretische Physik, Technische Universität Braunschweig, D-38106 Braunschweig — [2]Fakultät für Physik, Universität Bielefeld, D-33615 Bielefeld

Spin transport in the anisotropic Heisenberg chain is typically investigated theoretically w.r.t. the finiteness of transport coefficients only. Assuming their finiteness at high temperatures, we develop a concrete quantitative picture of the diffusion constant/(dc-)conductivity as a function of both the anisotropy parameter Δ and the spin quantum number s, going beyond the most commonly considered case $s = 1/2$. Using this picture, we enable the comparison of finite transport coefficients from complementary theoretical methods on a quantitative level, having more significance than the finiteness alone. Our method is essentially based on an application of the time-convolutionless projection operator technique to current autocorrelations. This technique, although being a perturbation theory in Δ, is found to be applicable, even if Δ is not small. This finding supports the applicability to a wider class of strongly interacting many-particle quantum systems.

DY 15.25 Tue 18:00 P1

Boltzmann approach to transport in weakly interacting fermionic 1-d systems — •Christian Bartsch and Jochen Gemmer — Fachbereich Physik, Universität Osnabrück, Barbarastrasse 7, D-49069 Osnabrück, Germany

We investigate the transport behavior of a system of weakly interacting 1-d (spinless) fermions featuring nearest and next nearest neighbor hopping and nearest neighbor interaction. By means of a leading order TCL (time-convolutionless) projection operator approach we set up a master equation for certain momentum mode occupation numbers and interpret the resulting rate matrix as scattering term of a linear(ized) quantum Boltzmann equation, from which one may extract a diffusion coefficient. One numerically finds that both the diffusion coefficient itself and the time scale, on which the diffusion coefficient becomes constant, are larger for smaller next nearest neighbor hoppings. In the absence of next nearest neighbor hopping (, in this case the model corresponds to an anisotropic Heisenberg spin chain in terms of a Jordan-Wigner-transformation,) this time scale diverges, which may indicate ballistic transport or a diffusion coefficient scaling in higher orders of the interaction strength that are beyond this leading order approach.

DY 15.26 Tue 18:00 P1

Absorption and energy transfer of molecular aggregates — •Gerhard Ritschel, Jan Roden, and Alexander Eisfeld — MPI-PKS Dresden

The coupling of electronic excitation to vibrational degrees of freedom strongly influences characteristic properties of molecular aggregates such as optical properties and energy transfer dynamics. We treat this complicated exciton-phonon coupling using a non-Markovian stochastic Schrödinger equation. Solving a Holstein-type model, we calculate spectra and energy transfer for a coupling to a realistic, complex phonon bath such that energy dissipation to the phonons is fully included. Our approach captures uniformly the transition from fully coherent to incoherent excitation transfer. Using this new method we are able to investigate decoherence and entanglement in mesoscopic molecular aggregates.

On the other hand, we compare experimental spectra of such molecular aggregates, that are obtained by helium nanodroplet isolation spectroscopy and resolve individual vibrational lines, with full quantum calculations. Here we are able to explain the effect of the many vibrational modes of the molecules on the aggregate absorption.

DY 15.27 Tue 18:00 P1

Quantum Correlations in Disordered Systems — •Dominik Hörndlein, Vivian França, and Andreas Buchleitner — Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg im Breisgau, Germany

In recent years, quantum correlations and entanglement in solid state systems have been examined with respect to their influence on the system's properties, as for example on charge transport. In this context, the impact of disorder in real-life solids is still an unclear issue. Therefore, we investigate the electronic correlations in one-dimensional atomic systems in the presence of disordered impurities. Our numerical studies are based on the Hubbard model, which is a standard model for describing electronic interactions in solids. Considering different probability distributions for the impurities, ranging from total order to total randomness, we analyse the usefulness of various types of quantum correlations for quantifying and characterizing the entanglement in these differently disordered systems.

DY 15.28 Tue 18:00 P1

Thermopower in Bilayer Graphene — •Aleksander Hinz — School of Engineering and Science, Jacobs University Bremen, Bremen 28759, Germany

In this work we present our theoretical approach to investigate Thermopower in Bilayer Graphene. Inspired by Seoung-Geol Nam's experimental work in late 2009 [1] as a member of the group of Hu-Jong Lee at Postech University, S.Korea, we seek to provide a theorecical underpinning for the observed phenomena concerning Bilayer Graphene.

Since our theoretical framework for Monolayer Graphene, which is

based upon the description of conductivity including diffusion on impurities by using the linear response theory within the diagrammatic description, is in good accordance with experimental data only for Monolayer and not for Bilayer Graphene, we devise a modification of this framework, taking into account additional physical effects beyond impurity diffusion.

The effect investigated in this work is the electron-phonon interaction, that leads to a Phonondrag component in Thermopower at low temperature, while at higher temperature this effect is suppressed by phonon-phonon interaction. In contrast to the diffusive part we here apply the Boltzmann equation description as well as the balance-equation-based examination, which appreas to be sufficient for our case. This serves as an approach to explain the observed disagreement between experimental results and corresponding calculations using the classical Mott formula in Seoung-Geol Nam's work [1].

[1] S. Nam, D. Ki, and H. Lee, arXiv:1005.4739

DY 15.29 Tue 18:00 P1

The density of Stone-Wales defects in a graphene nano-ribbon in terms of a Potts-like model — •Jaime E. Santos — Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden

We will discuss a 1d Potts-like model that accounts for the density of Stone-Wales defects along a zig-zag edge of a graphene nano-ribbon. The couplings of the model can be extracted from DFT, both in the case of H-passivated and non-passivated edges. Given that the couplings only involve nearest neighbouring sites, we can write the partition function of the model in terms of a transfer matrix that is easily diagonalisable, yielding the thermodynamics of the model.

DY 15.30 Tue 18:00 P1

Parity detection and entanglement with a Mach-Zehnder interferometer — •Géraldine Haack[1], Heidi Förster[2], and Markus Büttiker[1] — [1]University of Geneva, Geneva, Switzerland — [2]United Nations University, Bonn, Germany

A parity meter projects the state of two qubits onto two subspaces with different parities, the states in each parity class being indistinguishable. It has application in quantum information for its entanglement properties. In our work we consider the electronic Mach-Zehnder interferometer (MZI) coupled capacitively to two double quantum dots (DQDs), one on each arm of the MZI. These charge qubits couple linearly to the charge in the arms of the MZI. A key advantage of an MZI is that the qubits are well separated in distance so that mutual interaction between them is avoided. Assuming equal coupling between both DQDs and the arms and the same bias for each DQD, this setup usually detects three different currents, one for the odd states and two for each even state. Controlling the magnetic flux of the MZI, we can operate the MZI as a parity meter: only two currents are measured at the output, one for each parity class. In this configuration, the MZI acts as an ideal detector, its Heisenberg efficiency being maximal. For a class of initial states, the initially unentangled DQDs become entangled through the parity measurement process with probability one.

DY 16: Statistical Physics II

Time: Wednesday 10:30–11:30 Location: HÜL 186

DY 16.1 Wed 10:30 HÜL 186

Investigation of the Structure of the Energy Landscape Making Use of a Clustering Approach — •Johannes Josef Schneider and Michael Kwasnicki — Department of Physics, Mathematics, and Computer Science, Johannes Gutenberg University of Mainz, Staudinger Weg 7, 55099 Mainz, Germany

Recently, we have introduced the Traveling Salesman Problem with Clustering [1], in which we extended the original Traveling Salesman Problem with the constraint that nodes close to each other should be visited contiguously in the tour, if the detour for fulfilling this constraint is not too long. In this talk, we apply this approach to the ordering of quasi optimum configurations of the SK model, the Traveling Salesman Problem, and a multidisperse packing problem [2,3]. The distances between the quasi optimum configurations are given by the inverse overlaps between the configurations. We show that this approach leads to a block structure in the permuted overlap matrix, similarly to Parisi's block structure.

[1] Johannes J. Schneider, Thomas Bukur, and Antje Krause, Traveling Salesman Problem with Clustering, J. Stat. Phys. 141, 767-784, 2010.

[2] Johannes J. Schneider, Andre Müller, and Elmar Schömer, Ultrametricity property of energy landscapes of multidisperse packing problems, Phys. Rev. E 79, 031122, 2009.

[3] Andre Müller, Johannes J. Schneider, and Elmar Schömer, Packing a multidisperse system of hard disks in a circular environment, Phys. Rev. E 79, 021102, 2009.

DY 16.2 Wed 10:45 HÜL 186

Real-Time Monte Carlo Simulations for a two-level-system within a Sub-Ohmic environment — •Denis Kast[1], Charlotte Escher[2], and Joachim Ankerhold[1] — [1]Institut für Theoretische Physik, Universität Ulm — [2]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg

The two-level system (TLS) coupled to a dissipative environment (spin-boson-model) is studied within the numerically exact path integral Monte-Carlo (PIMC) approach. Well studied in all ranges of parameter space (e.g. temperature, coupling strength, cut-off frequency) is the real-time dynamics for ohmic spectral bath densities including a phase transition from a delocalized to localised regime at T=0. Much less is known for the sub-ohmic case which has recently gained considerable interest. Most studies, however, have been restricted to properties at T=0. Here we present real-time PIMC simulations for finite temperatures over a wide domain of parameters. Out of the TLS-dynamics estimates for the critical coupling strengths of the transition delocalized/localized are derived. Comparisons with alternative methods at T=0 are discussed.

DY 16.3 Wed 11:00 HÜL 186

Apollonian Breath Figures — •Johannes Blaschke, Tobias Lapp, and Jürgen Vollmer — Max Planck Institute for Dynamics and Self-Organization, 37073 Göttingen

The formation of dew droplets on planar surfaces is often referred to as Breath Figures. A scaling theory by Family and Meakin [1] predicts that the size distribution of the small droplets takes the form of a power law with exponent $-5/3$. Simulations show a clear deviation from this exponent by $\delta \simeq 0.1(0)$. This deviation had not been explained so far.

Taking insight from fractal packings [2], we have developed an extension to Family and Meakin's theory, which determines the correction to the size distribution for the small droplets. Knowing the fractal dimension of breath figures, d_f, we demonstrate how the correction, δ, is related to d_f: $\delta = 1/3(2 - d_f)$. This fractal dimension was subsequently measured from simulations to be $d_f = 1.6(9)$. Resulting in: $\delta = 0.103$

The case of breath figures forming on the underside of a horizontal surface constitutes another interesting, and previously unexplored, scenario: When droplets reach a critical size, they are distorted by gravity and eventually fall off the substrate. The previously published theories cannot be applied to this case. We report the results from our simulations and compare these to a kinetic theory.

[1] Family and Meakin. Phys. Rev. Lett. **61** (1988) 428-431
[2] Herrmann *et al.* Phys. Rev. Lett. **65** (1990) 3223-3226

DY 16.4 Wed 11:15 HÜL 186

How to describe bursty reaction kinetics? — •Stephan Eule — Max-Planck-Institut fuer Dynamik und Selbstorganisation

We introduce a generalization of the chemical master equation which is capable to describe reaction kinetics with non-Poissonian reaction statistics. Deviations from Poissonian reaction patterns have been observed in various systems ranging from reactions in cells to reactions involving polymers. Another application is the mathematical description of spreading rumors and infections that are usually modeled by simple reaction schemes. The corresponding dynamics is closely related to the interaction patterns of humans which are known to happen in bursts. We provide methods of solving the generalized chemical master equation and present an exact solution for a simple reaction scheme.

Furthermore we show how the generalized chemical master equation can be extended to include reactions following Poissonian statistics and apply it to a reaction where the production of a reactant happens in sudden bursts while the degradation is normal.

DY 17: Nonlinear Dynamics I

Time: Wednesday 10:15–13:15 Location: ZEU 255

Topical Talk DY 17.1 Wed 10:15 ZEU 255

Nonlinear Dynamics of Complex Hysteretic Systems — •Günter Radons — Institute for Physics, Chemnitz University of Technology, D-09107 Chemnitz.

Under the influence of external fields a large variety of materials and systems shows very complex hysteretic behavior. The latter means that in addition to major hysteresis loops, one finds many subloops or minor loops. Well-known examples range from the magnetization of magnetic materials and the deformation of shape memory alloys to capillary condensation in porous materials. Such a behavior is traditionally described by so-called hysteresis operators [1]. Correspondingly, the interaction of such hysteretic systems with its environment is naturally described by operator-differential equations. Despite its importance and its ubiquitous appearance, the dynamics resulting from such equations is not well understood.

In this talk I will review the working principles of the Preisach hysteresis operator and its applications. Subsequently recent results on dynamical systems with such hysteretic subsystems will be presented. They range from the appearance of 1/f-noise under simple input-output conditions [2] to the co-existence of infinitely many attractors for operator-difference equations or operator-differential equations describing e.g. the motion of an iron sphere in an inhomogeneous magnetic field.

[1] G. Bertotti, I.D. Mayergoyz (Eds.), The Science of Hysteresis, Vol. I-III, Elsevier, 2006. [2] G. Radons, Phys. Rev. Lett. 100, 240602 (2008), Phys. Rev E 77, 061133 (2008), Phys. Rev E 77, 061134 (2008).

DY 17.2 Wed 10:45 ZEU 255

Topological stability criteria for synchronized coupled systems of non-identical oscillators — •Anne-Ly Do[1], Stefano Boccaletti[2], and Thilo Gross[1] — [1]MPI for the Physics Complex Systems, Dresden, Germany — [2]CNR Istituto dei Sistemi Complessi, Sesto Fiorentino, Italy

Individual dynamical units that are coupled via an interaction network can synchronize spontaneously without central regulation. The propensity to synchronize depends on structural properties of the interaction network. The influence of certain network properties such as heterogeneity and diameter have extensively been studied, however sometimes with conflicting conclusions. This might indicate that beside global structural measures of the network also the actual local configuration plays a role that cannot be neglected. Here, we show that synchronization can only be achieved when the network obeys topological criteria that are independent of any statistical network measure. We analytically derive topological conditions for the stability of stationary and phase-locked states by constructing a graphical interpretation of Jacobi's signature criterion. Furthermore, we show that the proposed approach can be extended to an adaptive network version of the Kuramoto-model, in which the coupling topology co-evolves with the dynamics of the coupled units.

DY 17.3 Wed 11:00 ZEU 255

Nonlocal Generalized Models — •Christian Kuehn and Thilo Gross — MPI-PKS, Dresden

Generalized models have been applied successfully to understand the local dynamics of ordinary differential equations (ODEs) in equilibrium when the explicit functional forms of the ODE are only partially known. Hence the method is particularly successful in the context of biophysical problems. Generalized models allow us to draw conclusions about a large set of dynamical systems simultaneously using classical techniques from bifurcation analysis. In this talk, I will illustrate the mathematical and physical framework for generalized modeling and show that the method naturally applies to partial, stochastic and delay differential equations. Furthermore, a major extension to the analysis of periodic solutions will be introduced for ODEs. This new development marks the first step to a non-local dynamical analysis which is indispensable in many applications. The theory will be illustrated with a planar model system.

DY 17.4 Wed 11:15 ZEU 255

Boolean versus continuous dynamics on simple two-gene modules — •Eva Gehrmann and Barbara Drossel — Institut für Festkörperphysik, TU Darmstadt

We investigate the dynamical behavior of simple modules composed of two genes with two or three regulating connections. Continuous dynamics for mRNA and protein concentrations is compared to a Boolean model for gene activity. Using a generalized method, we study within a single framework different continuous models and different types of regulatory functions, and establish conditions under which the system can display stable oscillations. These conditions depend only on general features such as the ratio of the relevant time scales, the degree of cooperativity of the regulating interactions, and the logical structure of the interactions. Our results combine and generalize the findings of several disconnected previous studies.

DY 17.5 Wed 11:30 ZEU 255

Comparison of phase synchronization analysis methods in physiological data — •Anja Kuhnhold[1], Jan W. Kantelhardt[1], Aicko Y. Schumann[1,2], Axel Bauer[3], Petra Bartel[4], and Georg Schmidt[4] — [1]Institut für Physik, MLU Halle-Wittenberg, Halle (Saale), Germany — [2]Complexity Science Group, Dept. of Physics and Astronomy, Univ. of Calgary, Canada — [3]Med. Klinik, Abt. Kardiologie und Kreislauferkrankungen, Universitätsklinikum Tübingen, Germany — [4]1. Med. Klinik, Klinikum rechts der Isar, TU München, Germany

Phase synchronization between two weakly coupled oscillators occurs in many natural systems. Since it is difficult to unambiguously detect such synchronization in experimental data, several methods have been proposed for this purpose. Here, we systematically optimize and compare five approaches: the automated synchrogram method, the reduced synchrogram method, two variants of a very recently suggested gradient method, and the Fourier mode method. Studying real 24h data from 1455 patients recorded approximately one week after a myocardial infarction, real data with artificial inaccuracies, and corresponding surrogate data generated by Fourier phase randomization, we report characteristic differences as well as strengths and weaknesses of the five methods in detecting episodes of n:1 and n:2 cardio-respiratory phase synchronization. We also show that synchronization hardly depends on the patients' age in our large data base. However, a strong 24h cycle occurs with drastically increased n:1 and n:2 synchronization observed during night time by all five methods.

15 min. break.

DY 17.6 Wed 12:00 ZEU 255

Burst Event and Return Interval Statistics in Wikipedia Access and Edit Data — •Mirko Kämpf[1], Sebastian Tismer[1], Jan W. Kantelhardt[1], and Lev Muchnik[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle/Saale, Germany — [2]Leonard N. Stern School of Business, New York University, USA

Internet-based social networks often reflect extreme events in nature and society by drastic increases in user activity. We study the dynamics of hourly user access and edit time series for articles in the online encyclopaedia Wikipedia. Daily and weekly activity patterns occur in addition to fluctuations and bursting activity. The bursts are characterised by a power-law distribution of durations of increases and decreases; both sides seem rather uncorrelated. For describing the reoccurrence and clustering of bursts exceeding certain thresholds we investigate the statistics of the return intervals between them. We find stretched exponential distributions of return intervals with identical parameters for all thresholds in access time series, while edit time series yield a simple exponential distribution. We apply detrended fluc-

tuation analysis, finding that most article access time series are characterized by long-term correlations with fluctuation exponents $\alpha \approx 0.9$. Finally, we also analyse the cross-correlations between edits and access rates as well as multiple articles inside a subnet. The results help in understanding the complex process of collecting, processing, validating, and distributing information in self-organized social systems.

DY 17.7 Wed 12:15 ZEU 255

Pushing through the Arnold web: Hamiltonian ratchets in higher dimensions — •Armin Seibert, Sergey Denisov, and Peter Hänggi — Institute of Physics, University of Augsburg, Universitätsstr. 1, D-86135 Augsburg

In ac-driven, space-periodic Hamiltonian systems a ratchet effect [1] may occur: particles start to diffuse predominantly into one direction, producing constant flux, even when the driving field has a zero dc-component. This is a well-established phenomenon in the case of one-dimensional Hamiltonian transport, with experimental validations ranging from classical [2] to quantum [3] limits. Remarkably, two- and three - dimensional stationary transport is impossible {\it ab initio} in ac-driven Hamiltonian systems. The system can diffuse in its phase space - along resonance channels, which constitute the {\it Arnold web} [4], - so that even when the particle is initially placed at the bottom of a potential well, it can eventually be accelerated to any preassigned energy threshold. We demonstrate that although the ratchet current never saturates to an asymptotic value in the case of higher-dimensional Hamiltonian ratchets, the direction of the ratchet motion is fixed by the space-time symmetries of the underlying potentials, and can be predicted by using the symmetry analysis [5].

[1] P. Hänggi and F. Marchesoni, Rev. Mod. Phys. 81, 387 (2009) [2] M. Schiavoni et al., Phys. Rev. Lett. 90, 094101 (2003) [3] T. Salger et al., Science 326, 1241 (2009) [4] A. J. Lichtenberg and M. A. Lieberman, Regular and Chaotic Dynamics (New York, Springer-Verlag, 1992) [5] S. Denisov et al., Phys. Rev. Lett. 100, 224102 (2008)

DY 17.8 Wed 12:30 ZEU 255

Extractions of non-elliptic limit cycles from strong non-linear oscillations via the modified continuous wavelet transform — •Eugene Postnikov[1] and Elena Lebedeva[2] — [1]Kursk State University, Kursk, Russia — [2]St. Petersburg State Polytechnical University, St. Petersburg, Russia

Recently we have proposed the modification of the complex wavelet transform with the Morlet wavelet adapted for an analysis of strong non-linear oscillations [Phys. Rev. E 82, 057201 (2010)]. It has been shown that the rotation of transform modulus in a scale space allows to merge principal harmonics of non-sinusoidal oscillations into one line corresponding to the scale value coinciding with a main period.

The main goal of this presentation is to analyze the opportunity providing by this method to extract strongly non-elliptic instable limit cycles from chaotic signals. The following items are considered: restrictions, based on time-scale uncertainty, for the maximal number of loops extracted from a phase curve; correspondence between a global cascade of period-doubling bifurcations determined via the Fourier transform and a local loop decomposition based on the wavelet transform; the wavelet decomposition and bounding tori in a phase space.

This work was supported by the grant of the President of the Russian Federation for a support of young researchers Grant No. MK-7413.2010.1

DY 17.9 Wed 12:45 ZEU 255

A technique for identifying chaos in many body systems from time series analysis — •Tarek Elsayed, Benjamin Hess, and Boris Fine — Institute of Theoretical Physics, Heidelberg, Germany

We report a new possible signature of chaos that can be easily extracted from a time series produced by physical systems having many degrees of freedom. This technique can be helpful when conventional entropic approaches fail to distinguish between chaotic and nonchaotic time series due to insufficient statistics. We apply this approach to signals generated by integrable and nonintegrable classical spin systems and support our results by Lyapunov and power spectrum spectral analysis.

DY 17.10 Wed 13:00 ZEU 255

Properties of multi-particle correlation measures in complex systems — •Tobias Galla[1] and Otfried Gühne[2] — [1]School of Physics and Astronomy, University of Manchester, Manchester M13 9Pl, UK — [2]Fachbereich Physik, Universität Siegen, Walter-Flex-Strasse 3, 57068 Siegen

The characterisation of multi-particle correlations in classical complex systems is a non-trivial task, several quantative measures have been proposed and investigated. Some of these approaches are based on ideas from information geometry, and classify the invariant measures of dynamical systems according to their distance from the space of probability distributions generated by k-particle interactions. These methods have for example been applied to coupled chaotic maps and cellular automata. Motivated by recent findings in quantum information we investigate the extent to which these quantities fulfill desirable properties of correlation measures. For example local transformations applied to individual particles or integrating out individual degrees of freedom should not increase overall multi-particle correlation. However for some current correlation measures such behaviour is found. We discuss possible remedies for this problem.

DY 18: Networks: From Topology to Dynamics I (with BP, SOE)

Time: Wednesday 10:15–10:45 Location: GÖR 226

Invited Talk DY 18.1 Wed 10:15 GÖR 226

Impact of Single Links in Growing Networks — •Jan Nagler[1,2] and Marc Timme[1,2,3] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen — [2]Institute for Nonlinear Dynamics, Faculty of Physics, University of Göttingen — [3]Bernstein Center for Computational Neuroscience (BCCN) Göttingen

How a complex network is connected crucially impacts its dynamics and function. Until recently, random percolation processes were thought to exhibit continuous transitions in general. Numerical evidence for discontinuous changes of the order parameter in certain percolation processes, however, has triggered an ongoing scientific controversy about the conditions for discontinuous phase transitions in percolation [Achlioptas, D'Souza, and Spencer, Science 323, 1453 (2009); Nagler, Levina, and Timme, Nature Physics, in press; see also references therein.]. We study both numerically and analytically under which conditions certain "competitive" percolation processes exhibit macroscopic jumps in the order parameter.

DY 19: Networks: From Topology to Dynamics II (with BP, SOE)

Time: Wednesday 10:45–13:15 Location: GÖR 226

DY 19.1 Wed 10:45 GÖR 226

Stem Diseases: Efficient Immunization Strategies — •Christian M. Schneider[1], Tamara Mihaljev[1], Shlomo Havlin[2], and Hans J. Herrmann[1,3] — [1]Computational Physics, IfB, ETH Zurich, Schafmattstrasse 6, 8093 Zurich, Switzerland — [2]Minerva Center and Department of Physics, Bar-Ilan University, 52900 Ramat-Gan, Israel — [3]Departamento de Fisica, Universidade Federal do Ceara, 60451-970 Fortaleza, Ceara, Brazil

The spreading of diseases in social networks is crucial to the potential danger of the disease. We quantitatively analyze the effect of immunization strategies on the susceptibility to diseases. We introduce a novel immunization strategy and find for all studied networks that the spreading of diseases can be significantly suppressed compared to the known immunization strategies. As an example we show the results for the international airport network.

DY 19.2 Wed 11:00 GÖR 226

Vaccination Decisions with Limited Information — •Olivia Woolley Meza, Daniel Grady, and Dirk Brockmann — Northwestern University, Evanston, USA

Widely practiced vaccination can eradicate a disease from a population. However, if rational, self-interested individuals believe there is any risk associated with the vaccine, their strategic vaccination decisions can lead to insufficient aggregate vaccination. In fact, recent work has shown that in a well-mixed population with perfect information the disease will not be eradicated. We consider a finite-size stochastic system,where each individual has both a contact neighborhood, the group of others who can contact the individual, and an information neighborhood, the group of others about whom the individual can obtain information. We find that in this setting strategic vaccination decisions can lead to disease eradication. We further investigate how the likelihood of eradication changes with the extent of information on which individuals base their decisions. We find that when information is very limited, increasing the extent of information helps to eradicate the disease. However, as more information becomes available we find a second regime where additional information reduces the effectiveness of vaccination.The information region with high disease extinction is larger when the underlying topology is highly clustered. The cause of suboptimal behavior as we approach global information also depends on the underlying topology. We use simulations and analytical models to explain this behavior.

DY 19.3 Wed 11:15 GÖR 226

Optimal vaccination strategies in metapopulation networks — •Vitaly Belik — Massachusetts Institute of Technology, Cambridge, MA, USA — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Germany

Human infectious diseases remain a profound challenge for the humankind. Recently a lot of attention is devoted to theoretical modeling of geographical epidemic spread taking into account human mobility patterns obtained from the ubiquitous real data. This considerably advances the design of effective preventive and containment strategies. We investigate a problem of optimal vaccine distribution in a metapopulation network employing game theoretical approaches. We answer such an important question, as to what extent different regions are interdependent and where vaccination need to be subsidized to minimize the overall impact of the epidemic. In our extensive numerical simulation we employ the real data on human mobility in the USA.

DY 19.4 Wed 11:30 GÖR 226

What is the front velocity in wave propagation without fronts? - Epidemics on complex networks provide an answer — •Rafael Brune[1,2], Christian Thiemann[1,2], and Dirk Brockmann[1] — [1]Northwestern University, Evanston, USA — [2]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Deutschland

The spatiotemporal patterns of infectious diseases that spread nowadays typically lack a well defined wave front as human mobility is multi-scale. The structure of emergent patterns is difficult to assess quantitatively, in particular spreading speeds are difficult to define and compare in different scenarios. We present a novel way to look at contagion phenomena on complex networks using the underlying topological structure of the network. Shortest-path distances and arrival times are used to redefine the velocity of spreading patterns. We extend the idea of a wavefront that can be directly observed in simple networks like a regular lattice to the class of complex networks which in traditional views exhibit complicated patterns. This method substantially simplifies the way dynamics are analyzed and explains why patterns in complex modeling approaches share many similarities. Disease dynamics on various complex networks ranging from artificial to real human mobility networks show the benefit of representing the spatio-temporal patterns based on topological features of the network.

DY 19.5 Wed 11:45 GÖR 226

Limiting factors for the spread of infectious diseases in complex networks — •Hartmut H K Lentz[1,2], Mario Konschake[2], and Igor M Sokolov[1] — [1]Department of Physics, Humboldt University, Newtonstr. 15, 12489 Berlin, Germany — [2]Friedrich-Loeffler-Institut, Institute of Epidemiology, Seestr. 55, 16868 Wusterhausen, Germany

Epidemics are expected to spread rapidly in networks with heavy-tail degree distributions. On the other hand, many real world networks comprise complex substructures like modules. Modules are subsets of nodes being densely interconnected. This yields subgraphs which are in the limiting case 'isolated' from each other. Furthermore the directed character of a network might play a role in disease spread. Most social and human networks can be treated as undirected. But many networks, e.g. trade networks, are inherently directed since there is an underlying economic/logistic process. In directed networks the number of possible ways for a pathogen is dramatically reduced. Our results show that direction and community structure are limiting factors for disease spread.

15 min. break

DY 19.6 Wed 12:15 GÖR 226

Are motifs a myth? — •Jörg Reichardt[1], Roberto Alamino[2], and David Saad[2] — [1]Complexity Sciences Center, UC Davis and Würzburg University — [2]Aston University, Birmingham

Small subgraphs, called network motifs, have received considerable attention in network research over the last years and are suggested as simple building blocks of complex networks. Motifs are attributed functional significance due to their strong over- or underrepresentation when compared to random null models. However, the link randomized null models used for such comparisons generally match the observed networks only in terms of their microscopic structure, destroying all mesoscopic features and hence give biased estimates of the statistical significance of motif counts in real world networks.

We present a generative probabilistic model based on Exponential Random Graphs plus an algorithm to infer model parameters from a given network. This model allows to generate an ensemble of random null models that matches the observed network with respect to both its microscopic *and* mesoscopic structural features.

We show that such random null models may result in a much more conservative estimation of the statistical significance of motif counts in real world networks. Further, they maintain the parsimonious explanation of complex networks as a collection of conditionally independent edges.

DY 19.7 Wed 12:30 GÖR 226

Is there a bias in the generation of simple random graphs with the configuration model? — •Hendrike Klein-Hennig and Alexander K. Hartmann — Institute of Physics, University of Oldenburg

The configuration model is an often used and well known procedure to generate random graphs with an arbitrary degree sequence. The basic idea is to assign a fixed degree to each vertex, which create edges emerging from the vertex called stubs. In a second step random pairs of stubs are connected until there are no stubs left. This procedure generates every possible graph realization with the same probability. In this work two generation procedures are compared how to deal with self-loops and multiple edges (forbidden edges) to generate undirected simple graphs. In the first procedure the entire graph is disregarded and the generation process is restarted from the beginning as soon as a forbidden edge is encountered. Another method, which is frequently applied [1], is to disregard only the forbidden edge, restoring the stubs and drawing a new pair, while keeping the rest of the graph. An analysis of small example graphs shows that for the second generation procedure the graphs are not necessarily created with equal probability. For large graph sizes the behavior is studied using statistical tests on computer generated graphs [2].

[1] M.Catanzaro, M.Boguñá and R. Pastor-Satorras, *Generation of uncorrelated random scale-free networks*, Phys. Rev. E *71* 027103 (2005)

[2] A.K. Hartmann, *Practical Guide to Computer Simulations*, (World Scientific, 2009)

DY 19.8 Wed 12:45 GÖR 226

Surrogates and significance testing for spatially embedded complex networks — •Jonathan F. Donges[1,2], Reik V. Donner[1], Norbert Marwan[1], and Jürgen Kurths[1,2] — [1]Potsdam Institute for Climate Impact Research, P.O.Box 60 12 03, 14412 Potsdam, Germany — [2]Department of Physics, Humboldt University of Berlin, Newtonstr. 15, 12489 Berlin, Germany

The analysis of spatially embedded complex networks, i.e., networks with vertices embedded in a metric space, is of increasing interest in many fields of science. Examples are power grids in electrical engineering, the internet and world wide web in computer science or social

networks in social science. In many cases, there is some degree of uncertainty about the network structure, e.g., edges might be missing in the network that exist in the system under study (the opposite may also be true). This is particularly relevant for networks constructed from multivariate data using the tools of time series analysis. Given this uncertainty, it is very important to evaluate the significance of measured network properties such as clustering coefficient, average path length, degree distribution or various vertex centrality sequences with respect to a given null hypothesis. Here we present different types of surrogates for spatially embedded networks, i.e., random networks with prescribed spatial constraints such as fixed edge distance distribution or a fixed average edge distance sequence, and show how to use them for testing the associated null hypotheses. The method is illustrated using diverse example networks, e.g., the european power grid or a climate network representing correlation structure of the surface air temperature field.

DY 19.9 Wed 13:00 GÖR 226

Backbones and borders from shortest-path trees — •Daniel Grady, Christian Thiemann, and Dirk Brockmann — Northwestern University, Evanston, IL, USA

One of the most important tasks in complex network research is to distinguish between vertices and edges that are topologically essential and those that are not. To this end, a variety of vertex and edge centrality measures have been introduced, ranging from measuring local properties (degree, strength) to quantities that depend on the global structure of the graph (betweenness). Here we introduce a novel technique based on the family of shortest-path trees, which is applicable to strongly heterogeneous networks. This approach can identify significant edges in the network, distinct from conventional edge betweenness, and these edges make up a network backbone relevant to dynamical processes that evolve on such networks. We will show that important network structures can be extracted by investigating the similarity and differences of shortest-path trees and show that tree dissimilarity in combination with hierarchical clustering can identify communities in heterogeneous networks more successfully than ordinary reciprocal-weight distance measures. We demonstrate the success of this technique on complex multi-scale mobility networks.

DY 20: Glasses I (jointly with DF and CPP)

Time: Wednesday 10:15–13:00 Location: KÖN Farb

DY 20.1 Wed 10:15 KÖN Farb

Boson-peak in glasses and random-matrix statistics — •Walter Schirmacher — Institut für Physik, Univ. Mainz — Physik-Department E13, TU München

The enhancement of the vibrational density of states (DOS) with respect to the Debye expectation ("boson peak"), which is universally observed in glasses, is considered by means of of symmetry arguments. Low-frequency wave-like excitations in a disordered solids probe a homogeneous and isotropic material. Due to these symmetries the vibrational wave-like states are highly degenerate (Debye regime). This degeneracy is lifted at higher frequencies. In this regime the discretized equation of motions are governed by a sparse random matrix. The eigenvalues of this matrix are non-degenerate and show the distance statistics of the Gaussian orthogonal ensemble ("level repulsion"). It is conjectured that the integrated density of levels in this regime increases linearly. The cross-over from the Debye regime to the random-matrix regime leads in three dimensions to an enhancement of the DOS. In two dimensions this is not the case. Model calculations using a field-theoretical approach [1] and inspection of simulation data [2] confirm this reasoning.

[1] W. Schirmacher, Europhys. Lett. Europhysics Letters, 73, 892 (2006); [2] see e.g. S. K. Sarkar, G. S. Matharoo, A. Pandey, Phys. Rev. Lett. 92,215503 (2004)

DY 20.2 Wed 10:30 KÖN Farb

Identification of facilitation effects in supercooled liquids — •Andreas Heuer and Christian Rehwald — Institute of Physical Chemistry, University of Muenster

In a first step we analyze the information content of the finite-size effects of a glass-forming system. Interestingly, the diffusion constant shows a very weak and the structural relaxation time a very strong finite-size effect [1]. This result reflects the dynamic coupling of different regions in real space via a facilitation mechanism. We can formulate a minimum model of the glass transition which can reproduce in detail the observed features of these finite-size effets. It can be regarded as a generalization of the kinetically constrained models [2].

In a second step we search for a direct evidence of this facilitation mechanism in computer simulations. Using the setup of a highly non-equilibrium configuration these causal relations between successive relaxation events can indeed be found and characterized.

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

[2] Y. J. Jung, J. P. Garrahan, and D. Chandler, Phys. Rev. E 69, 061205 (2004).

DY 20.3 Wed 10:45 KÖN Farb

Dynamics of shear transformation zones during mechanical cycling of glassy CuTi - a molecular dynamics study — •Lennart Fricke und S. G. Mayr — Leibniz-Institut fuer Oberflaechenmodifizierung, Translationszentrum fuer regenerative Medizin und Fakultaet fuer Physik und Geowissenschaften der Universitaet Leipzig, 04318 Leipzig

Plastic deformation of bulk metallic glasses at low temperatures occurs in highly localized regions, called shear-transformation-zones (STZ) [1] - as corroborated recently in detailed experimental and simulational studies. After activation, these STZs should possess a memory of their configuration prior to transformation due to confinement by the surrounding elastic matrix, i.e. the Eshelby back-stress. While this picture surely is intuitive, it is particularly interesting whether it applies in a strict or only statistical sense and up to what strain levels. With this background we study shear behavior during mechanical cycling of CuTi with a maximum of 1% to 10% shear strains in large–scale MD simulations using realistic embedded atom method (EAM) potentials. Evaluating suitable quantities, including non-affine displacements and atomic-level Basinski–Duesbery–Taylor (BDT) stresses, we address the reversibility of STZs and the underlying physics on the atomic scale.

[1] A. S. Argon, Acta Metall. 27, 47 1979

This project is funded by the German DFG - PAK 63

DY 20.4 Wed 11:00 KÖN Farb

Describing experimentally obtained stress overshoots in sheared colloidal dispersions with schematic MCT — •Christian Peter Amann[1], Matthias Fuchs[1], Miriam Siebenbürger[2], and Matthias Ballauff[2] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Helmholtz Zentrum für Materialien und Energie, 14109 Berlin, Germany

Sheared viscoelastic media show a stress overshoot between elastic and plastic deformation regime, i.e. a maximum in the shear stress vs. strain plot after switching on a constant shear rate. We found a way to model such overshoots with the $F_{12}^{(\dot\gamma)}$ model, a schematic model of a microscopic mode-coupling theory (MCT) approach to describe glass forming liquids. The enhancement of the schematic model is tested by fitting experimental strain-stress curves from sheared colloidal dispersions of thermosensitive core-shell particles. Flow curves and linear stress response moduli of the same experimental setup could be fitted well with the $F_{12}^{(\dot\gamma)}$ model [1]. Furthermore this model has been able to describe nonlinear stress response to oscillatory shear rates [2]. The implementation of stress overshoots in this schematic model was motivated and guided by the recently identified mechanism within microscopic MCT framework causing such overshoots to occur [3]. This mechanism is also identified to be highly connected to a super-diffusive motion regime of the colloids [3].

[1] M. Siebenbürger et al., *J. Rheol.* **53**, 707–726 (2009)
[2] J.M. Brader et al., arXiv:1010.2587v1 (2010)
[3] J. Zausch et al., *J. Phys.: Condens. Matter* **20**, 404210 (2008)

DY 20.5 Wed 11:15 KÖN Farb

Evaluation of MD force fields for ion transport in glassy materials — •Christian Trott[1], Martin Körner[1], Michael Schuch[2], and Philipp Maass[2] — [1]Theoretical Physics II, Technische Univer-

sität Ilmenau, 98684 Ilmenau, Germany. — [2]Fachbereich Physik, Universität Osnabrück, 49076 Osnabrück, Germany

Ion conducting glasses are an interesting class of materials with a wide range of possible applications, including batteries, supercapacitors, and smart windows. Considerable efforts have been undertaken to understand their properties with the help of experimental and theoretical investigations such as molecular dynamics (MD) simulations. Most of the previous MD studies of ion conducting glasses have been limited to structural analysis and the existing investigations of ion transport were almost all performed at comparatively high temperatures just below the "computer glass transition" temperature. Recent advances in hardware and MD software, namely the development of the GPU-MD code $\text{LAMMPS}_{\text{CUDA}}$, allow for a much more comprehensive investigation of long term dynamics. We assess the power of a number of interaction models for investigating long range ion transport in glasses. Specifically we determine diffusion constants and selected activation energies in several ion conducting glass systems for which force fields have been suggested in the literature.

DY 20.6 Wed 11:30 KÖN Farb

Lorentz-like power-law decay of velocity anti-correlations in a supercooled liquid — •Felix Höfling[1] and Peter Colberg[2,3] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, and Institut für Theoretische und Angewandte Physik, Universität Stuttgart — [2]Chemical Physics Theory Group, Department of Chemistry, University of Toronto, Canada — [3]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln

Harnessing the compute power of recent graphics processors, we have measured the velocity-autocorrelation function (VACF) in the supercooled Kob-Andersen mixture for large systems of 50,000 particles, providing data with an excellent signal-to-noise ratio. The emergence of glassy dynamics upon supercooling is systematically accompanied by a power-law decay of the VACF at intermediate times with exponent 5/2 and negative prefactor, similarly as observed recently for the hard sphere liquid (Williams *et al.*, PRL 2006). Such anti-correlations are reminiscent of the well-known, universal long-time tail in the Lorentz model with the same exponent and sign. The role of dynamic heterogeneities for the power-law decay is addressed by considering correlation functions that are restricted to the most mobile or immobile particles. We find that the Lorentz-like decay is absent in the VACF of the most mobile particles and conclude that the power law is *not* a manifestation of dynamic heterogeneities. For the most immobile particles, however, the power-law decay is well pronounced and we propose that the relevant mechanism is given by repeated encounters with the quasi-arrested, microscopic particle cages.

DY 20.7 Wed 11:45 KÖN Farb

Universal jamming phase diagram in the hard-sphere limit and comparison of the dynamics of soft and hard spheres — •Michael Schmiedeberg[1], Thomas K. Haxton[2], Sidney R. Nagel[3], and Andrea J. Liu[4] — [1]Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany — [2]Theory of Nanostructured Materials, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — [3]The James Franck Institute, The University of Chicago, Chicago, IL 60637, USA — [4]Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104, USA

We present a new formulation of the jamming phase diagram for a class of glass-forming fuids consisting of spheres interacting via finite-ranged repulsions. Our phase diagram is universal at low pressure, i.e. observables such as the relaxation time are insensitive to details of the interaction potential and collapse onto the values for hard spheres.

Furthermore, we show that the dynamics of soft spheres can be described in terms of the dynamics of hard spheres. By introducing an effective hard sphere diameter that is determined from the soft-sphere pair potential via the Andersen-Weeks-Chandler approximation, the relaxation times of soft spheres can be mapped onto the curve known for hard-sphere liquids. These results indicate that the dynamics of soft spheres depend on an effective free volume in a universal way.

DY 20.8 Wed 12:00 KÖN Farb

Investigation of the dephasing of tunneling systems in glasses using two-pulse polarisation echo experiments — •Masoomeh Bazrafshan, Paul Fassl, Martin Schwarze, Angela Halfar, Annina Luck, Andreas Fleischmann, and Christian Enss — Kirchhoff Institut für Physik, Universität Heidelberg

Low temperature properties of glasses are governed by atomic tunneling systems. Many aspects are well described within the phenomenological standard tunneling model. Tunneling systems couple to their local strain fields which gives rise to a strain-mediated coupling among them. These interactions cause time-dependent variations in the energy splittings of tunneling systems when their neighbors undergo thermal transitions. This is the basis of the spectral diffusion model, which describes the dephasing of tunneling systems at very low temperatures. Experimentally, this dephasing of tunneling systems can be studied by two-pulse polarisation echo experiments. We have performed such echo decay measurements with an improved setup allowing us to observe echoes at very long delay times where the echo has decayed five orders of magnitude from its original amplitude. We have analysed the time and temperature dependent results in the framework of spectral diffusion model, finding very good qualitative agreement for the echo decay, but clear shortcoming in terms of the temperature dependence.

DY 20.9 Wed 12:15 KÖN Farb

Structural investigations on Eu-doped fluorobromozirconate glass ceramics. — •Marie-Christin Wiegand[1], Bernd Ahrens[2], Bastian Henke[2,3], and Stefan Schweizer[2,3] — [1]Department of Physics, University of Paderborn, Warburger Str. 100, 33100 Paderborn, Germany — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale), Germany — [3]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale), Germany

Modified Eu-doped fluorozirconate glasses are regarded as promising materials for photovoltaic and medical applications. In these glasses, a substantial fraction of the fluorine ions was replaced by bromine ions resulting in the formation of $BaBr_2$ nanocrystals upon subsequent thermal treatment of the as-made glass. Interestingly, the metastable hexagonal phase of $BaBr_2$ is always formed first before further annealing leads to the formation of orthorhombic phase $BaBr_2$, i.e., a phase transition from hexagonal to orthorhombic phase $BaBr_2$ occurs upon annealing. During the annealing a part of the doped Eu^{2+} is incorporated into the $BaBr_2$ nanocrystals enabling fluorescent transitions of Eu^{2+} in hexagonal and orthorhombic $BaBr_2$, respectively, upon ultraviolet excitation. The nanocrystal size and the structural phase depend on the addition of InF_3 and YF_3 and on the Br/(F+Br)-ratio, which was investigated by differential scanning calorimetry and x-ray diffraction. In addition, photoluminescence experiments were performed to monitor the phase transition by optical means.

DY 20.10 Wed 12:30 KÖN Farb

Optical and structural properties of fluorozirconate-based glass ceramics doped with divalent and trivalent europium. — •Christian Passlick[1], Bastian Henke[1,2], Jacqueline Anne Johnson[3], and Stefan Schweizer[1,2] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale) — [3]Department of Materials Science and Engineering, University of Tennessee Space Institute, Tullahoma, TN 37388, USA

Eu-doped fluorozirconate-based glass ceramics can be used for x-ray detection in medical diagnostics as well as for down-converting top layers in photovoltaics. A modified ZBLAN composition consisting of a mixture of Zr, Ba, La, Al, and Na fluorides was additionally doped with chlorine ions to initiate the formation of $BaCl_2$ nanocrystals upon thermal treatment of the as-poured glasses. During annealing some of the Eu^{2+} ions are incorporated into the nanocrystals enabling a strong blue fluorescence upon ultraviolet excitation or x-ray irradiation. In this work, focus is put on the amount of divalent and trivalent Eu fluoride and chloride additives since it is known that the expensive Eu^{2+} can be produced by melting the cheaper Eu^{3+} raw material. Influences of the different Eu oxidation states on the $BaCl_2$ crystallization and the optical response of the glass ceramics are presented.

DY 20.11 Wed 12:45 KÖN Farb

Multi-phonon relaxation in Eu-doped fluorozirconate-based glasses and glass ceramics — •Charlotte Pfau[1], Christian Bohley[1], Manuela Miclea[1], Paul-Tiberiu Miclea[2,3], and Stefan Schweizer[2,1] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle — [3]Institute of Physics, Martin-Luther-University of Halle-Wittenberg, Heinrich-

Damerow-Str. 4, 06120 Halle

Eu-doped fluorozirconate(FZ)-based glasses are of interest for various fluorescence applications such as photon down-conversion layers for high efficiency solar cells or ionizing radiation imaging plates. Multi-phonon relaxation (MPR) is one of the major quenching processes of the rare-earth (RE)-related fluorescence therein. The MPR is significantly reduced in hosts providing low phonon frequencies such as FZ-based glasses and glass ceramics; the latter contain barium halide nanocrystals with even lower phonon frequencies. However, the MPR rate depends not only on the phonon frequency, but also on the electron-phonon coupling between the rare-earth ion and the host lattice. The local vibrational environment of the RE ion is investigated by phonon sideband spectroscopy. To analyze the vibrational spectra and their influence on the fluorescence properties, a series of Eu-doped FZ-based glasses and glass ceramics has been studied by Raman, phonon sideband, and fluorescence spectroscopy. The MPR rate is determined for the levels involved in the fluorescence process.

DY 21: Thermodynamics and Statistical Physics of Small Systems (contributed talks)

Time: Wednesday 11:45–13:15 Location: HÜL 186

DY 21.1 Wed 11:45 HÜL 186

Stochastic energetics of the Büttiker-Landauer Brownian Motor and Refrigerator — •Ronald Benjamin — German Aerospace Center, Cologne, Germany

The energetics of a Brownian motor and refrigerator driven by position dependent temperature, known as the Büttiker-Landauer motor and refrigerator, is investigated by extensive numerical simulations of the inertial Langevin equation. We identify parameter values for optimal performance of the motor and refrigerator. Inertial effects strongly affect the thermodynamic behavior of the system even in the over-damped limit. The behavior of the motor and refrigerator, in the linear response regime, is examined under finite time conditions and we find that the efficiency can never reach that of an endoreversible engine working under the same condition. Finally, we investigate the role of different potential and temperature profiles to enhance the efficiency of the system. Our simulations show that optimizing the potential and temperature profile leads only to a marginal enhancement of the system performance and the reasons for this are given.

DY 21.2 Wed 12:00 HÜL 186

Measurements in optimal finite-time thermodynamics — •David Abreu and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

The second law states the impossibility of extracting work from a system in a single thermal bath. However, as Sagawa and Ueda recently showed [1], this becomes possible if we extract information out of the system through measurements. We show here a basic example of an isothermal engine based on the conversion of information into work.

Our model system consists in a Brownian particle confined in a harmonic potential that we want to displace from its initial position to a fixed final position in finite time. Performing one or more measurements of the position of the particle at the beginning or during the process leads to work extraction from the thermal bath. We optimize the output work of such a process and build a cyclic engine based on it. We observe the presence of an optimal cycle-time which depends on the precision of the measurements.

We then quantify the information obtained during the measurements and show that we can transform it all into useful work in the quasistatic limit, given that we control not only the position but also the stiffness of the potential. We compare this result to a discrete two-level system, analogous to the Szilard engine, and show that the expressions of the total extractable work in both cases are similar and consistent with each other.

[1] T. Sagawa and M. Ueda. Phys. Rev. Lett. 104, 090602 (2010).

DY 21.3 Wed 12:15 HÜL 186

Free gold clusters in CO and O_2 atmosphere: an ab initio study. — •Elizabeth C. Beret, Luca M. Ghiringhelli, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft Berlin, Germany

The marked catalytic activity of gold nanoparticles has inspired a large number of scientific contributions from different fields. However, many questions still lack a satisfying answer, for example what are the structures and stoichiometries of the gold particles in the presence of the reactive gases, and how do their catalytic properties depend on the particle size [1].

We answer these questions for neutral gold clusters modeled in a gas phase atmosphere containing CO and O_2 in variable compositions, and in a temperature range between 100 and 600 K. To this aim, DFT (PBE)–based *ab initio atomistic thermodynamics* technique [2] is applied, including full account of the vibrational contribution to the free energy. As a result, the preferred cluster+adsorbate structures for different environmental conditions are obtained and interpreted as candidate intermediates in the catalytic CO oxidation reaction.

[1] R. Meyer, C. Lemire, S. K. Shaikhutdinov and H. J. Freund, *Gold Bull.* **2004**, *37*, 72–124. [2] K. Reuter and M. Scheffler, *Phys. Rev. B* **2001**, *65*, 035406; C. M. Weinert and M. Scheffler, *Mat. Sci. Forum* **1986**, **10–12**, 25–30; M. Scheffler and J. Dabrowski, *Phil. Mag. A* **1988**, *58*, 107–121.

DY 21.4 Wed 12:30 HÜL 186

Interaction effects and performance of a photoelectric device — Marcel Dierl[1,2] and •Mario Einax[1,2] — [1]Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau, Germany — [2]Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück, Germany

We investigate a one-dimensional photoelectric device, where charge carriers interact via coupling constant V. Based on classical time-dependent density functional theory calculations, we find that nearest-neighbor interactions are of crucial importance for the current, the power as well as the efficiency of the nano-device. To point out the validity of this analytical approach, kinetic Monte Carlo simulations are performed.

DY 21.5 Wed 12:45 HÜL 186

Kramers barrier crossing as a cooling machine — •Philip Schiff and Abraham Nitzan — School of Chemistry, Tel Aviv University, Israel

The achievement of local cooling is a prominent goal in the design of functional transport nanojunctions. One generic mechanism for local cooling is driving a system through a local uphill potential step. In this talk we examine the manifestation of this mechanism in the context of the Kramers barrier crossing problem. For a particle crossing a barrier, the local effective temperature and the local energy exchange with the thermal environment are calculated, and the coefficient of performance of the ensuing cooling process are evaluated. These results represent a heuristic demonstration of a mechanism for pumping heat in a nanosystem.

DY 21.6 Wed 13:00 HÜL 186

Effects of polymer grafting on the thermodynamic equilibrium behavior of single polymer adsorption — •Monika Möddel[1], Wolfhard Janke[1], and Michael Bachmann[2] — [1]Institut für Theoretische Physik, Universität Leipzig — [2]Institut für Festkörperforschung, Theorie II, Forschungszentrum Jülich

The adsorption of single polymers onto flat attractive substrates has been the subject of several studies in the past. Especially for numerical studies of finite chains it is popular to consider the chain to be grafted, i.e. permanently attached to the substrate at one end. Compared to non-grafted polymer adsorption, translational entropy is strongly suppressed, and thus the phase space lacks completely desorbed conformations some distance away from the substrate. We systematically show how the competition between translational and conformational entropies changes the character of the adsorption transition. We present a comparison of the thermodynamic behavior of free and grafted chains for a range of different surface attraction strengths and temperatures. This is done by parallel tempering simulations of an off-lattice coarse-grained homopolymer [1] and a combined canonical

and microcanonical analysis of energetic and steric observables.

[1] M. Möddel, M. Bachmann, and W. Janke, J. Phys. Chem. B 113, 3314 (2009); M. Möddel, W. Janke, and M. Bachmann, Phys. Chem. Chem. Phys. 12, 11548 (2010).

DY 22: Granular Matter/ Contact Dynamics

Time: Wednesday 14:00–18:00 Location: HÜL 186

DY 22.1 Wed 14:00 HÜL 186

Where to Dig for Gold? - Density Segregation inside Migrating Dunes — Christopher Groh[1], Ingo Rehberg[1], and •Christof A. Krülle[1,2] — [1]Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth, Germany — [2]Maschinenbau und Mechatronik, Hochschule Karlsruhe - Technik und Wirtschaft, D-76133 Karlsruhe, Germany

Spatiotemporal patterns in nature, such as ripples or dunes, formed by a fluid streaming over a sandy surface show complex behavior despite their simple forms. Below the surface, the granular structure of the sand particles is subject to self-organization processes, exhibiting such phenomena as reverse grading when larger particles are found on top of smaller ones. Here we report results of an experimental investigation with downscaled model dunes revealing that, if the particles differ not in size but in density, the heavier particles, surprisingly, accumulate at the crest of migrating dunes while lighter particles are buried at the bottom. As a side effect we show that the migration velocity of bidense dunes scales with the mean density of the grains as a power law function with an exponent of -3/2. This insight into the sedimentology of dunes composed of different types of sand has, loosely speaking, the implication, that in a ripple or dune mixed of gold and sand, the gold nuggets are likely to be found at the top, close to the surface at the crest.

DY 22.2 Wed 14:15 HÜL 186

Axial segregation and convection of a granular mixture in a quasi-2d rotating container — •Frank Rietz and Ralf Stannarius — Universität Magdeburg, Abt. Nichtlineare Phänomene

A bimodal mixture of glass spheres is filled into a long, flat rectangular container. The flatness of the container allows the particles to arrange only in a quasi 2d layer. The cell is slowly rotated along the horizontal axis. We observe in most cases demixing of the beads in lateral bands. In some cases the mixture does not segregate and the beads circulate in convection patterns. With this simple system we can reproduce well-known three-dimensional phenomena like axial segregation banding in half filled rotated cylinders[1] and convection rolls in flat rotated cells[2]. By reducing the complexity from 3d to 2d we show that models based on the angle of repose are not relevant for 2d cells and thus might be not relevant in general.

[1] K.M. Hill, A. Caprihan, and J. Kakalios, *Phys. Rev. Lett.* **78**, 50 (1997).
[2] F. Rietz and R. Stannarius, *Phys. Rev. Lett.* **100**, 078002 (2008).

DY 22.3 Wed 14:30 HÜL 186

Traffic jams, gliders, and bands in a simple lattice swarming model — •Fernando Peruani[1], Tobias Klauss[2], Andreas Deutsch[2], and Anja Voss-Boehme[2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]ZIH - Technische Universitaet Dresden, Dresden, Germany

In this talk, we will introduce a simple swarming model on a two-dimensional lattice where the self-propelled particles exhibit a tendency to align ferromagnetically. Volume exclusion effects are present: particles can only hop to a neighboring node if the node is empty. We will show that such effects lead to a surprisingly rich variety of self-organized spatial patterns. As particles exhibit an increasingly higher tendency to align to neighbors, they first self-segregate into disordered particle aggregates. Aggregates turn into traffic jams. Traffic jams evolve toward gliders, triangular high density regions that migrate in a well-defined direction. Maximum order is achieved by the formation of elongated high density regions - bands - that transverse the entire system. Numerical evidence suggests that below the percolation density the phase transition associated to orientational order is of first-order, while at full occupancy it is of second-order.

DY 22.4 Wed 14:45 HÜL 186

Amplitude-dependent phase-separation in vibrated dry granular matter — •Klaus Röller[1], James P.D. Clewett[2], Roger M. Bowley[2], Stephan Herminghaus[1], and Michael R. Swift[2] — [1]MPI for Dynamics and Self-Organization, Bunsenstr. 10, D-37073 Göttingen, Germany — [2]School of Physics and Astronomy, University of Nottingham, Nottingham, NG7 2RD, United Kingdom.

A new phase transition is observed experimentally and by simulation in a dry granular gas subject to vertical vibration between two horizontal plates. Molecular dynamics simulations allow to investigate the observed phase separation in detail. We find a high-density, low temperature gas, coexisting with a low-density, high temperature gas moving coherently. A simple scaling argument approximately gives the amplitude dependence of the temperature in each phase. The characteristic dependence of the phase separation on the vibration amplitude distinguishes this phase separation from other known transitions in driven granular media.

DY 22.5 Wed 15:00 HÜL 186

Phase transitions of two dimensional wet granular matter under swirling motion — •Christopher May, Kai Huang, and Ingo Rehberg — Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth, Germany

Wetting triggered phase transitions of granular matter may lead to natural disasters such as landslide. To shed light on phase transitions of wet granular matter in general, we study experimentally the dynamical behavior of two dimensional wet glass beads under horizontal swirling motion. The cohesion induced by capillary bridges formed between adjacent particles tends to keep wet granular clusters rigid against 2D swirling motion. How the rigidity varies with wetting liquid added and how the change of rigidity in turn influences the phase transitions of the 2D system are going to be addressed. The structures of the clusters are investigated by particle tracking techniques and their solid-, fluid- and gaslike states are characterized by means of bond-orientational order parameters.

DY 22.6 Wed 15:15 HÜL 186

Spiral Patterns in Vertically Vibrated Wet Granular Matter — •Kai Huang and Ingo Rehberg — Experimentalphysik V, Universität Bayreuth, D-95440, Germany

Spiral patterns widely exist in nature and have been extensively studied in various non-equilibrium systems. As a peculiar example, we report here spiral patterns in a few layers of cohesive glass beads driven by vertical vibrations. The cohesion is introduced by adding few percent of wetting liquid into the sample so that the particles are bonded with each other by liquid bridges. As the vibration amplitude reaches a certain threshold, traveling waves or rotating spiral patterns start to appear. These spiral patterns have typically a meandering core and three rotating arms which are associated with the three phases of a parametrically driven oscillation with period 3. The phase diagram for the pattern forming system will be presented and the mechanism for the spiral patterns will be discussed.

DY 22.7 Wed 15:30 HÜL 186

Fluidization of wet granulates under hydrodynamic stresses — •Ilenia Battiato and Jürgen Vollmer — Max Planck Institute for Dynamics and Self-Organization, 37073, Göttingen

We investigate the fluidization threshold of three-dimensional wet granulates under hydrodynamic drag exerted by a creeping flow. A continuum model of flow through porous media provides a closed form expression for the average drag force on a single grain. The balance equation for the forces and a force propagation model are then used to investigate the effects of porosity and different packing structures (e.g. Face Centered and Hexagonal Close Packing) on the stability of the pile.

DY 22.8 Wed 15:45 HÜL 186

Temperature-sensitive wet granular matter — •Christoph Gögelein, Martin Brinkmann, Matthias Schröter, and Stephan Herminghaus — MPI für Dynamik und Selbstorganisation,

Bunsenstr. 10, 37073 Göttingen

We present our recent experimental studies on the temperature-induced formation of capillary bridges in granular matter. We will demonstrate that we can precisely tune the bridge size and force by immersing our glass spheres in a binary liquid mixture [1]. Furthermore, we will discuss the effect of capillary bridges on random sphere packing's using a fluidized bed setup.

[1] C. Gögelein, M. Brinkmann, M. Schröter, and S. Herminghaus, Langmuir 26 (2010) 22, 17184.

15 min. break

DY 22.9 Wed 16:15 HÜL 186

Refraction, exclusion and reflection of shear zones in layered granular materials — •Balázs Szabó[1], Sandra Wegner[2], Tamás Unger[3], Frank Angenstein[4], Ralf Stannarius[2], and Tamás Börzsönyi[1] — [1]Research Institute for Solid State Physics and Optics, H-1525 Budapest, PoB. 49, Hungary — [2]Otto-von-Guericke-University, D-39106 Magdeburg, Germany — [3]HAS-BUTE Condensed Matter Research Group, Budapest University of Technology and Economics H-1111 Budapest, Hungary — [4]Leibniz Institute for Neurobiology, D-39118 Magdeburg, Germany

When granular materials deform under external stress the deformation is often localized into narrow regions. These shear zones develop along the most optimal path (weakest bonds break), thus, in an inhomogeneous material the shear zone tries to escape the high friction regions. In a layered system the zone can change direction when crossing the layer boundaries, which is very similar to the refraction of light beams in geometric optics [1]. We show experimentally and numerically, that for the case of shear zones the refraction law is in striking analogy with geometric optics, but here the frictional properties of the materials take the role of the optical index of refraction [2]. We also explore other configurations, where the zone is refracted from the layer boundary. Visualization of the zone inside the material was achieved by two independent techniques: (i) excavating the system layer by layer and (ii) Magnetic Resonance Imaging.

[1] T. Unger, Phys. Rev. Lett. 98, 018301 (2007). [2] T. Börzsönyi et al., Phys. Rev. E 80, 060302(R) (2009).

DY 22.10 Wed 16:30 HÜL 186

Tailoring the frictional properties of granular media — •Sonia Utermann[1,2], Philipp Aurin[1], Markus Benderoth[1], and Matthias Schröter[1] — [1]Max Planck Institute for Dynamics and Self-organization — [2]Georg-August-Universität Göttingen

Where the theorist often neglects friction, this most intriguing of granular interactions, the experimentalist cannot, and instead must embrace it. Here, we go a step further and develop a protocol which allows us to use friction between grains as an experimental control parameter. We present two simple chemical etching procedures which alter the roughness of soda-lime glass spheres: a procedure to smoothen the surface and one to roughen it. The roughness has an influence on the frictional properties of the grains because it alters the topology and size of the microscopic contacts between grains. We characterise the spheres using white light interferometry. Additional underwater angle-of-repose measurements on our etched samples give us a measure of frictional properties in the bulk.

DY 22.11 Wed 16:45 HÜL 186

Nanoindentation on sedimented colloids — •Marcel Roth[1], Carsten Schilde[2], Philipp Lellig[1], Arno Kwade[2], and Günter K. Auernhammer[1] — [1]MPI for Polymer Research, Mainz, Germany — [2]Institute for Particle Technology, TU Braunschweig, Germany

The mechanical properties of colloidal and granular matter depend on the mutual interplay of inter-particle forces as well as structural and material properties. While attractive forces are directly connected to the mechanical strength of the sample, particle rearrangements under gravity or external loads are critically affected by the particle density and surface properties.

In the present paper we investigate the mechanical properties of dense amorphous and semi-crystalline colloidal sediments made from monodisperse PMMA particles (diameter: $1.6\,\mu m$) via nanoindentation in combination with confocal microscopy. In doing so the bare mechanical data are complemented by three-dimensional trajectories of all particles during the indentation. Reorganization processes are identified and the average deformation field is calculated. Although the indent extension is only ten times larger than the particle size the deformation field of the amorphous structure is in reasonable agreement with the predictions from the continuum theory. In semi-crystalline assemblies heterogeneities and generation of dislocation defects are observed. As a consequence measured force-depth curves can be quantitatively analyzed with the theory of Oliver and Pharr to extract average values for hardness and effective elastic modulus characteristic for the tested structure.

DY 22.12 Wed 17:00 HÜL 186

Length scales of volume correlations in disk packings — •SongChuan Zhao and Matthias Schröter — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen

In a static granular packing particles influence their nearest neighbors e.g by force chains [1]. More recently, building on the ideas of Edwards and co-workers [2], experiments on the distribution of Voronoi volumes in 2D granular packing have found that the logarithm of the free volume distribution scales in a non-extensive way with the cluster size. This implies the existence of the correlation between Voronoi cells [3]. We present experimental data how the length of this correlation depends on packing fraction. We vary the packing fraction in the range 0.820˜0.838. Three length scales related to the correlation are identified. Two of them only appear for denser packing (> 0.826). They characterize anti-correlation between Voronoi volumes. One of them increases strongly with packing fraction.

[1] T.S. Majmudar, R.P. Behringer Nature (2005) 435:1079-1082
[2] S.F. Edwards and R.B.S. Oakeshott, Physica A, 157 1080 (1989)
[3] F. Lechenault, F. da Cruz, O. Dauchot and E. Bertin. J. Stat. Mech. (2006) P07009

DY 22.13 Wed 17:15 HÜL 186

Tagged particle dynamics close to the glass transition of a driven dissipative system — •Till Kranz[1,2], Matthias Sperl[3], and Annette Zippelius[1,2] — [1]Institut für Theoretische Physik, Göttingen — [2]MPI für Dynamik und Selbstorganisation, Göttingen — [3]Institut für Materialphysik im Weltraum, DLR Köln

In order to reach a steady state, granular (dissipative) systems need an external driving. One of the many possible methods is to fluidize the system by a fluctuating driving force. We have been able recently to establish the existence of a granular glass transition by extending mode coupling theory to nonequilibrium systems [1]. A similar extension of the mode coupling formalism for the incoherent scattering function $\phi_s(q,t)$ of a granular fluid shall be discussed in this contribution. Close to the critical density $\varphi_c(\epsilon)$, that depends on the coefficient of restitution ϵ, the incoherent scattering function $\phi_s(q,t)$ as well as the mean square displacement $\delta r^2(t)$ are found to exhibit a plateau for intermediate times. Related observables that are also meaningful for the nonequilibrium steady state of a granular fluid are the long time diffusion coefficient $D_\infty = \lim_{t\to\infty} \delta r^2(t)/t$ close to the glass transition and the localization length r_c at the glass transition. Evidence for a granular glass transition as indicated by the tagged particle dynamics has been found both in experiments and in simulations [2,3]. We will discuss our theoretical findings in relation to the experimental data.

[1] W. T. Kranz, M. Sperl and A. Zippelius, PRL **104**, 225701 (2010)
[2] A. R. Abate and D. J. Durian, PRE **74**, 031308 (2006)
[3] A. Fiege *et al.*, PRL **102**, 098001 (2009)

DY 22.14 Wed 17:30 HÜL 186

Superdiffusive, heterogeneous, and collective particle motion near the jamming transition in athermal disordered materials — •Claus Heussinger[1], Ludovic Berthier[2], and Jean-Louis Barrat[3] — [1]Institute for Theoretical Physics, University of Goettingen, Germany — [2]LCVN, Univ. Montpellier 2, France — [3]LPMCN, Univ. Lyon I, France

Many materials, from emulsions and suspensions to foams and granular materials are dense assemblies of non-Brownian particles. In these systems a fluid-to-solid "jamming" transition can be observed when the particle volume fraction is increased beyond a critical value. In this contribution, we use computer simulations to study the microscopic dynamics of an assembly of soft, frictionless particles near their jamming transition. We observe superdiffusive, spatially heterogeneous, and collective particle motion over a characteristic scale which displays a surprising non-monotonic behavior across the transition. Establishing a connection between single particle dynamics and collective particle motion, we develop an intuitive and appealing picture of jamming as the consequence of the diverging size of rigid particle clusters.

DY 22.15 Wed 17:45 HÜL 186

Jamming of frictional tetrahedra — •Max Neudecker[1], Stephan Ulrich[2], Stephan Herminghaus[1], and Matthias Schröter[1] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation, Bunsenstr. 10, 37073 Göttingen — [2]Universität Göttingen, Institut für theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen

We present experimental results on the packing of polypropylene tetrahedra with 7mm side length. Analysis via X-ray-tomography allows for a detailed analysis of the radial distribution function and the number and type of geometrical contacts. We focus particularly on the dependence of these packing properties on the bulk packing fraction.

DY 23: Nonlinear Waves/ Nonlinear Lattices

Time: Wednesday 14:00–16:15 Location: ZEU 255

Topical Talk DY 23.1 Wed 14:00 ZEU 255

Nonlinear waves in localizing media — •Sergej Flach — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany

Linear wave propagation is inhibited in a variety of structured media, such as disorder potentials (Anderson localization), Wannier-Stark ladders (Bloch oscillations), quantum kicked rotors (dynamical localization), and quasiperiodic potentials (Aubry-Andre localization). All cases were experimentally studied with light and/or matter waves, and confirmed the expected localization of waves. An additional nonlinear response couples the localized eigenmodes of the linear equations and makes them nonintegrable. Wave packets tend to spread subdiffusively. I will review recent theoretical studies of the dynamical details of wave packet spreading, and discuss recent experimental data obtained with interacting matter waves.

DY 23.2 Wed 14:30 ZEU 255

Strong and weak chaos regimes of wave spreading in nonlinear disordered media — •Tetyana Laptyeva, Joshua Bodyfelt, Dmitry Krimer, Charalampos Skokos, and Sergej Flach — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, D-01187 Dresden, Germany

The spreading behavior of multiple-site excitations was analyzed for anharmonic disordered 1-D lattices with cubic nonlinearity, where all linear modes are exponentially localized by disorder. Due to chaotic nonlinear interaction, the initial localization is destroyed and a finite part of the wave packet spreads subdiffusively [1]. In addition to our previous results [1], we find a qualitatively new dynamical regime, where the second moment m_2 of the wave packet grows as $t^{1/2}$, with a crossover to an asymptotic $t^{1/3}$ law at larger times [2]. This novel effect is attributed to the strong chaos regime, in contrast to the previously observed weak chaos. The crossover between the regimes is controlled by the ratio of the nonlinear frequency shift and the average eigenvalue spacing of the linear problem eigenstates within one localization volume. The details of these spreading regimes were analyzed using extensive numerical simulations over large times with ensemble averaging [2].

[1] S Flach DO Krimer Ch Skokos, Phys. Rev. Lett. **102**, 024101 (2009); Ch. Skokos DO Krimer S Komineas S Flach, Phys. Rev. E **79**, 056211 (2009)

[2] TV Laptyeva JD Bodyfelt DO Krimer Ch Skokos S Flach, EPL **91**, 30001 (2010)

DY 23.3 Wed 14:45 ZEU 255

A generalized spreading conjecture in $2D$ nonlinear disordered media — •Joshua Bodyfelt and Sergej Flach — Max Planck Institut für Physik komplexer Systeme, Dresden

It is generally accepted that the presence of nonlinearity in a random lattice couples the lattice's localized Anderson modes. This coupling then allows mode resonances, which in turn are responsible for spreading of initially compact, localized wavepackets. The spreading is measurable via several moments, all showing a characteristic subdiffusive behavior of t^{α}, where $\alpha < 1$. Numerical investigations confirm the validity of these measures, including a recent work [1] which discusses the novel appearance of a dynamical crossover from strong to weak resonances (please see talk by T.V. Laptyeva). The concept of a tunable nonlinearity (with power order of $\sigma > 0$) also holds great interest [2], in that a critical power order is observed seperating the two regimes of strong and weak resonances. However, these works mainly focus on $1D$ systems. Within [3] a generalization was made to multidimensional lattices, with resonances on a wavepacket's surface (as opposed to those within the internal volume) being claimed as the main mechanism for spreading. Here, we present for $2D$ lattices further numerical investigations into this claim.

[1] T.V. Laptyeva et al., *Europhys. Lett.* **91**, 30001 (2010).
[2] Ch. Skokos & S. Flach, *Phys. Rev. E* **82**, 016208 (2010); M. Mulansky & A. Pikovsky *Europhys. Lett.* **90**, 10015 (2010); H. Veksler et al., *Phys. Rev. E*, **80** 037201 (2009).
[3] S. Flach, *Chemical Physics* **375**, 548 (2010).

DY 23.4 Wed 15:00 ZEU 255

A Coupled-Map Lattice Model for the Puff-Slug-Transition in Turbulent Pipe Flow — Christian Marschler and •Jürgen Vollmer — Max Planck Institute for Dynamics and Self-Organizaton, 37073 Göttingen

Pipe flow shows long-lived localised turbulent regions (*puffs*) that are convected down the flow when increasing the Reynolds number $\mathrm{Re} = UL/\nu$ beyond $\mathrm{Re} \gtrsim 1500$. Here Re is the flow velocity U nondimensionalized by the pipe diameter L and the kinematic viscosity ν. Beyond $\mathrm{Re} \simeq 2300$ the turbulent regions start to grow in size. Eventually, they can fill macroscopic portions of the pipe. The resulting turbulent regions are called *slugs*. Recent experiments and simulations have provided a wealth of data on the life-time of puffs [1], and the structure and growth of slugs [2].

In order to contribute to understanding the nature of the transition from puffs to slugs, we constructed a coupled-map lattice where laminar flow is mimicked by a fixed point of the on-site dynamics, and turbulence amounts to long-lived chaotic structures that propagate through the lattice. In this model the transitions from puffs to slugs is related to an intermittency crisis of the dynamics. Implications for the interpretation of pipe-flow data will be given.

[1] B. Hof, et al, *Phys Rev Lett* **101** (2008) 214501.
[2] D. Moxey and D. Barkley, PNAS **107** (2010) 8091.

DY 23.5 Wed 15:15 ZEU 255

Controlling the non-equilibrium particle density in block-structured driven lattices — •Christoph Petri[1], Florian Lenz[1], Benno Liebchen[1], Fotis Diakonos[2], and Peter Schmelcher[1] — [1]Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Department of Physics, University of Athens, GR-15771 Athens, Greece

We study the dynamics of noninteracting particles loaded into a one-dimensional lattice formed by laterally oscillating barriers. By tuning parameters of the driven barriers it is possible to create blocks in the lattice with locally different transport or localization properties. At the interfaces between these blocks crossovers of trajectories from chaotic to ballistic dynamics and vice versa are observed. Thereby different time-scales are introduced which leave their hallmark in properties of the system like the spatial density of particles for an ensemble propagating in the lattice.

DY 23.6 Wed 15:30 ZEU 255

Using symmetry breaking for the directed transport of paramagnetic colloids on garnet films — •Saeedeh Aliaskarisohi[1], Tom.H Johansen[2], and Thomas.M Fischer[1] — [1]Institut für Experimentalphysik, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Department of Physics, University of Oslo, P.O.Box 1048, Blindern, 0316 Oslo, Norway

The transport behavior of paramagnetic particles on top of a ferrimagnetic garnet film is investigated in a modulated external magnetic field. Broken symmetries are required to direct the transport of the particles. We provide such symmetry breaking by tilting the external field modulation with respect to the garnet film normal and by the intrinsic geometrical symmetry breaking of the garnet film magnetic pattern. The interplay of both symmetry breaking mechanisms cause

a rich variety in transport behavior and direction. We corroborate our experimetal transport directions by comparing experimental with theoretical transport phase diagrams. Directing the transport of paramagnetic colloids will be useful when they are loaded with biomedical cargo on a magnetic lab-on-a-chip device.

DY 23.7 Wed 15:45 ZEU 255

Synchronization in monolayer transfer onto prepatterned substrates: A novel perspective for controlled nanopatterning of surfaces — •Michael H. Köpf, Svetlana V. Gurevich, and Rudolf Friedrich — Institut für Theoretische Physik, Universität Münster

Solid substrates can be endued with self-organized regular stripe patterns of nanoscopic lengthscale by Langmuir-Blodgett transfer of organic monolayers [1]. Here, we present an extension of the recent theoretical description of these phenomena [2,3], considering the effect of periodically prepatterned substrates on this process of spatiotemporal pattern formation. It leads to a time periodic forcing of the oscillatory behavior at the meniscus. Utilizing higher order synchronization with this forcing, complex periodic patterns of predefined wavelength can be created. The dependence of the synchronization on the amplitude and the wavelength of the wetting contrast is investigated in one and two spatial dimensions and the resulting patterns are discussed. Furthermore, the effect of prepatterned substrates on the pattern selection process is investigated [4].

[1] M. Gleiche, L. F. Chi, H. Fuchs, *Nature*, **403** (2000) 173-175

[2] M. H. Köpf, S. V. Gurevich, R. Friedrich, *EPL (Europhysics Letters)*, **86** (2009) 66003 (6 pages)

[3] M. H. Köpf, S. V. Gurevich, R. Friedrich, L. F. Chi, *Langmuir*, **26** (2010) 10444-10447

[4] M. H. Köpf, S. V. Gurevich, R. Friedrich, *submitted to PRE*, arXiv:1011.1140v1 [nlin.PS] (2010)

DY 23.8 Wed 16:00 ZEU 255

Lattice dynamics in the itinerant helical magnet MnSi — •Daniel Lamago[1,2], Evgeni Clementyev[3,4], Alexander Ivanov[5], Rolf Heid[1], Jean-Michel Mignot[2], A.E. Petrova[6], and Pavel A. Alekseev[3] — [1]Karslruhe Institut für Technologie (KIT), Institut fuer Festkoerperphysik, P.O.B. 3640, 76021 Karlsruhe, Germany — [2]Laboratoire Leon Brillouin, CEA Saclay, 91191 Gif sur Yvette Cedex, France — [3]ISSSPh, Russian Research Centre Kurchatov Institute, 123182 Moscow, Russia — [4]LNS, Institute for Nuclear Research, Russian Academy of Sciences, Troitsk, Moscow Region, Russia — [5]Institut Laue Langevin, 38042 Grenoble Cedex 9, France — [6]Institute for High Pressure Physics, Russian Academy of Sciences, Troitsk 142190, Moscow Region, Russia

The phonon dispersion relations in MnSi were measured using inelastic neutron scattering. At the same time, calculations of the lattice dynamics of MnSi were carried out in the framework of the density-functional theory using both the local-density and the generalized gradient approximations. The calculations match most of the phonon modes in the frequency range up to 40 meV, if they are performed using the experimental lattice constant. Spin-polarized calculations for ferromagnetic ground states result in subtle modifications of the dispersion curves, which further improve the description, in particular, for the acoustic branches.

DY 24: Focus Session: Computational Polymer Physics - New Developments (jointly with CPP)

Time: Wednesday 14:00–16:45 Location: MOL 213

Invited Talk DY 24.1 Wed 14:00 MOL 213

Multiscale Simulation of Soft Matter: Challenges — •Florian Müller-Plathe — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie and Centre of Smart Interfaces, Technische Universität Darmstadt, Germany

Systematic coarse-graining approaches to the simulation of soft materials are now commonplace. Structural coarse-graining can be performed by a variety of methods such as Iterative Boltzmann Inversion and Force Matching. There remain, however, substantial challenges to the coarse-grained models, such as: (i) Dynamical properties. Current structure based coarse-graining methods predict too fast mobilities. (ii) Scale-bridging between particle models (e.g molecular dynamics) and continuum models (e.g. finite elements). (iii) The application of coarse-graining techniques to real-world problems. This lecture will highlight the challenges and survey approaches to overcome them.

Invited Talk DY 24.2 Wed 14:30 MOL 213

A self-consistent field approach for crosslinked polymer materials — •Friederike Schmid — KOMET 331, Institut fuer Physik, JGU Mainz

The Self-Consistent Field (SCF) theory is one of the most powerful approaches to studying inhomogeneous polymer melts and solutions. It is nowadays a standard method to calculate nanoscale structures at polymer-coated surfaces or at interfaces in polymer mixtures, self-organization of amphiphilic polymers, phase transitions between block copolymer mesophases, to name just a few examples. However, the original SCF theory has a major drawback: It can only treat polymeric fluids. Many polymeric materials have a network structure, which means that they respond elastically to stress and that deformations are restored. In the talk, a generalized SCF theory for networks shall be proposed. As a first application, it is used to study the effect of crosslinking on the order-disorder transition in ordered lamellar block copolymer phases.

Invited Talk DY 24.3 Wed 15:00 MOL 213

Mechanical separation of short double stranded DNA: Effect of pulling geometry — •Sanjay Kumar — Department of Physics, Banaras Hindu University, Varanasi 221 005, India

Using the Exact Enumeration technique and Molecular Dynamics simulation, we study the influence of force on the melting of DNA. A force is applied perpendicular to the helix direction to study the DNA unzipping. The force-temperature diagram is consistent with the experiment but differs significantly with the theoretical predictions. However, when a force is applied along the helix direction, we have a situation similar to the DNA rupture. We show that the rupture force increases linearly with the chain length and approaches to the asymptotic value. This is consistent with the experiment. We also observed that the rupture force depends logarithmically on the loading rate. It was found that below a certain loading rate, rupture force decreases with temperature, whereas above it, increases with temperature. Using phenomenological argument, we explain why the rupture force has distinctively different behavior for two temperatures above and below a certain loading rate. We substantiate our argument with the simulation.

15 min. break

Invited Talk DY 24.4 Wed 15:45 MOL 213

Soft coarse-grained models for multi-component polymer melts — •Marcus Müller — Institut für Theoretische Physik, Georg-August-Universität, Göttingen, Germany

The universal equilibrium properties of dense multi-component polymer systems can be described by minimal coarse-grained models that only incorporate the relevant interactions – connectivity along the molecular backbone, limited compressibility of the polymer liquid, and repulsion between unlike segment species – via simple potentials. In such a model an effective segment corresponds to many monomeric repeat units of a chemically realistic representation and the interactions between effective segments are soft. This large degree of coarse-graining allows for a computationally efficient description of large three-dimensional systems characterized by a large invariant degree of polymerization.

I will discuss simulation techniques for studying the structure formation in block copolymer materials and illustrate the advantages and limitations of this coarse-grained description.

Invited Talk DY 24.5 Wed 16:15 MOL 213

Simulations of Polymer Electrolytes for Lithium-Ion Batteries Highly Accurate Polarizable Potentials — •Grant Smith — University of Utah, Salt Lake City, UT, USA

There is increasing interest in using polymer electrolytes for secondary lithium batteries due to improved safety and mechanical properties compared to conventional electrolytes based on organic solvents. In polymer electrolytes a lithium salt is dissolved in a polymer matrix. In principle molecular dynamics (MD) simulations can provide important insight into the mechanism of Li+ cation coordination and transport in polymer electrolytes, facilitating the development of materials with improved properties. Such simulations require the development of potential energy functions, or force fields, that are able to faithfully reproduce polymer-polymer, salt-polymer and salt-salt interactions. We have developed such potentials based upon high-level quantum chemistry studies of model compounds, and have found that the inclusion of polarization effects is critical in obtaining an accurate description of polymer electrolytes. I will discuss the nature of these potentials as well as insights into polymer electrolytes we have gained through extensive MD simulations utilizing them.

DY 25: Networks: From Topology to Dynamics III (with BP, SOE)

Time: Wednesday 15:30–17:00 Location: GÖR 226

DY 25.1 Wed 15:30 GÖR 226

Traveling Salesman Problem with Clustering — •Johannes Josef Schneider[1], Thomas Bukur[2], and Antje Krause[2] — [1]Department of Physics, Mathematics, and Computer Science, Johannes Gutenberg University of Mainz, Staudinger Weg 7, 55099 Mainz, Germany — [2]Fachhochschule Bingen – University of Applied Sciences, 55411 Bingen, Germany

In the original traveling salesman problem, the traveling salesman has the task to find the shortest closed tour through a proposed set of nodes, touching each node exactly once and returning to the initial node at the end. For the sake of the tour length to be minimized, nodes close to each other might not be visited one after the other but separated in the tour. However, for some practical applications, it is useful to group nodes to clusters, such that all nodes of a cluster are visited contiguously. Here we present an approach which leads to an automatic clustering with a clustering parameter governing the sizes of the clusters.

[1] Johannes J. Schneider, Thomas Bukur, and Antje Krause, Traveling Salesman Problem with Clustering, J. Stat. Phys. 141, 767-784, 2010.

DY 25.2 Wed 15:45 GÖR 226

Importance of Industrial Sectors within the Overall Economy — •Christian Hirtreiter[1] and Johannes Josef Schneider[2] — [1]Faculty of Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, Mathematics, and Computer Science, Staudinger Weg 7, 55099 Mainz, Germany

We have a look at the overall economy of a state focussing on the exchange of goods and services between the various sectors of that economy. Depending on the market theory, either the best seller (the sector selling the largest value of goods and services to other sectors) or the best buyer (the sector buying the largest value of goods and services from other sectors) is the most important sector within the overall economy. We generate a sequence of sectors depending on their importance using the exchange matrix between these sectors. Furthermore, we show that this problem is an extreme case of the Traveling Salesman Problem with Clustering, which was recently introduced by us [1].

[1] Johannes J. Schneider, Thomas Bukur, and Antje Krause, Traveling Salesman Problem with Clustering, J. Stat. Phys. 141, 767-784, 2010.

DY 25.3 Wed 16:00 GÖR 226

Emergent bipartiteness in an adaptive social network — •Charo Del Genio and Thilo Gross — Max-Planck-Institut für Physik komplexer Systeme – Nöthnitzer Straße 38 – D-01187 Dresden – Deutschland

Representing complex systems as adaptive networks has become a very important method for analysing the properties of many real-world networks, with fields of application ranging from epidemiology to the Internet to social sciences.

We present a model of a social network in which the nodes belong to two different species, which we call "truthfuls" (T) and "liars" (L) and the existence or permanence of a link between next-neighbouring nodes is determined by the "advice" of the common neighbour. In particular, an agent node connects to one of its next-neighbours, or maintains a link with it, if the common neighbour reports the target node as truthful. Vice versa, the link is removed if the common neighbour reports the target node as a liar. Also, truthfuls always state the real species of a target node, while liars always report the false.

We show that if the fractions of truthfuls and liars are close enough, the network self organizes in a perfectly bipartite graph. On the other hand, if the excess of one of the two species is greater than a size-dependent critical value, the network splits into two components, of which one is bipartite and the other contains only the excess species and is densely connected.

DY 25.4 Wed 16:15 GÖR 226

The emergence of critical behavior in evolving economies — João da Cruz[1,2] and •Pedro Lind[1,3] — [1]Departamento de Física, Faculdade de Ciências da Universidade de Lisboa, 1649-003 Lisboa, Portugal — [2]Closer Consultoria Lda, Avenida Engenheiro Duarte Pacheco, Torre 2, 14^o-C, 1070-102 Lisboa, Portugal — [3]Center for Theoretical and Computational Physics, University of Lisbon, Av. Prof. Gama Pinto 2, 1649-003 Lisbon, Portugal

We address the controversy in the study of financial systems, sometimes taken as brownian-like processes and other as critical systems with fluctuations of arbitrary magnitude, by introducing a model of financial networks which reproduces critical behavior. The model considers a collection of economical agents which establish trade connections among them according to basic economical principles properly translated into physical properties and interaction. Agents accumulate asset or liability by means of internal energy storage, as a product of energy balance that takes into account the labor performed by the agent and the payment it gets in return. With such model we are able to reproduce the evolution of macroscopic quantities, namely the logarithmic return of the total internal energy taken as a financial index. Furthermore, we correctly retrieve the common exponent value characterizing several indices in financial markets.

DY 25.5 Wed 16:30 GÖR 226

Evolutionary dynamics and conditional cooperation in the iterated prisoner's dilemma — •Jelena Grujić, José A. Cuesta, and Angel Sánchez — Grupo Interdisciplinar de Sistemas Complejos (GISC), Departamento de Matemáticas, Universidad Carlos III de Madrid, Leganés, Madrid, Spain,

We have recently performed an experiment to test the emergence of cooperation in the presence of an underlying structure [Grujic et al., PLoS ONE 5(11): e13749 (2010)]. Human subjects played a PD with each of their neighbors in a 13x13 square lattice. The results show that the population consisted of cooperators and defectors, who respectively cooperate or defect with high probability regardless of their and their neighbors' previous actions, and conditional cooperators, whose behavior does depend on those previous actions.

Here we take a first step towards an evolutionary explanation of the experimental results. Specifically, we use replicator dynamics to describe the evolution of a set of strategies that mimics the observations, in a simplified context consisting of a well-mixed population of players confronted in iterated Prisoner's Dilemma games. The dynamics exhibits two attractors: one for a population consisting only of defectors, and an interior point with population frequencies comparable to those observed in the experiment. The former has a much smaller basin of attraction than the latter, which therefore becomes the most probable evolutionary outcome. This is the first hint that the experiment may be amenable to an evolutionarily explanation.

DY 25.6 Wed 16:45 GÖR 226

The role of short-cuts for the emergence of cooperation in random topologies. — •Daniele Vilone[1], Angel Sánchez[1], and Jesús Gómez-Gardeñes[2] — [1]GISC - Mathematics Department, Universidad Carlos III de Madrid, Spain — [2]Biocomputation and Complex Systems Institute, Universidad de Zaragoza, Spain

We present a detailed study about the role of the short-cuts of a net-

work in promoting the emergence of cooperation in a population of agents playing the Prisoner's Dilemma Game (PDG). We introduce a model which allows to tune the topology of the system from the one-dimensional euclidean lattice (a ring) to the complete graph just changing the value of one parameter (the probability p to add a link between two nodes not already connected in the euclidean configuration). We show that there is a region of values of p in which cooperation is largely enhanced, whilst for smaller values of p only a few cooperators are present in the final state, and for p->1 cooperation is totally suppressed. We present analytical arguments that provide a very plausible interpretation of the simulation results. Our work makes it clear how short-cuts can be decisive in promoting (or suppressing) cooperation in the absence of other mechanisms such as clustering. Implications for other dynamics are also drawn.

DY 26: Nonlinear Dynamics II

Time: Wednesday 16:30–18:15 Location: ZEU 255

DY 26.1 Wed 16:30 ZEU 255

Nonlinear dynamics of the internal degrees of freedom and transport of benzene on graphite — •Astrid S. de Wijn — IMM, Radboud University Nijmegen, the Netherlands

The presence of internal degrees of freedom has been connected to the diffusion and friction of molecules on surfaces. In this work, the chaotic internal degrees of freedom of a benzene molecule adsorbed on a graphite substrate [1], their interplay with thermal noise, and their effects on the diffusion and friction are investigated analytically and numerically by making use of the presence of two different time scales. It is found that that the substrate temperature affects the dynamics of the internal degrees of freedom only weakly, yet still influences the friction and diffusion.

The contributions from different degrees of freedom to diffusion and friction are identified analytically and numerically and found to be sufficiently large to account for the high friction found in experiments [2]. In atomistic molecular dynamics simulations of the system, various internal degrees of freedom can be investigated separately. Torsion of the benzene molecule dominates the chaotic dynamics and the effects of the internal degrees of freedom on the diffusion and friction. Based on the analytical and numerical results, suggestions are made for experimental conditions under which the effects of internal degrees of freedom might be more directly observable.

[1] A. S. de Wijn and A. Fasolino, Journal of Physics: Condensed Matter, 21, 264002 (2009).

[2] H. Hedgeland, er al., Nature Physics, 5, 561 (2009).

DY 26.2 Wed 16:45 ZEU 255

Asymmetries in delay coupled systems: mismatches and their impact on dynamics and synchronization of two coupled lasers — •Konstantin Hicke[1,2], Otti D'Huys[3], Valentin Flunkert[2], Eckehard Schöll[2], Jan Danckaert[3,4], and Ingo Fischer[1] — [1]Instituto de Fisica Interdisciplinar y Sistemas Complejos, IFISC (UIB-CSIC), Campus Universitat de les Illes Balears, E-07122 Palma de Mallorca, Spain — [2]Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [3]Department of Physics (DNTK), Vrije Universiteit Brussel, Pleinlaan 2, 1050 Brussel, Belgium — [4]Department of Applied Physics and Photonics (TONA), Vrije Universiteit Brussel, Pleinlaan 2, 1050 Brussel, Belgium

We study the dynamics and synchronization properties of two mutually delay-coupled semiconductor lasers. We concentrate on a configuration in which the lasers are coherently coupled via a partially transparent mirror. We investigate the influence of mismatches of the delay times and of the coupling strengths for self-feedback and coupling. We show that the former mismatch alters the lasers' dynamics significantly but does not affect the synchronization quality. The latter mismatch has a considerable effect on the stability of the zero-lag synchronized state of the system, but does not change the dynamics within the synchronization manifold. Finally, we discuss the implications of our analytical and numerical results.

DY 26.3 Wed 17:00 ZEU 255

Leaking chaotic systems — •Jefferson S. E. Portela[1], Eduardo G. Altmann[1], and Tamás Tél[2] — [1]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Institute for Theoretical Physics, Eötvös University, Pázmány P. s. 1/A, Budapest, H–1117, Hungary

A large class of problems have been addressed by relating the properties of a closed dynamical system, where the main dynamical properties are well defined asymptotically in time, to the relevant properties of its open, leaked counterpart, where typically all trajectories eventually escape and the relevant quantities are dependent on the escape procedure, as described by transient chaos theory.

Using a billiard – a system of point particles moving freely inside a bounded area and colliding specularly with its boundary – we illustrate the effects of a leak, emphasizing the dependence of the orbits decay on the leak characteristics.

Billiards model a number of relevant physical systems, such as optical microcavities and wave/quantum-chaos systems, and also are, due to their symmetries, particularly convenient for numerical simulation and visualization purposes. We consider the family of Robnik billiards, defined by limaçon curves ($\rho(\phi) = 1 + \varepsilon\cos(\phi)$, in polar coordinates), which has already been extensively studied in both its classical and quantum versions.

DY 26.4 Wed 17:15 ZEU 255

The Geometry of Chaotic Dynamics - A Complex Network Perspective — •Reik V. Donner[1], Jobst Heitzig[1], Jonathan F. Donges[1,2], Yong Zou[1], Norbert Marwan[1], and Jürgen Kurths[1,2] — [1]Potsdam Institute for Climate Impact Research, Potsdam, Germany — [2]Department of Physics, Humboldt University of Berlin, Germany

Among the different existing complex network approaches to time series analysis, ε-recurrence networks most faithfully represent the geometrical fine structure of the underlying chaotic attractors. We demonstrate that the well known graph theoretical properties local clustering coefficient and global network transitivity can meaningfully be exploited to define new local and global measures of dimension in phase space. Rigorous analytical as well as numerical results for self-similar sets and simple chaotic model systems suggest that these measures are well-behaved in most non-pathological situations and that they can be estimated reasonably well using ε-recurrence networks constructed from relatively short time series. These findings theoretically explain why the networks' transitivity properties are particularly well suited for identifying dynamically invariant objects as well as regime shifts in non-stationary time series. Our results demonstrate that ε-recurrence networks exhibit an important link between dynamical systems and graph theory.

DY 26.5 Wed 17:30 ZEU 255

Algorithms for the integration of variational equations of multidimensional Hamiltonian systems — Enrico Gerlach[1], Siegfried Eggl[2], and •Charalampos Skokos[3] — [1]Lohrmann Observatory, Technical University Dresden, D-01062 Dresden, Germany — [2]Institute for Astronomy, University of Vienna, Türkenschanzstrasse 17,A-1180 Vienna, Austria — [3]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, D-01187 Dresden, Germany

We investigate the efficiency of different algorithms for the integration of the variational equations of multidimensional Hamiltonian systems. In particular we consider the tangent map (TM) method (Skokos Ch. and Gerlach E., 2010, PRE, 82, 036704 - Gerlach E. and Skokos Ch., 2010, arXiv:nlin.CD/1008.1890), a scheme based on symplectic integration techniques, as well as non-symplectic schemes, like the DOP853 general-purpose integrator and methods based on Taylor and Lie expansions. The numerical verification of well-known properties of chaos indicators like the Lyapunov Characteristic Exponents (LCEs) and the Generalized Alignment Indices (GALIs) is used for characterizing the efficiency of the various integration schemes. Besides discussing the methods theoretically, we will apply them exemplarily to the Fermi-Pasta-Ulam (FPU) β lattice model and to an astronomical N body problem to demonstrate the differences between them regarding parameters of practical importance, as e.g. CPU time requirements and reliability of the results.

DY 26.6 Wed 17:45 ZEU 255

Conditional Mutual Sorting Information for Coupling Analysis of Time Series — •Jakob Runge[1] and Bernd Pompe[2] — [1]Potsdam-Institut für Klimafolgenforschung — [2]Universität Greifswald

We propose a method to detect couplings between two simultaneously measured time series. It is based on conditional mutual sorting information. By setting suitable conditions, we are able to diminish misleading effects of auto dependencies within each series. This enables the detection of the right coupling delays also in the case of bidirectional couplings. Our approach is based on ordinal properties of time series. This makes the analysis invariant with respect to monotonous distortions which is very useful, e.g., in the analysis of proxy data in climatology. Moreover, ordinal analysis is robust to some trend, and easy and fast to compute. We consider also the problem of reliable estimation from finite time series. Finally, we apply the proposed method to nonlinear models as well as to some climate data.

DY 26.7 Wed 18:00 ZEU 255

Effects of Janus particles in a phase-separating binary mixture — Alexei Krekhov, •Vanessa Weith, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany

A new class of colloidal particles, so-called Janus particles, have been synthesized in large quantities [1], recently. Janus particles represent colloids with a different chemical composition of the surface of the two hemispheres of a particle. Each half of a particle may be wetted preferentially by one component of a binary mixture.

We suggest a mean field approach for the dynamics of phase separation in binary mixtures in the presence of Janus particles. The numerical results on the dynamics of Janus particles are presented. The different wetting properties of the two hemispheres of a Janus particle cause a spatial variation of the concentration in their neighborhood. Accordingly, the Janus particles are trapped to interfaces in the two-phase region, leading to a complex particle and interface dynamics. The Janus particles also induce an interesting interface ordering in one and two dimensions, leading to layered structures with small tunable length scale.

[1] A. Walther and A. H. E. Müller, Soft Matter 4, 663 (2008)

DY 27: ISS Transport and Localization of Interacting Bosons I

Time: Wednesday 16:30–18:00 Location: HSZ 02

DY 27.1 Wed 16:30 HSZ 02

Observation of Absolute Negative Mobility in Driven Quantum Systems — •Tobias Salger[1], Sebastian Kling[1], Sergey Denisov[2], Alexey Ponomarev[2], Peter Hänggi[2], and Martin Weitz[1] — [1]Institut für Angewandte Physik, Wegelerstrasse 8, 53115 Bonn — [2]Institut für Physik, Universitätsstrasse 1, 86135 Augsburg

Here we report on the observation of absolute negative mobility (ANM) of a Bose-Einstein condensate in an ac-driven quantum system. This effect describes the paradoxial situation, when the motion of a particle is always in oppositve direction to an applied external gradient field. Based on successful experiments, demonstrating a directed motion of a Bose-Einstein condensate in a Hamiltonian quantum ratchet, we investigate the dynamics of atoms when exerted to an external bias field [1].

Up to now, the presence of strong decoherence mechanisms has been considered to be crucial for absolute negative mobility [2]. However here we demonstrate for the first time that this phenomenon can also be observed in a coherent quantum system. Our experimental results are in good agreement with a theoretical model, based on numerical simulations.

[1] T. Salger et al., Science **326**, 1241 (2009)
[2] A. Ros et al., Nature **436**, 928 (2005)

DY 27.2 Wed 16:45 HSZ 02

Direct observation of quasi-local relaxation with strongly correlated bosons in an optical lattice — •Stefan Trotzky[1,2,3], Yu-Ao Chen[1,2,3], Andreas Flesch[4], Ian P. McCulloch[5], Ulrich Schollwöck[1,6], Jens Eisert[6,7], and Immanuel Bloch[1,2,3] — [1]Ludwig-Maximilians Universität München — [2]MPI für Quantenoptik, Garching — [3]Johannes-Gutenberg Universität Mainz — [4]Forschungszentrum Jülich — [5]University of Queensland — [6]Institute for Advanced Study, Berlin — [7]Universität Potsdam

The question of how closed quantum systems far from equilibrium come to rest lies at the heart of statistical mechanics. We report the experimental observation of the relaxation dynamics of a one-dimensional bosonic density wave in an optical lattice. Using an optical superlattice, we are able to load Bose-Hubbard chains with each second lattice site occupied. Furthermore, the superlattice allows us to monitor the non-equilibrium dynamics emerging after rapidly switching on the tunnel coupling along the chain in terms of quasi-local densities, currents and correlations. We find a rapid relaxation of all these quantities to steady-state values compatible with those of a maximum entropy state. We compare the experimental results to parameter free time-dependent DMRG simulations, finding excellent agreement. The system thus can be seen as an accurate dynamical quantum simulator for the systematic study of equilibration phenomena in strongly correlated many-body systems.

DY 27.3 Wed 17:00 HSZ 02

Observation of subdiffusion of a disordered interacting system — •Eleonora Lucioni[1], Benjamin Deissler[1], Luca Tanzi[1], Chiara D'Errico[1], Giacomo Roati[1], Matteo Zaccanti[1,2], Michele Modugno[1,3], Massimo Inguscio[1], and Giovanni Modugno[1] — [1]LENS and Università di Firenze, and CNR-INO, Italy — [2]Institut für Quantenoptik und Quanteninformation, Innsbruck, Austria — [3]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain

We study the transport dynamics of matter-waves in the presence of disorder and non-linearity. A Bose-Einstein Condensate of 39K atoms is let free to expand in a quasiperiodic lattice realized by superimposing two laser beams of incommensurate wavelength in standing wave configuration. By means of a broad magnetic Feshbach resonance it is possible to tune the scattering length between atoms at will. In the noninteracting case this system is an experimental realization of the Aubry-André model: if the disorder is strong enough, the system is localized and no expansion is permitted (Anderson localization).

The presence of a weak repulsive interaction allows the coupling between orthogonal localized single particle states and destroys localization. In this case we observe a change of shape of the atomic cloud during the expansion and a slow increase of the width σ of the sample that follows a subdiffusive law: $\sigma(t) \propto t^{\alpha}$, with $\alpha = 0.2 - 0.4$. We find that the exponent increases with the initial interaction energy and the localization length.

DY 27.4 Wed 17:15 HSZ 02

Coherent transport of a BEC in the presence of disorder and nonlinearity — •Tobias Geiger, Thomas Wellens, and Andreas Buchleitner — Physikalisches Institut der Universitaet Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg

For a dilute cloud of weakly interacting ultracold bosons subject to a random disorder potential, the Gross-Pitaevskii equation, in its limits, produces reliable results. However, for increasing amounts of disorder and interaction, the stationary solution of the mean field description [1] – and eventually also the mean field description itself – breaks down.

In our approach, we treat the full bosonic N-body problem microscopically in a nonlinear scattering setup. By employing a diagrammatic technique relying on the assumption of a weakly scattering disorder potential [2], one is in principle able to sum up all different orders of the nonlinear scattering series.

Here, we present first preliminary results of different scattering orders and compare them to findings predicted by the Gross-Pitaevskii equation.

[1] T. Paul, M. Albert, P. Schlagheck, P. Leboeuf, and N. Pavloff, Phys. Rev. A **80**, 033615 (2009)
[2] T. Wellens and B. Grémaud, Phys. Rev. A **80**, 063827 (2009)

DY 27.5 Wed 17:30 HSZ 02

Interaction-based reduction of weak localization in coherent

transport of Bose Einstein Condensates — •Josef Michl[1], Timo Hartmann[1], Juan Diego Urbina[1], Cyril Petitjean[2], Thomas Wellens[3], Peter Schlagheck[4], and Klaus Richter[1] — [1]Institute of Theoretical Physics, University of Regensburg, Germany — [2]SPSMS-INAC-CEA, Grenoble, France — [3]Physics Department, University of Fribourg, Switzerland — [4]Physics Department, University of Liège, Belgium

Based on the Gross-Pitaevskii-equation, we investigate reflection amplitudes and reflection probabilities in the transport of coherent bosonic matter waves through a fully-chaotic two-dimensional billiard-system. Like in the case of electronic transport, one can observe the effect of weak-localization in this setting. Our interest lies now in the influence of a weak interaction between particles on the weak-localization-peak and its behaviour in the presence of a weak magnetic field in the billiard.

Numerical results on this topic predict a reduction of the weak-localization-peak for small magnetic fields and a vanishing influence of the interaction with an increasing one. Trying to explain that, an analytical technique based on a semiclassical treatment in form of a diagrammatic perturbation theory in the parameter representing the interaction will be presented. Its results are compared to the numerical findings.

DY 27.6 Wed 17:45 HSZ 02

Anderson orthogonality catastrophe in ultracold quantum gases — •Daniel Kotik[1], Martina Hentschel[1], and Walter Strunz[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 83, 01187 Dresden — [2]Institut für Theoretische Physik, TU Dresden, 01062 Dresden

Ultracold quantum gases have attracted a lot of attention in recent years, not least due to their exquisite experimental control and the resulting versatile possibilities to manipulate them.

Here, we study impurity potentials in ultracold bosonic quantum gases and specifically in their Bose-Einstein condensed phase, that result, e.g., from unavoidable defects contained in the material or from deliberately placed perturbations. Our emphasis will be on spatio-temporal perturbations that are suddenly switched-on and spatially localized, as can be realized by switching on an additional laser beam. The many-body response of the quantum gas to this impurity potential is studied numerically and analytically.

We will pay particular attention to the consideration of the bosonic analogue known from solid state theory as Anderson orthogonality catastrophe.

DY 28: Statistical Physics far from Equilibrium

Time: Thursday 10:15–13:15 Location: HÜL 186

DY 28.1 Thu 10:15 HÜL 186

Nonequilibrium steady states in contact: Approximate thermodynamic structure and zeroth law for driven lattice gases — •Punyabrata Pradhan, Christian Amann, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

We explore a class of nonequilibrium systems, called driven lattice gases, for the existence of an intensive thermodynamic variable which could determine "equilibration" between two such nonequilibrium systems kept in weak contact [1]. We numerically check that there exists an intensive thermodynamic variable, like equilibrium chemical potential, which equalize in the final "equilibrated" steady state when two initially separated driven lattice gases are brought into contact and allowed to exchange particles with total number of particles conserved. We find that these systems satisfy surprisingly simple thermodynamic laws, such as the zeroth law and the fluctuation-response relation between the particle-number fluctuation and the corresponding susceptibility remarkably well. However at higher densities, small but observable deviations from these laws occur due to nontrivial contact dynamics and the presence of long-range spatial correlations.

Reference: [1] P. Pradhan, C. P. Amann and U. Seifert, Phys. Rev. Lett. **105**, 150601 (2010).

DY 28.2 Thu 10:30 HÜL 186

Crooks fluctuation theorem for the fluctuating lattice-Boltzmann model — •Léo Granger[1], Markus Niemann[2], and Holger Kantz[1] — [1]Max Planck Institut für Physik komplexer Systeme, Dresden, Germany — [2]Carl von Ossietzky Universität Oldenburg, Institut für Physik, Oldenburg, Germany

We probe the validity of Crooks' fluctuation relation on the fluctuating lattice-Boltzmann model (FLBM), a highly simplified lattice model for a thermal ideal gas. Crooks' relation is one of the only rigorous results known about non-equilibrium thermodynamics. It links a dynamic quantity, the probability to perform a certain amount of work during a non quasi-static process, to a thermodynamic quantity, the difference in equilibrium free energy between the initial and the final states.

We simulate am ideal gas submitted to a force field. By gradually switching on and off the force field, we drive the system frome one thermondynamic equilibrium state to another, performing some work on the gas. By comparing the distributions of the work performed during the forward driving and time reversed driving, we show that the system satisfies Crooks' relation.

DY 28.3 Thu 10:45 HÜL 186

Investigations of unconventional quantum statistics in isolated spin clusters — •Kai Ji and Boris Fine — Institute for Theoretical Physics, University of Heidelberg, Philosophenweg 19, 69120 Heidelberg, Germany

Quantum micro-canonical (QMC) ensemble refers to an isolated quantum system with fixed average energy but unrestricted participation of eigenstates. The QMC ensemble reveals marked deviation from the conventional Boltzmann-Gibbs (BG) statistics [1]. In this work, based on an anisotropic Heisenberg model, we perform numeral investigations on the statistics of QMC ensemble and discuss the physical realization of it in isolated spin clusters. The exploration for superpositions of quantum states in the Hilbert space is proposed to be driven by strong perturbations with a series of magnetic pulses. It is demonstrated that starting from a BG distribution, the occupation numbers universally evolve to the distribution obtained in Ref. [1] before reaching the infinite temperature limit, indicating the onset of QMC ensemble. Possible ways for detecting the established QMC ensemble is to be addressed as well.

[1] B.V. Fine, Phys. Rev. E 80, 051130 (2009).

DY 28.4 Thu 11:00 HÜL 186

Nonequilibrium entropy production for open quantum systems — •Sebastian Deffner and Eric Lutz — Department of Physics, University of Augsburg, D-86135 Augsburg, Germany

We consider a driven quantum system weakly coupled to a thermal environment. We provide a microscopic expression for the irreversible entropy production for general far from equilibrium processes and show that it fulfills an integral fluctuation theorem. Our derivation is solely based on thermodynamic arguments and does not rely on master equations or quantum trajectories.

DY 28.5 Thu 11:15 HÜL 186

Absence of Boltzmann-Gibbs equilibrium in an isolated quantum system with fixed energy and unrestricted participation of eigenstates. — •Boris Fine — Institute for Theoretical Physics, University of Heidelberg, 69120 Heidelberg, Germany

Usual approach to the foundations of quantum statistical physics is based on conventional micro-canonical ensemble as a starting point for deriving Boltzmann- Gibbs (BG) equilibrium. It leaves, however, a number of conceptual and practical questions unanswered. Here we discuss these questions, thereby motivating the study of a natural alternative known as Quantum Micro-Canonical (QMC) ensemble. The QMC ensemble includes all possible superpositions of eigenstates of a large isolated quantum system provided all these superpositions have the same energy expectation value. We obtain analytically the statistics associated with the QMC ensemble for both the entire system and its small subsystem[1]. In a significant departure from the BG statistics, the average occupation numbers of quantum states exhibit in the present case weak algebraic dependence on energy. In the macroscopic

limit, this dependence is routinely accompanied by the condensation into the lowest-energy quantum state. The above unconventional kind of equilibrium may be realizable after strong perturbations in small isolated quantum systems having large number of levels. We further suggest that the reason, why BG equilibrium commonly occurs in nature rather than the QMC-type equilibrium, has something to do with the notion of quantum collapse. [1] B.V. Fine, Phys. Rev. E v.80, p. 051130 (2009).

DY 28.6 Thu 11:30 HÜL 186

Monte-Carlo sampling of energy-constrained quantum superpositions in high-dimensional Hilbert spaces — •Frank Hantschel and Boris Fine — Institute for Theoretical Physics, Heidelberg, Germany

The quantum microcanonical (QMC) ensemble is an alternative to conventional statistical ensembles, which results in a deviation from the usual Gibbs distribution. The resulting statistics is computed by performing a Monte-Carlo simulation on high-dimensional Hilbert space.

A straightforward Monte-Carlo routine would enclose the energy constrained manifold within a larger manifold, which is easy to sample, e.g., a hypercube. We observed that the efficiency of such a sampling routine decreases exponentially with the increase of the dimension of the Hilbert space, because the volume of the enclosing manifold becomes exponentially larger than the volume of the manifold of interest. This fact imposes a problem, because it strongly limits the size of the system of interest.

The talk explores the ways to optimize the above routine by varying the shapes of the manifolds enclosing the energy-constrained manifold. The resulting improvement in the sampling efficiency is about a factor of five for a 14-dimensional Hilbert space. The advantage of the above algorithm is that it does not compromise on the rigorous statistical nature of the sampling outcome and hence can be used to test other more sophisticated Monte-Carlo routines. The present attempts to optimize the enclosing manifolds also bring insights into the geometrical properties of the energy-constrained manifold itself.

15 min. break.

DY 28.7 Thu 12:00 HÜL 186

Non-perturbative renormalization of a diffusion-limited decay process — •Anton Winkler and Erwin Frey — Arnold Sommerfeld Center and CeNS, Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, 80333 München, Germany

Many quantitative results for stochastic processes are restricted to one dimension, where a plethora of methods is available. However, in higher dimensions they often fail. Furthermore, the major part of renormalization group analysis focuses on low dimensions, i.e. lower than or equal to the upper critical dimension. For magnetic $O(n)$ models this is of course very reasonable since in this case the upper critical dimension is four.

In our work we have studied the decay process $A + A \to 0$ in the framework of reaction diffusion processes. The critical dimension of our decay process is two. In three dimensions, fluctuations are not strong enough to obliterate the microscopic structure of space and the shape of the particles. This poses a problem to the usual perturbative approach because it works best for studying universal features.

Our non-perturbative approach is known to cope also with non-universal properties. It allowed us to tackle the intriguing question of how the microscopic structure enters the dynamics of the process in three and higher dimensions by providing exact results for the non-equilibrium Gibbs energy.

DY 28.8 Thu 12:15 HÜL 186

The influence of temperature gradients on protein folding — •Bernhard Reuter[1], Pedro Ojeda-May[2], and Martin E. Garcia[1] — [1]Universität Kassel, Fachbereich Naturwissenschaften, Institut für Theoretische Physik, Heinrich-Plett-Straße 40, 34132 Kassel, Germany — [2]Institute for Computational Physics, Universität Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany

Using Monte Carlo techniques in the framework of the lattice model we addressed the folding of proteins under extreme temperature gradients.

This analysis is inspired by the recent work of Zia [Zia et al., EPL, 89 (2010) 50001] in which a 2D Ising model with two different temperature regions was studied and the presence of persistent currents at the interface between the temperature regions was observed. The relevant fact is that no gravity and no shear forces are necessary to induce those nonequilibrium effects but only the temperature gradient.

In the present work we aim at determining if temperature gradients are also capable of inducing nonequilibrium patterns in more sophisticated models such as proteins in a lattice. We analyze the influence of the magnitude of the temperature difference on the attained protein conformations. Also we compare the so obtained structures with those of the thermodynamic equilibrium.

DY 28.9 Thu 12:30 HÜL 186

Analysis of non-equilibrium fluctuations of quantum mechanical expectation values — •Christian Bartsch and Jochen Gemmer — Fachbereich Physik, Universität Osnabrück, Barbarastrasse 7, D-49069 Osnabrück, Germany

For certain abstract, closed quantum systems the dynamics of expectation values, obtained by exact diagonalization, may be interpreted as a composition of some "regular" dynamics, e.g., an exponential decay into equilibrium, and some "irregular" part, which we call fluctuations. We numerically find that the latter may typically be regarded as Gaussian white noise in good approximation. Furthermore, we analyze particularly the non-equilibrium fluctuations on the basis of a Langevin-type equation describing the time evolution of the expectation value, where the fluctuations are incorporated as a stochastic force. We moreover define an entropy as a function of the analyzed expectation value, similar to the common von Neumann-entropy. As long as the fluctuations correspond to a stochastic Gaussian variable, the entropy production over time may as well be viewed as a Gaussian stochastic variable, for which then the fluctuation theorem holds. Additionally, we analyze the scaling of the fluctuations with fundamental system parameters.

DY 28.10 Thu 12:45 HÜL 186

Energy current magnification in coupled oscillator loops. — •Rahul Marathe — Max Planck Institute for Colloids and Interfaces, 14476, Potsdam, Germany.

Motivated by studies on current magnification in quantum mesoscopic systems, we consider sound and heat transmission in classical models of oscillator chains. A loop of coupled oscillators is connected to two leads through which one can either transmit monochromatic waves or white-noise signal from heat baths. We look for the possibility of current magnification in this system due to some asymmetry introduced between the two arms in the loop. We find that current magnification is indeed obtained for particular frequency ranges. However, the integrated current shows the effect only in the presence of a pinning potential for the atoms in the leads. We also study the effect of anharmonicity on current magnification.

DY 28.11 Thu 13:00 HÜL 186

Endoreversible Modeling using the example of fuel cells — •Katharina Wagner and Karl Heinz Hoffmann — Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany

In endoreversible thermodynamics irreversible processes and systems are split into reversible subsystems and interactions in between them. Subsystems can either be reservoirs storing energy and extensive quantities or engines transferring energy between different extensive quantities. The irreversibilities of the system are completely described by the interactions between the reversible subsystems. This separation leads to a block of balance equations, which characterize the reversible subsystems, and transport equations, which describe the interactions. The entropy production can thus be localized within the whole system. Using the formalism of endoreversible thermodynamics a PEM fuel cell is modeled and the power output as well as the efficiency are investigated.

DY 29: Quantum Chaos I

Time: Thursday 10:15–12:30 Location: ZEU 255

DY 29.1 Thu 10:15 ZEU 255

Planar anharmonic two-electron quantum dots — •Sebastian Schröter, Johannes Eiglsperger, Moritz Schönwetter, and Javier Madroñero — TU München, Physik Department

As a first attempt to understand from first principles an unusual behaviour of the coherence of many-body systems [1,2,3] we propose an *ab initio* quantum approach for planar two-electron quantum dots. In our approach the quantum dot is approximated by an harmonic potential with an additional quartic perturbation. An appropriate coordinate transformation leads to a finite exact representation of the eigenvalue problem in creation and annihilation operators. In order to investigate the dynamics of the system a novel explicit time propagation method [4,5] is utilised to solve the time dependent Schrödinger equation.

Within this approach we focus on the study of the complex dynamics of the system. In particular we address the quantum fidelity of wave packets to investigate the loss of coherence of the system.

[1] G. Manfredi, P.-A. Hervieux, New J. Phys. **11**(2009), 013050.
[2] G. Manfredi, P.-A. Hervieux, Phys. Rev. Lett. **100**(2008), 050405.
[3] G. Manfredi, P.-A. Hervieux, Phys. Rev. Lett. **97**(2006), 190404.
[4] S. O. Fatunla, Math. Comput. **34**(1980), 373.
[5] J. Madroñero, B. Piraux, Phys. Rev. A **80**(2009), 033409.

DY 29.2 Thu 10:30 ZEU 255

Phase-Space Properties of a Classical Non-Harmonic Two-Electron Quantum Dot — •Moritz Schönwetter, Javier Madroñero, Sebastian Schröter, and Johannes Eiglsperger — Physik Department, Technische Universität München, James-Franck-Str. 1, D-85748 Garching

Recent investigations of the fidelity in many body systems – which include trapped BEC [1], many electrons in nonparabolic quantum wells [2], and electron gases [3] – have shown an unusual behaviour of the quantum fidelity: it stays equal to unity until a critical time, then drops suddenly to much lower values. In order to understand the origin of this phenomenom the dynamics of a non-harmonic two-electron quantum dot is investigated. We present our first results in an attempt to characterize the coherence of this system in terms of the underlying mixed regular-chaotic classical dynamics.

[1] G. Manfredi, P.-A. Hervieux, Phys. Rev. Lett. **100** (2008), 050405.
[2] G. Manfredi, P.-A. Hervieux, New J. Phys. **11** (2009), 013050.
[3] G. Manfredi, P.-A. Hervieux, Phys. Rev. Lett. **97** (2006), 190404.

DY 29.3 Thu 10:45 ZEU 255

Collective versus Single-Particle Motion in Quantum Many-Body Systems from the Perspective of an Integrable Model — •Jens Haemmerling, Boris Gutkin, and Thomas Guhr — Theoretische Physik Universität Duisburg-Essen

We study the emergence of collective dynamics in the integrable Hamiltonian system of two finite ensembles of coupled harmonic oscillators. After identification of a collective degree of freedom, the Hamiltonian is mapped onto a model of Caldeira-Leggett type, where the collective coordinate is coupled to an internal bath of phonons. In contrast to the usual Caldeira-Leggett model, the bath in the present case is part of the system. We derive an equation of motion for the collective coordinate which takes the form of a damped harmonic oscillator. We show that the distribution of quantum transition strengths induced by the collective mode is determined by its classical dynamics.

DY 29.4 Thu 11:00 ZEU 255

Transport moments beyond the leading order — Gregory Berkolaiko[1] and •Jack Kuipers[2] — [1]epartment of Mathematics, Texas A&M University, College Station, TX 77843-3368, USA — [2]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

For chaotic cavities with scattering leads attached, transport properties can be approximated in terms of the classical trajectories which enter and exit the system. With a semiclassical treatment involving fine correlations between such trajectories we show by using graphical recursions how we can obtain the moments of various transport quantities. In particular we give the moment generating function of the transmission and reflection eigenvalues at the first two subleading orders in the inverse channel number for systems with and without time reversal symmetry. These results suggest patterns which could hold for higher order corrections and which would match the low order moments derived from random matrix results. The techniques can also incorporate an energy dependence which allows us to show that the gap in the density of states of chaotic Andreev billiards is robust against the subleading corrections and to obtain the next orders of the moment generating function of the Wigner delay times. Furthermore, the graphical representation provides an intuitive picture for non-linear statistics and we conclude with some generating functions for the correlation between transport moments.

DY 29.5 Thu 11:15 ZEU 255

Whispering Gallery Modes by Partial Barriers in Deformed Microcavities — •Jeong-Bo Shim[1], Jan Wiersig[1], and Hui Cao[2] — [1]Institut für Theoretische Physik, Otto-von-Guericke-Universität Magdeburg, D-39106, Magdeburg, Germany — [2]Department of Applied Physics, Yale University, New Haven, Connecticut 06520-8482, USA

The idea of deformed optical micorcavities was first suggested to induce a directional light emission from the whispering gallery modes. However, it is still not easy to control the optical properties of the whispering gallery modes such as the emission directionality or the quality factor due to the chaotic internal ray dynamics.

In this work, we introduce the possibility that the remnant of a dynamical invariant structure in the phase space of the deformed microcavity, the so-called partial barrier play a role of an unbroken tori due to the openness of the system. Using the semiclassical approach, the spectrum of the microcavity is qualtitatively analyzed in the short wavelength regime. As a result, we are able to predict the spectral and emissional properties of the microcavity along with a good agreement between the theoretical analysis and the numerically obtained spectrum.

DY 29.6 Thu 11:30 ZEU 255

A spectrum and the eigenfunctions of a rectangular microwave Dirac billard — Stefan Bittner[1], Barbara Dietz[1], •Maksym Miski-Oglu[1], and Achim Richter[1,2] — [1]Institut für Kernphysik, Technische Universität Darmstadt, D-64289 Darmstadt, Germany — [2]ECT*, Villa Tambosi, I-38100 Villazzano (Trento), Italy

A spectrum and the eigenfunctions of a rectangular microwave Dirac billard have been measured. The microwave Dirac billiard is a rectangular microwave billiard filled with a photonic crystal consisting of a triangular lattice of metallic cylinders. In the frequency range around the Dirac point two bands approach each other as a pair of cones, i.e. the dispersion relation of the photonic crystal resembles the spectrum of relativistic massless fermions. Microwave power is coupled into (out of) the microwave billiard via dipole antennas and the transmitted power is measured. The eigenvalues of a Dirac billiard correspond to resonances in the transmission spectra. The eigenfunctions are measured by a so-called perturbation body method. Arround the Dirac frequency the eigenfunctions show a clear localization along the ΓK direction of the photonic crystal which corresponds to the zigzag edge in graphene. The observed states are analogous to edge states in graphene nanoribbons.

This work has been supported within the DFG grant SFB634.

DY 29.7 Thu 11:45 ZEU 255

Random caustics and the branching of two-dimensional flows — •Jakob J. Metzger, Ragnar Fleischmann, and Theo Geisel — Max-Planck-Institut für Dynamik und Selbstorganisation

When particles or waves emitted from a source travel through a weak, correlated disorder potential, strong density fluctuations in the form of branches appear on scales much smaller than the mean free path. This branching of the flow has been observed on length scales ranging from a few micrometres, affecting the transport properties of semiconductor devices [1], up to several thousand kilometres, influencing sound propagation through the ocean [2]. It is also responsible for the appearance of large and hazardous freak waves and tsunamis [3].

We present recent results on the statistics of branches which are universal for many types of disorder [4] and their implication on the

statistics of the flow density.

[1] e.g. M. A. Topinka et al., Nature **410**, 183 (2001), M. P. Jura et al., Nature Physics **3**, 841 (2007)

[2] M. Wolfson & S. J. Tomsovic, Acous. Soc. Am., **109**, 2693 (2001)

[3] M. V. Berry , New J. Phys. **7**, 129 (2005); M. V. Berry, Proc. R. Soc. A **463**, 3055 (2007); E. J. Heller, L. Kaplan & A. Dahlen, J. Geophys. Res., **113**, C09023 (2008)

[4] J. J. Metzger, R. Fleischmann and T. Geisel, Phys. Rev. Lett. **105**, 020601 (2010)

DY 29.8 Thu 12:00 ZEU 255

Flooding Signatures in Spectral Statistics — Arnd Bäcker[1,2], Steffen Löck[1], Normann Mertig[1], and •Torsten Rudolf[1] — [1]Technische Universität Dresden, Institut für Theoretische Physik, 01062 Dresden — [2]MPI für Physik komplexer Systeme, 01187 Dresden

We investigate the consequences of flooding on spectral statistics in systems with a mixed phase space, where regions of regular and chaotic motion coexist. Quantum mechanically, eigenstates are typically concentrated on regular tori or in the chaotic sea. However, when increasing the coupling between the regular and the chaotic region, the chaotic states flood the regular island and simultaneously the regular states disappear. We demonstrate that flooding has a significant impact on the level-spacing distribution, which shows a transition from Berry-Robnik statistics in the semiclassical regime to Wigner statistics in the flooding regime.

DY 29.9 Thu 12:15 ZEU 255

How long is the chaotic boundary of a billiard? — Arnd Bäcker[1,3], Roland Ketzmerick[1,3], •Steffen Löck[1], and Holger Schanz[2,3] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden — [2]Institut für Maschinenbau, Hochschule Magdeburg-Stendal, 39114 Magdeburg — [3]MPI für Physik komplexer Systeme, 01187 Dresden

For two-dimensional quantum billiards we derive a partial Weyl law, i.e. the average density of states for a subset of eigenstates concentrating on an invariant region Γ of phase space. The leading term is proportional to the area of the billiard times the phase-space fraction of Γ. The boundary term is proportional to the fraction of the boundary where *parallel* trajectories belong to Γ. Agreement with numerical data will be presented for the mushroom and the cosine billiard, where we determine the boundary lengths associated with chaotic and regular states, and for the elliptical billiard, where we consider rotating and oscillating states.

DY 30: Reaction-Diffusion Systems

Time: Thursday 10:15–12:30 Location: ZEU 118

DY 30.1 Thu 10:15 ZEU 118

Interaction of a pair of scroll waves — •Dennis Kupitz and Marcus Hauser — Abteilung Biophysik, Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Scroll waves are the three-dimensional counterparts of spiral waves occurring in excitable media. Single scroll waves may undergo a series of instabilities that play an important role in the formation of cardiac arrhythmias, like ventricular tachycardia. While the dynamics of single scroll waves have attracted some experimental effort, the interaction of scroll waves has so far received much less attention.

We present an experimental study of the interaction of two scroll waves created in a Belousov-Zhabotinsky reaction medium and observed by optical tomography with a parallel beam technique. The scroll waves may either rotate in the same or in an opposite sense of rotation, thus leading to situations with different topological charges. The organising centres of the scrolls, the so-called filaments, were originally straight, and depending on the selected experimental conditions, they may either describe a circular or a meandering trajectory. The dynamics of pairs of co- and counter-rotating scroll waves were studied for both rigidly rotating and meandering filaments, leading to different types of collective filament behaviour.

DY 30.2 Thu 10:30 ZEU 118

A reactive-flow model of phase separation in fluid binary mixtures with continuously ramped temperature — Izabella Benczik and •Jürgen Vollmer — Max Planck Institute for Dynamics and Self-Organization, 37073 Göttingen

We suggest to revisit the phase separation of binary mixtures subjected to a sustained change of temperature from the point of view of reactive flows. Exploiting this new perspective, we describe the demixing dynamics by a spatial model of advection-reaction-diffusion completed with nucleation and coaguation of droplets. In this approach several features of the dynamics — in particular an oscillatory variation of the droplet density — become numerically and analytically accessible. Hence, this model helps to clarify why the oscillation frequency is hardly affected by the flow.

I.J. Benczik and J. Vollmer, EPL **91** (2010) 36003.

DY 30.3 Thu 10:45 ZEU 118

Reaction-diffusion system with continuous distributions of binding energies — •Andrea Wolff[1], Ingo Lohmar[2], Joachim Krug[1], and Ofer Biham[2] — [1]Institut für theoretische Physik, Universität zu Köln — [2]Racah Institute of physics, The Hebrew University, Jerusalem, Israel

We study pair reactions on a periodic square lattice with continuous deposition, diffusion, and spontaneous desorption of particles. The characteristic quantity of the system's steady state is the efficiency, which is the fraction of incoming particles, that react before desorption.

Since spatial inhomogeneity is of theoretical and applied interest, we want to study the influence of disorder in the process rates systematically. We start with binary disorder, where each site has one of two possible different binding energies. The behaviour of this system has been well-understood qualitatively and quantitatively [1]. In contrast, the case of continuously distributed binding energies cannot be treated exactly anymore. We use the knowledge of the binary system to derive a mapping from the system with a continuous distribution to an effective binary model, where all the different binding energies are pooled into two effective ones. Comparison of this effective model with Monte Carlo simulations shows remarkable agreement.

[1] A. Wolff, I. Lohmar, J. Krug, Y. Frank, O. Biham, Phys. Rev. E 81, 061109 (2010)

DY 30.4 Thu 11:00 ZEU 118

Reentries generated by a random heterogeneous region in cardiac tissue — •Sergio Alonso and Markus Bär — Physikalisch-Technische Bundesanstalt

Wave propagation in the heart has a discrete nature due to the discrete intercellular connections via gap junctions. Cardiac diseases may result on the reduction of conductivities of the gap junctions. The distribution of the disrupted connections can be inhomogeneous and some part of the heart can accumulate a major density.

We study the effect on homogeneous wave propagation with a region where a random distribution of connectivities between cells are eliminated. This region can produce the appearance of reentries. We consider the Fenton-Karma model for cardiac tissue to perform a systematic study of the reentry generation depending on the topology of the connectivity network.

DY 30.5 Thu 11:15 ZEU 118

Coupling of pacemakers and irregular excitation patterns in reaction-diffusion systems — •Claudia Lenk[1], Mario Einax[2], J. Michael Koehler[1], and Philipp Maass[2] — [1]Institut für Physik, Technische Universität Ilmenau, Germany — [2]Fachbereich Physik, Universität Osnabrück, Germany

Reaction-diffusion (RD) systems describe pattern formation in many areas as, e.g., chemical reactions, population dynamics, and the propagation of electrical excitations in the brain or heart. They allow one also to study the mechanisms that lead to irregular, chaos-like excitation patterns and related pathological states in physiologic applications. In this talk we report on the generation of irregular excitation patterns due to coupling of different pacemakers in two types of spatially separated RD-systems, the Belousov-Zhabotinsky reaction (BZR) and a simple model for atrial fibrillation. Theoretical

calculations are carried out for two different RD-models, the FitzHugh-Nagumo equations and the minimal model of Bueno-Orovio *et al* [1]. Experiments of the BZR are conducted in a gel system with periodic pattern of the catalyst Ferroin. The regularity of the excitation patterns is analyzed by the entropy of the frequency distribution and by the synchronization properties between the two pacemakers.

[1] A. Bueno-Orovio, E. M. Cherry, F. H. Fenton, JTB **253**, 544 (2008).

DY 30.6 Thu 11:30 ZEU 118

Dynamics of scroll rings interacting with boundaries — •Arash Azhand, Peter Kolski, and Harald Engel — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Undamped propagation of three-dimensional travelling waves has been observed in a variety of dissipative active media including chemical waves, temperature waves in solid fuel combustion and waves of electric activity during cardiac arrhythmias, for example. Here, we present experimental and numerical results for the dynamics of scroll rings in thin layers of the photosensitive Belousov-Zhabotinsky reaction. The study is focused on boundary effects that modify the intrinsic dynamics of the scroll ring under these geometrically confined conditions. The experimental findings are compared to results obtained by numerical simulations with the underlying Oregonator model. The reported results do not depend, however, on a particular kinetics but apply to a large class of excitable media.

DY 30.7 Thu 11:45 ZEU 118

Control of spatiotemporal chaos by flow in a reaction-diffusion-advection system — •Igal Berenstein and Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Germany

We report spatiotemporal chaos in the Oregonator model of the Belousov-Zhabotinsky (BZ) reaction. Uniform oscillations and traveling waves are unstable and spatiotemporal chaos spontaneously develops in a regime, where the underlying local dynamics show stable limit cycle oscillations (diffusion-induced turbulence). We show that spatiotemporal chaos can be suppressed by a unidirectional flow in the system. With increasing flow velocity, we observe a transition scenario from spatiotemporal chaos via a regime of travelling waves to a stationary steady state. At large flow velocities we recover the known regime of flow distributed oscillations (stationary structure). We also investigated systems with a gradient in one of the parameters. We show that in such systems, localized domains of spatiotemporal chaos can be found if the gradient is sufficiently small, i.e., if the size of the chaotic domain is large compared to the diffusive length scale. Finally, we show that spatiotemporal chaos can be suppressed by allowing diffusive exchange of the activator between the reaction- diffusion system and a non-reacting layer. The type of pattern that is formed is independent of a flow in the non-reactive layer.

DY 30.8 Thu 12:00 ZEU 118

Hysteresis in the pinning-depinning transition of a spiral wave close to a circular defect — •Jan Frederik Totz and Harald Engel — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

A non-monotonous dependence of the rotation period on the defect radius with coexistence between freely rotating and pinned spiral waves in a certain parameter range has been reported first by Pertsov et al. [1]. Recently, these results were confirmed in a detailed numerical bifurcation analysis using the continuation software AUTO [2]. Within a free-boundary formulation the role of curvature and dispersion effects has been clarified [3]. By doing so, quantitative agreement between theoretical predictions and results obtained by numerical simulations was achieved. The experimental verification of the hysteresis phenomenon in an open gel reactor with the photosensitive Belousov-Zhabotinsky reaction is the topic of the talk.

[1] A. M. Pertsov, E. A. Ermakova, A. V. Panfilov, Physica D 14, 117 (1984).

[2] G. Bordyugov, H. Engel, Physica D 228, 49 (2007).

[3] V. Zykov, G. Bordyugov, H. Lentz, H. Engel, Physica D 239, 797 (2010).

DY 30.9 Thu 12:15 ZEU 118

Activation parameters of model redox reactions and their variation from classical molecular simulation — •Christof Drechsel-Grau and Michiel Sprik — University of Cambridge, Department of Chemistry, Cambridge, CB2 1EW, United Kingdom

Transition states are dynamical bottlenecks of chemical reactions, and an understanding of their energetic properties and location can provide insight into the reactions' mechanism. In particular, the variation of the activation free energy with temperature yields the activation entropy and the activation energy, whereas the variation of the activation free energy with reaction free energy defines the charge-transfer symmetry factor, which indicates the location of the transition state relative to the stable states. The calculation of activation parameters is not only computationally demanding, but traditionally also relies on knowledge of the reaction coordinate, which is usually unavailable. Thus, we employ transition path sampling, which does not require knowledge of the reaction coordinate, to compute activation energies and their variation with reaction free energy for a model system. Exploiting knowledge of the reaction coordinate for the model system, we also calculate the activation free energies and the charge-transfer symmetry factor from umbrella integration and from free energy perturbation simulations. We find that the activation energies are smaller than the activation free energies. In addition, the variation of the latter with reaction free energy is larger than that of the former.

DY 31: Glasses and Glass Transition (jointly with CPP, DF)

Time: Thursday 10:45–13:00 Location: ZEU 114

Topical Talk DY 31.1 Thu 10:45 ZEU 114

Local Anisotropy of Fluids, Glasses and Jammed Bead Packs — •Gerd Schroeder-Turk — Theoretische Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstr 7B, 91058 Erlangen

The local structure of particle ensembles is important for physical properties of normal or super-cooled fluids, jammed bead packs or structural glass phases. It is often characterized by order parameters such as q_4 or q_6, defined by spherical harmonics of particle neighborhoods. Here we show that a Minkowski tensor analysis of the particles' Voronoi cells provides shape indices that give a clear signature of various structural transitions in particle systems. In particular, all of the above mentioned systems consist of locally anisotropic environments. We show that the degree of cell anisotropy shows a clear signature of the jamming transition in bead packs, the transition to partially ordered states at the random close packing limit, and of the transitions from fluid to ordered phases in simple liquids. For jammed bead packs, these findings suggest an inherent geometrical reason why anisotropic shapes can fill space more efficiently than spheres.

[1] Schröder-Turk *et al*, Europhys. Lett., **90**(3), 34001 (2010)
[2] Kapfer *et al*, J. Stat. Mech. (2010) P11010

DY 31.2 Thu 11:15 ZEU 114

In-situ characterization of vapor-deposited glasses of toluene by differential AC chip nanocalorimetry — •Mathias Ahrenberg[2], Heiko Huth[2], Katie Whitaker[1], Mark D. Ediger[1], and Christoph Schick[2] — [1]University of Wisconsin - Madison — [2]University of Rostock

We use ac nanocalorimetry to investigate extraordinarily stable glasses of toluene prepared by vapor deposition. For that purpose we have built a vapor deposition chamber that allows in-situ characterization of vapor-deposited organic glasses down to liquid nitrogen temperature. With highly sensitive nanocalorimeters in a differential setup, we are able to measure ng-samples over a frequency range from 0.1 Hz up to 8 kHz. The device was used to investigate the transformation of as-deposited stable toluene glasses into ordinary glasses. For films about 100 nm thick, the transformation was studied as a function of time at constant temperature above the common glass transition and as function of temperature at constant heating rate. The stability of the thin films was investigated as a function of substrate temperature

and deposition rate.

DY 31.3 Thu 11:30 ZEU 114

Structural relaxation times in high-density amorphous ice (HDA) — •Philip H. Handle[1], Markus Seidl[1], Erwin Mayer[2], and Thomas Loerting[1] — [1]Institute of Physical Chemistry, University of Innsbruck, Austria — [2]Institute of General, Inorganic & Theoretical Chemistry, University of Innsbruck, Austria

Solid water (H2O) exists in a variety of different forms. Besides common hexagonal Ice (Ih) today 15 different crystalline and three different amorphous forms are known. It is under discussion whether the amorphous forms are glassy (related to liquid water [1]) or nano-crystalline (related to ice). In case of high-density amorphous ice (HDA) this question has been addressed in some studies [2-4], yet remains controversial. In our work we measured structural relaxation times of HDA at elevated pressures (0.1 and 0.2 GPa) and different temperatures (125-135 K) on the basis of differential scanning calorimetry (DSC) at 1 bar. Our data suggest that at 135 K the structural relaxation time is only slightly higher than 100s, i.e., HDA is on the borderline to the glass transition.

[1] Poole, P. H.; et al.; Nature 360, 324-328 (1992). [2] Tse, J. S.; et al.; Nature 400, 647-649 (1999). [3] Mishima, O.; J. Chem. Phys. 115, 4199-4202 (2001). [4] Andersson, O.; Phys. Rev. Lett. 95, 205503-205507 (2005).

DY 31.4 Thu 11:45 ZEU 114

Dynamics of glass forming liquids in soft confinement — •Emmanuel Gouirand[1], Thomas Blochowicz[1], Andreas Blank[1], Bernd Stühn[1], and Bernhard Frick[2] — [1]Institut für Festkörperphysik, TU Darmstadt — [2]Institut Laue-Langevin, Grenoble, France

In search of a characteristic length scale associated with cooperative dynamics at the glass transition, intensive effort has been devoted to investigating the influence of confinement on the dynamics of glass forming liquids. Nevertheless, no generally accepted picture exists so far because of the complex interplay of surface, pressure and finite size effects affecting the dynamics. We investigate the dynamics in confinements of different nature in order to be able to disentangle these various effects. Therefore, we apply photon correlation spectroscopy and quasi elastic neutron scattering on glass formers confined within microemulsion droplets, the structure of which proved to remain stable over the whole temperature range by means of small angle scattering. First, we report on the dynamics of glycerol confined in AOT micelles where the glass transition temperature (T_g) of the matrix is chosen to be smaller than T_g of the glycerol core (fast soft confinement). We find glycerol to relax faster than in bulk with an Arrhenius temperature dependence [1]. Then we compare the dynamics of toluene in Cremophor ELP micelles. Contrary to the former situation, here the matrix relaxes slower than the core and slows down the latter due to interfacial effects. Finally, below T_g of the matrix actual hard confinement of toluene within the droplets is realized.

[1] Blochowicz et al., CPL 475, 171-174 (2009)

DY 31.5 Thu 12:00 ZEU 114

Crystallization and induced glass transition of n-alcohols in silicon-nanochannels — •Rolf Pelster, Rene Berwanger, Carsten Biehl, and Christoph Schuhmacher — FR 7.2 Experimentalphysik, Universität des Saarlandes, D-66123 Saarbrücken, Germany

We have investigated the molecular dynamics of n-alcohols (C_4H_9OH - $C_{11}H_{23}OH$) confined in mesoporous silicon and silicon oxide with pore radii ranging from 3.5 to 7 nm. Using dielectric and infrared spectroscopy we show that the temperature of the liquid-solid phase transition and the structure of the solid phase depend on both the chain length and the radius of the pores:

Long-chain alcohols exhibit a crystalline structure at low temperatures. The confinement induces a lowering of the freezing temperature. The shorter the chain length or the smaller the pore radius, the lower the freezing temperature. Below the phase transition only the dynamics of amorphous wall layers are observable [1].

Short-chain alcohols behave differently. While bulk alcohols still freeze upon slow cooling, we observe a glass transition for the confined phase. The glass transition temperature is close to that reported for quenched bulk alcohols. We thus conclude that nano-confinement suppresses the crystallization process and induces a glass transition.

[1] R. Berwanger, Ch. Schumacher, P. Huber, and R. Pelster, Eur. Phys. J. Special Topics 189, 239-249 (2010)

DY 31.6 Thu 12:15 ZEU 114

Glass Transition in Confined Geometry — •Simon Lang[1,2], Viatlie Botan[1], Martin Oettel[1], David Hajnal[1], Thomas Franosch[2], and Rolf Schilling[1] — [1]Johannes Gutenberg-Universität Mainz, Germany — [2]Universität Erlangen/Nürnberg, Germany

Confinement of a simple liquid is accompanied by introducing a further length scale in addition to the average distance of the particles. The interplay between them strongly influences the glass transition according to numerous significant experiments and simulations.

To achieve a theoretical description, we extend the microscopic mode-coupling theory to a liquid confined between two parallel flat hard walls [1]. The theory contains the standard mode-coupling equations in bulk and in two dimensions as limiting cases and requires as input solely the equilibrium density profile and the static structure factors of the fluid in confinement. We evaluate the phase diagram for a hard-sphere liquid as a function of the distance of the plates and obtain an oscillatory behavior of the glass transition line as a result of the structural changes related to layering. We detect a facilitation of the glass transition at half-integer values of the distance with respect to the hard-sphere diameter. In contrast, at commensurate packing particles can more easily slide along the walls and therefore the liquid phase remains favored for higher packing fractions.

[1] S. Lang, V. Botan, M. Oettel, D. Hajnal, T. Franosch, and R. Schilling, Phys. Rev. Lett. 105 125701 (2010)

Topical Talk DY 31.7 Thu 12:30 ZEU 114

Concentration fluctuations and intrinsic confinement effects in binary glass forming liquids: Insights from neutron scattering and X-ray photon correlation spectroscopy — •Thomas Blochowicz[1], Sebastian Schramm[1], Emmanuel Gouirand[1], Philipp Gutfreund[2], Bernd Stühn[1], Bernhard Frick[2], and Yuriy Chushkin[3] — [1]TU-Darmstadt, Darmstadt, Germany — [2]ILL, Grenoble, France — [3]ESRF, Grenoble, France

We investigate the dynamics in a series of binary glass forming liquids using dielectric spectroscopy (DS) in combination with quasielastic neutron scattering, dynamic light scattering and X-ray photon correlation spectroscopy (XPCS). It turns out that, although macroscopically the systems are fully miscible in the whole temperature range, two glass transitions can be clearly distinguished due to the high T_g contrast of the components. By means of DS the corresponding relaxation processes are identified, and it turns out that contrary to expectation the small molecules take part in both glass transitions, which suggests that two dynamical species can be distinguished among the small molecules. Moreover, the relaxation connected with the lower glass transition shows properties typical of dynamics in confinement like an Arrhenius-type temperature dependence and a broad distribution of relaxation times. On the other hand it is revealed by XPCS that the concentration fluctuations exhibit a significantly weaker temperature dependence than the α-relaxation and show a crossover from a diffusive to a so-called ballistic wave vector dependence and from stretched to compressed relaxation functions around the upper T_g.

DY 32: Statistical Physics in Biological Systems III (organised by BP)

Time: Thursday 10:15–13:00 Location: ZEU 260

Invited Talk DY 32.1 Thu 10:15 ZEU 260

Bacterial Games — •Erwin Frey — Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universitaet Muenchen, Theresienstrasse 37, D-80333 Muenchen

Microbial laboratory communities have become model systems for studying the complex interplay between nonlinear dynamics of evolutionary selection forces, stochastic fluctuations arising from the probabilistic nature of interactions, and spatial organization. Major research goals are to identify and understand mechanisms that ensures viabil-

ity of microbial colonies by allowing for species diversity, cooperative behavior and other kinds of social behavior. A synthesis of evolutionary game theory, nonlinear dynamics, and the theory of stochastic processes provides the conceptual framework for a deeper understanding of these ecological systems. In this talk, we give an introduction into the modern formulation of these theories and illustrate their effectiveness focussing on selected examples of microbial systems. We also discuss current challenges and future perspectives in quantifying bacterial population dynamics, and how this might have an impact on research in non-equilibrium physics.

DY 32.2 Thu 10:45 ZEU 260

Transport efficiency governs the morphology of the plasmodial arterial network in slime moulds — •Werner Baumgarten and Marcus Hauser — Abteilung Biophysik, Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

The plasmodium of the slime mould Physarum polycephalum is a single multi-nucleate giant amoeboid cell. It forms a characteristic two-dimensional arterial network, where the apical end of the plasmodium extends to search for new food sources, while the dense network of tubular arteries is in charge of transport of protoplasm throughout the giant cell. The tubular network forms a regular graph [1,2] and displays characteristic distributions of the lengths, widths, and surface area of the tubes [2]. With time, the originally dense network coarsens as tiny arterial segments are deleted. Taking into account the laminar flow inside the arterial network [3], the conductivity and drag inside the arteries are estimated. From these data it will be shown that the evolution of the network strongly depends on the efficiency of the protoplasmic transport in the arteries.

[1] W. Baumgarten, M.J.B. Hauser, J. Comp. Interdisc. Sci. 2010, 1, 241-249.

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

[3] N. Kamiya, Protoplasma 1950, 39, 344-357.

DY 32.3 Thu 11:00 ZEU 260

A Thermal Trap for DNA Replication — •Christof B. Mast and Dieter Braun — Systems Biophysics, Physics Department, Center for Nanoscience, Ludwig Maximilians Universität München, Amalienstr. 54, 80799 München, Germany

The hallmark of living matter is the replication of genetic molecules and their active storage against diffusion. We implement both in the simple non-equilibrium environment of a temperature gradient. Convective flow both drives the DNA replicating polymerase chain reaction (PCR) while concurrent thermophoresis accumulates the replicated 143 base pair DNA in bulk solution. The time constant for accumulation is 92 s while DNA is doubled every 50 s. The length of the amplified DNA is checked with thermophoresis. Finite element simulations confirm the findings. The experiments explore conditions in pores of hydrothermal rock which can serve as a model environment for the origin of life.

DY 32.4 Thu 11:15 ZEU 260

Negative design in protein folding: The role of correlations — •Jonas Minning[1], Ugo Bastolla[2], and Markus Porto[3] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Germany — [2]Centro di Biología Molecular 'Severo Ochoa', Madrid, Spain — [3]Institut für Theoretische Physik, Universität zu Köln, Germany

Assessing the stability of a protein sequence folded into its native structure is a crucial aspect of protein design and of understanding protein evolution. Folding stability has two sides: (i) stability against the unfolded ensemble, which is usually achieved by evolution providing the native state with native contacts that are attractive enough to compensate for the loss of conformational entropy (positive design), and (ii) stability against incorrectly folded (misfolded) structures with low free energy, which is achieved through negative design.

A simple approximation based on the Random Energy Model (REM) and hence on the neglect of correlations predicts that negative design can be achieved by reducing the variance of the contact interaction energies of all possible residue-residue contacts. We verify that this approximation provides a good fit of the minimum free energy of misfolded structures. Nevertheless, our results suggest that negative design in protein evolution follows actually a completely different strategy, namely utilizing structural correlations between pairs of positions in the misfolded ensemble, which are neglected in the REM approach. We discuss how the REM approach might be generalized to include these correlations.

15 min. break

DY 32.5 Thu 11:45 ZEU 260

Assessing the asymptotic fitness distribution of beneficial mutations from incomplete data sets — •Ivan G. Szendro[1], Martijn Schenk[2], J. Arjan G.M. de Visser[2], and Joachim Krug[1] — [1]Institut für Theoretische Physik, Universität zu Köln — [2]Laboratory of Genetics, Wageningen University

Since seminal work by Gillespie [1] and Orr [2] it is expected that the distributions of fitness effects of beneficial mutations are determined by the universality classes of extreme value theory. More specifically, it is commonly assumed that the distributions of fitness fall into the Gumbel class, implying an exponential decay at large values. However, there have been recent claims that for some viruses the distribution belongs to the Weibull class [3].

In this contribution, we assess the effect of not observing existing beneficial mutations on the assignment of fitness distributions to one of the three extreme value classes. We assume that the probability to observe a specific mutant depends on its selective disadvantage with respect to the fittest observed mutants. In the light of our considerations, we analyze data collected in an experimental evolution study of the TEM-1 β-lactamase enzyme, which confers antibiotic resistance to *Escherichia coli*.

[1] J.H. Gillespie, Theor. Popul. Biol. 23, 202 [2] H.A. Orr, Genetics 163, 1519 [3] D.R. Rokyta et al., J. Mol. Evol. 67, 368

DY 32.6 Thu 12:00 ZEU 260

Stochastic tunneling in a two-locus system with recombination — •Andrej Fischer, Ivan Szendro, Joachim Krug, and Alexander Altland — Institut für Theoretische Physik, Universität zu Köln, D-50973 Köln, Germany

The analysis of minimal models in population genetics is an important conceptual task. The effects of mutation, selection and drift (finite population size) on evolution are captured by Kimura's well-known one-locus model with two alleles. Here, we analyze a model that includes additionally the effects of epistasis and recombination in a two-locus setting. For sign epistasis, i.e. the over-compensation of an initial deleterious point mutation by a beneficial secondary mutation at the other locus, the fixation of the fittest genotype is dominated by the presence of several bottlenecks. The interplay of both finite size effects and meta-stability induced by recombination make for intricate fixation dynamics in this paradigmatic model system. Both analytical and numerical results are presented.

DY 32.7 Thu 12:15 ZEU 260

How to cross a fitness valley - A network approach — •Hinrich Kielblock[1], Marc Timme[1,2], and Stefan Grosskinsky[3] — [1]Network Dynamics Group, Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Bernstein Center for Computational Neuroscience Göttingen, Germany — [3]Centre for Complexity Science, University of Warwick, Conventry, UK

How fast does a population evolve from one fitness peak to another in a fitness landscape? This question has recently received much attention as the answer may strongly affect the speed of evolution.

Here we analyze the problem in the stochastic tunneling regime, where almost always almost all individuals are found near one fitness peak but once in a while the population switches to another peak. We derive an analytical expression for this switching time considering finite polulation sizes. We first analyze the dynamics of a population existing in only two different genotypes. The results of such a simple system enable us to derive a formula for an effective mutation rate between the peaks of a fitness valley. This effective rate makes it possible to determine the mean switching times in more complex setups, as e.g. multiple fitness valleys or other structures.

DY 32.8 Thu 12:30 ZEU 260

A dynamical phase transition in a model for evolution with migration — •Bartlomiej Waclaw, Rosalind Allen, and Martin Evans — Department of Physics & Astronomy, University of Edinburgh, JCMB, The King's Buildings, Mayfield Road, Edinburgh EH9 3JZ, United Kingdom

Migration between different habitats is ubiquitous among biological populations. Here I will discuss a simple model for evolution of asex-

ual organisms in two different habitats coupled by one-way migration as well as mutations. This gives rise to clusters of closely related genotypes (quasispecies). The habitats are assumed to have different fitness landscapes, i.e., organisms which are well-adapted in the primary habitat are likely to be maladapted in the secondary habitat. The model undergoes a dynamical phase transition: at a critical value of the migration rate, the time to reach the steady state diverges. Above the transition, the population is dominated by immigrants from the primary habitat. Below the transition, the genetic composition of the population is highly non-trivial, with multiple coexisting "quasispecies" which are not native to either habitat. Using results from localization theory, I will show that the critical migration rate may be very small — demonstrating that evolutionary outcomes can be very sensitive to even a small amount of migration.

DY 32.9 Thu 12:45 ZEU 260

The role of population size in the evolution of microbial populations — •Joachim Krug[1], Kavita Jain[2], and Su-Chan Park[3] — [1]Institut für Theoretische Physik, Universität zu Köln, Cologne, Germany — [2]Theoretical Sciences Unit and Evolutionary and Organismal Biology Unit, Jawaharlal Nehru Centre, Bangalore, India — [3]Department of Physics, The Catholic University of Korea, Bucheon, Korea

The speed of adaptation of a population placed into a new environment is generally expected to increase with increasing population size, for at least two reasons: The supply of beneficial mutations is proportional to population size, and the probability of fixation of deleterious mutations is negligible in large populations. Contrary to this expectation, recent experiments on microbial populations have shown that small populations evolving in a complex nutrient medium may achieve a higher fitness than large ones due to the increased heterogeneity of adaptive trajectories. We introduce a class of haploid three-locus fitness landscapes that allows to investigate this scenario in a precise and quantitative way. Our main result derived analytically shows how the probability of choosing the path of largest initial fitness increase grows with the population size. This makes large populations more likely to get trapped at local fitness peaks and implies an advantage of small populations at intermediate time scales. Additional studies using ensembles of random fitness landscapes show that the results achieved for a particular choice of three-locus landscape parameters are robust and also persist as the number of loci increases.

DY 33: Brownian Motion, Stochastic Processes, Transport I

Time: Thursday 14:00–17:00 Location: HÜL 186

DY 33.1 Thu 14:00 HÜL 186

Dynamics of self-assembly of flower-shaped magnetic colloidal clusters — •Ayan Ray, Saeedeh Aliaskarisohi, and Thomas M. Fischer — Institute of Physics, Universität Bayreuth, Bayreuth 95440, Germany

In a static magnetic field paramagnetic and nonmagnetic colloids immersed in a ferrofluid self-assemble into fluctuating colloidal flowers. Adsorption and desorption of nonmagnetic petals to larger paramagnetic cores and changes in the petal conformation around the paramagnetic core induce a fluctuating dynamics. We track the motion of colloidal petals on the paramagnetic core. Adsorption and desorption of petals occur on a larger time scale than the rotational diffusion of the petals. Magnetic dipole interactions split the motion of the petals into different modes of rotational diffusion. Modes of rotational diffusion that change the petal conformation are suppressed compared to the conformation invariant rotational diffusion of all petals. The suppression of higher modes of rotational diffusion results in a subdiffusive dynamics of the individual petals.

DY 33.2 Thu 14:15 HÜL 186

Escape rate of an active Brownian particle — •P. Sekhar Burada and Benjamin Lindner — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We study the dynamics of an active Brownian particle in a spatial cubic potential, in particular, its rate of escape over the potential barrier. Here, we consider an effective nonlinear friction function, which acts as an energy pump for the Brownian particle, and study the escape dynamics of the particle by varying the amplitude of spatial cubic potential. In contrast to the Arrhenius law for the escape rate found for a normal ("passive") Brownian particle, the escape rate of an active particle shows a non-monotonic dependence on the strength of fluctuations. We explain the stochastic mechanism for this remarkable effect.

DY 33.3 Thu 14:30 HÜL 186

Quantum master equation in phase space applied to the Brownian motion in a tilted periodic potential — •William Coffey[1], Yuri Kalmykov[2], Sergey Titov[3], Liam Cleary[4], and William Dowling[1] — [1]Department of Electronic and Electrical Engineering, Trinity College, Dublin 2, Ireland — [2]Laboratoire de Mathématiques, Physique et Systèmes, Université de Perpignan, 52, Avenue de Paul Alduy, 66860 Perpignan Cedex, France — [3]Institute of Radio Engineering and Electronics, Russian Acad. Sci., Vvedenskii Square 1,Fryazino 141190, Russia — [4]Massachusetts Institute of Technology

Quantum effects in the Brownian motion of a particle in a tilted cosine potential are treated in the high temperature and weak bath-particle coupling limit using the semiclassical master equation for the time evolution of the Wigner distribution function in phase space proposed by Coffey et al. [PCCP 9, 3361, 2007]. The differential recurrence relation generated from the quantum master equation by expanding the distribution function in Fourier series are solved using matrix continued fractions yielding both the time-independent and the time-dependent periodic solutions. The time-independent periodic solution is of interest in calculating quantum effects in the dc current-voltage characteristic of a Josephson junction including the capacitance, while the time-dependent periodic solution governs dynamical properties of the junction in the locked state such as the impedance, etc. In the limit of high damping the results reproduce those yielded by the semiclassical Smoluchowski equation [W. Coffey et.al, PRE 78, 031114, 2008].

DY 33.4 Thu 14:45 HÜL 186

Langevin equation of a system nonlinearly coupled to a heat bath — •Mykhaylo Evstigneev and Peter Reimann — Universität Bielefeld, 33615 Bielefeld, Deutschland

We derive the generalized Langevin equation for a system in contact with a heat bath. In contrast to the previous treatments focusing on linear system-bath coupling, we consider a general case where the corresponding interaction potential has an arbitrary functional form, but is weak in comparison to the coupling between the bath particles. The validity of our results is demonstrated on two simple models.

DY 33.5 Thu 15:00 HÜL 186

Feedback-controlled transport in an interacting colloidal system — •Ken Lichtner and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We consider a non-equilibrium system of interacting colloidal particles driven by a constant tilting force through a periodic, symmetric "washboard" potential. As a framework for solving the equation of motion for the time-dependent density profile, we employ the Dynamical Density Functional Theory (DDFT)[1], where the microscopic particle interactions enter via a free energy functional. In [2] we demonstrate that, despite pronounced spatio-temporal correlations, the particle current can be reversed by adding suitable feedback control terms, similar to what has been found for single-particle transport[3]. We explore two distinct control protocols with time delay, focussing on either the particle positions or the density profile. Our study shows that the DDFT is an appropriate framework to implement time-delayed feedback control strategies widely used in other fields of nonlinear physics.

[1] A. J. Archer and R. Evans, J. Chem. Phys., 121 (2004) 4246.
[2] K. Lichtner and S. H. L. Klapp, Europhys. Lett., accepted.
[3] D. Hennig, Phys. Rev. E, 79 (2009) 041114.

DY 33.6 Thu 15:15 HÜL 186

Entropic transport in energetic potentials — P. Sekhar Burada[1], Yunyun Li[2], Wolfgang Riefler[2], and •Gerhard Schmid[2] — [1]MPI für Physik komplexer Systeme, Germany —

[2]Universität Augsburg, Germany

We study the transport of point size particles in micro-sized two dimensional periodic channels [1]. The channels exhibit periodically varying cross sections. The particles are subjected to a constant external force acting alongside the direction of the longitudinal channel axis and a varying force stemming from a periodic substrate potential. While particle transport in tilted periodic potentials is facilitated by noise, the transport through pores with periodically varying cross-section worsens with increasing noise level, i.e. increasing temperature. The competition between the noise-assisted propagation for energetic potentials and the hampered transport in confined structures leads to a striking, non-monotonic behavior which sensitively depend on the phase lag of the periodic channel structure and the periodic potential. By controlling this phase lag the symmetry could be broken and rectification observed.

[1] P.S. Burada, Y. Li, W. Riefler, G. Schmid, Chem.Phys. **375**, 514 (2010).

15 min. break.

DY 33.7 Thu 15:45 HÜL 186

Nano-Mechanical Single-Electron Devices — •Alex Croy and Alex Eisfeld — MPI-PKS Dresden

The fabrication and utilization of nanoscale machines and devices is one of the great promises of the 21st century. In particular, so-called *nanoelectromechanical systems* provide intriguing possibilities for applications beyond common paradigms. The involvement of mechanical parts promises increased robustness, low power-consumption and higher operating temperature compared to conventional devices. One paradigm in this regard is the *nanomechanical single-electron transistor (NEMSET)* proposed by Gorelik et al. which can exhibit mechanically assisted charge transport.

In this context, we present theoretical results for two new nanomechanical single-electron devices, which promise interesting applications. The first device consists of two couples NEMSETs and can be used for storage of information. The second device is a single-electron rotor, which generalizes the NEMSET concept and can act as a charge pump.

DY 33.8 Thu 16:00 HÜL 186

Diffusion of active Brownian particles with coloured angular noise — •Christian Weber and Lutz Schimansky-Geier — Department of Physics, Humboldt Universität zu Berlin, Germany

Motivated by the motion of biological agents we introduce a model of a self-propelled particle with coloured angular noise given by an Ornstein-Uhlenback process (OUP). The consideration of OUP driven noise leads to trajectories which are reminiscent of searching behaviour of animals. We derive analytical results for the angular correlation function and the mean square displacement (MSD). The impact of the correlation time of the OUP on the MSD is discussed for different scalings of the noise intensity in the OUP. A possible connection to polymer physics (worm-like chains) will be briefly discussed.

DY 33.9 Thu 16:15 HÜL 186

Brownian motion with active fluctuations — •Pawel Romanczuk and Lutz Schimansky-Geier — Department of Physics, Humboldt Universität zu Berlin, Germany

We analyze dynamics of particles with fluctuating velocity and orientation in two spatial dimensions. We distinguish passive (e.g. thermal fluctuations) and active fluctuations which emerge in active systems far from equilibrium as for example living organisms or chemically driven colloids. We derive analytical expressions for the speed and velocity distributions for generic models of (active) Brownian particles in two spatial dimensions. The presence of active fluctuations already for simple Stokes friction results in speed and velocity distributions which differ from the classical Maxwell distribution. Active Gaussian fluctuations lead to speed distributions increasing as $\sim |v|^\alpha$ with $\alpha < 1$ at small speeds $|v| \ll 1$ which results in a divergence of the corresponding stationary Cartesian velocity distributions at the origin. Finally we show that such a behavior occurs also for non-Gaussian active fluctuations (shot noise).

Topical Talk DY 33.10 Thu 16:30 HÜL 186

Motion States in Intracellular Transport — •Doris Heinrich — Faculty of Physics and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Geschwister-Scholl-Platz 1, 80539 München, Germany

The living cell's cytoskeleton is a fascinating active network, in which diffusion is intercepted by distinct phases of directed transport. To dissect temporal phases (i) of active, directed motion of a tracer particle along a cellular filament and (ii) motion in the diffusive regime, a time-resolved statistical mean-squared-displacenment (MSD) analysis was applied. In living amoeba, the distribution of active lifetimes for an intracellular particle, moving along microtubules via ATP-driven biomotors, is found to decay exponentially with a characteristic lifetime of about t=0.5s [1]. However in motor neurons, cellular vesicles show very efficient directed transport for large distances, whereas inserted non-functionalized nanoparticles mostly undergo subdiffusion [2]. To investigate the time-dependent contributions of cytoskeletal components on diffusive motion states in the crowded cellular interior, a local, lag-time dependent MSD analysis was employed. Cellular fine-tuning from Brownian to subdiffusive motion could be extracted, which enables effective interplay of intracellular molecules on the nanoscale. This active actin-microtubule interplay is not only important for intracellular transport, but also contributes to active cellular stability and other cell functions, like cellular migration [3].

[1] PRL101:248103(2008) [2] ChemPhysChem10:2884(2009)
[3] Annu.Rev.Condens.MatterPhys.1:257(2010)

DY 34: Fluid Dynamics and Turbulence II

Time: Thursday 14:00–16:15 Location: ZEU 255

Topical Talk DY 34.1 Thu 14:00 ZEU 255

Dynamics of particles in turbulent flow: size matters — •Holger Homann[1,2], Jérémie Bec[1], and Rainer Grauer[2] — [1]Laboratoire Cassiopée, OCA, Nice, France — [2]Theoretische Physik I, Ruhr-Universität Bochum

This presentation aims at a detailed understanding of the dynamical properties of finite-size particles transported by a turbulent flow. The statistics of these particles is of great importance in many engineering and environmental problems. Up to now mostly simple models are used which on the one hand consider those particles as point-like objects and one the other hand neglect their back-reaction on the carrier-flow (passive particles). Experiments have recently shown the limits of such models. We are going beyond these simple models by means of direct numerical simulations of particles larger than the small-scale structures in high Reynolds number turbulence. The combination of a standard pseudo-spectral and a penalty technique allows us to precisely control the carrier-flow and to impose the no-slip boundary condition at the surface of the particles. A selection of questions we are going to discuss: What is the range of validity of the point-models? How is turbulence modified in the vicinity of a particle? How to build a finite-size model?

DY 34.2 Thu 14:30 ZEU 255

Pressure boundary conditions for multiphase lattice-Boltzmann simulations — •Ariel Narváez[1] and Jens Harting[1,2] — [1]Departament of Applied Physics, TU Eindhoven, P.O. Box 513. NL-5600MB Eindhoven, The Netherlands — [2]Institut für Computerphysik, Universität Stuttgart, 70569 Stuttgart

For a broad range of applications of multiphase fluid systems, the lattice-Boltzmann (LB) method together with the Shan&Chen (SC) model [1] has been successfully applied. A number of boundary conditions are available to be provided for such simulations, i.e., periodic, no-slip and wettability boundary conditions on solid surfaces. Even though, numerous applications require pressure or flux boundary conditions, an implementation of those together with the SC model has not been presented so far. We developed an implementation of the well known D3Q19 LB method integrating the SC model for multiphase flows together with Zou&He [2] on-site boundary conditions. To demonstrate the applicability of the method we show results of simulations of capillary flow and of a flow focussing device.

[1] X. Shan and H. Chen. Phys. Rev. E, 47:1815-1820 (1993)
[2] Q. Zou and X. He. Phys. Fluids., 9:1591-1598 (1997)

DY 34.3 Thu 14:45 ZEU 255

LES using Lattice Boltzmann Methods — •Georg Eitel-Amor, Matthias Meinke, and Wolfgang Schröder — Aerodynamisches Institut, RWTH Aachen University, Aachen

Over the last two decades the Lattice Boltzmann Method (LBM) has received a growing interest due to its efficient handling of complex geometries and its parallel scalability. The LB approach is based on the Boltzmann equation and describes macroscopic quantities using a simplified model of microscopic kinetics. The present work focuses on the application of LBM to large-eddy simulations (LES) of wall-bounded turbulent flows on hierarchically refined meshes. The single-relaxation time model, the multiple-relaxation time model, and the cascaded LBM have been analyzed concerning their stability and numerical dissipation. Besides the standard Smagorinsky technique, a dynamic eddy-viscosity model has been introduced and both techniques are validated for different flow regimes.

DY 34.4 Thu 15:00 ZEU 255

Dynamical model for the formation of patterned deposits at receding contact lines — •Uwe Thiele, Lubor Frastia, and Andrew J. Archer — Department of Mathematical Sciences, Loughborough University, Loughborough, Leicestershire, LE11 3TU, UK

We describe the formation of deposition patterns that are observed in many different experiments where a three-phase contact line of a volatile nanoparticle suspension or polymer solution recedes [1]. A dynamical model based on a long-wave approximation predicts the deposition of irregular and regular line patterns due to self-organised pinning-depinning cycles corresponding to a stick-slip motion of the contact line [2]. We analyze how the line pattern properties depend on the evaporation rate and solute concentration.

[1] R. D. Deegan et.al, Nature 389, 827 (1997); G. Berteloot et. al, Phys. Rev. E (2010), submitted; H. Yabu and M. Shimomura, Adv. Funct. Mater. 15, 575 (2005); J. Xu et al., Phys. Rev. Lett. 96, 066104 (2006); S. W. Hong, J. F. Xia, and Z.Q. Lin, Adv. Mater. 19, 1413 (2007); H. Bodiguel, F. Doumenc, and B. Guerrier, Langmuir 26, 10758 (2010).

[2] L. Frastia, A. J. Archer and U. Thiele, submitted (2010), at arxiv: http://arxiv.org/abs/1008.4334v1

DY 34.5 Thu 15:15 ZEU 255

Sound scattering on irrotational vortices — •Piotr Marecki — Uni Duisburg-Essen

In the talk I will discuss the current status of the problem of sound scattering on typical vortex lines in superfluids. I will use hydrodynamical approximation, in which sound will be regarded as small (test) perturbation of a given background flow. I will use the acoustic-spacetime approach, which quite directly leads to the central issues of the problem. Curiously, this classical subject has deep connections to other important problems of theoretical physics, including: Bohm-Aharonov scattering, spectral analysis of systems with singular potentials, and behavior of classical/quantum fields in rotating spacetimes. Despite many efforts over the last 130 years, in the opinion of the author, the subject cannot be regarded as closed, and new important advances continue to be made. In particular, I will draw attention to the issues of boundary conditions at the vortex core and at infinity, and to the consequences of various (mathematically allowed) choices for the physical scattering characteristics.

DY 34.6 Thu 15:30 ZEU 255

Vortex-dipole chaos solves last enigma of classical physics: turbulence. — •Helmut Baumert — IAMARIS, Bei den Mühren 69 A, 20457 Hamburg

The talk sketches a statistical quasi-particle approach to idealized fluid turbulence at asymptotically high Reynolds numbers, based on an ensemble of dipole vortex tubes realized in geometrically non-trivial forms like rings etc. In a cross sectional area through a vortex tangle, taken locally orthogonal through each individual tube, the dipoles are moving with the classical dipole velocity. The effective vortex radius is related with Prandtl's classical mixing length.

A quasi-particle is dressed, embedded in a cloud of others. Its energy is finite. It performs a local quasi-2D dipole chaos, reminding of real gases. Collisions between stable quasi-particles lead either to scattering (turbulent diffusion) or to particle annihilation (formation of unstable couples as stationary dissipative patches via the "devil's gear" of Herrmann, 1990, down to a scale of size zero).

This geometrization allows to derive equations of turbulent motions and of fundamental constants like von Karman's or two Kolmogorov spectral constants - in agreement with observations. In particular, it allows a better understanding of stratified flows (collapsing turbulence, whitecapping of internal gravity waves).

This work relates to Department of the Navy Grant N62909-10-1-7050 issued by Office of Naval Research Global. The talk will be given in German.

DY 34.7 Thu 15:45 ZEU 255

Stochastic modeling of lift dynamics under turbulent conditions — •Muhammad Ramzan Luhur, Patrick Milan, Jörge Schneemann, Matthias Wächter, and Joachim Peinke — ForWind, Centre for Wind Energy Research, University of Oldenburg, D-26111, Germany.

This paper presents stochastic modeling of the lift dynamics of an airfoil placed in turbulent inflows. The measurements were taken in the closed wind tunnel of the University of Oldenburg, for an airfoil FX 79-W-151A. The turbulent flows were generated using different grids including a fractal one, installed in front of the wind tunnel test section nozzle. The measurements were performed by two methods i.e. using force sensors and wall pressure sensors. The force sensors were installed at the two ends of an airfoil in the flap-wise direction and the pressure sensors at the test section walls.

For the stochastic modeling of the lift dynamics, force measurements with the fractal grid are used here because the force sensors give better results than the pressure sensors. The modeling of the lift coefficient is based on measurement time series of lift coefficient. This is done using a first-order stochastic differential equation called the Langevin equation. The results are optimized using a chi-square test on the probability distribution functions. The modeled time series and their probability distribution functions show good agreement with the actual measurement. The model is being developed with the aim to integrate it into a general wind energy converter model.

DY 34.8 Thu 16:00 ZEU 255

Generation of homogeneous shear turbulence by using an active grid — •Erwin Renken, Pascal Knebel, and Michael Hölling — Carl von Ossietzky Universität Oldenburg

We generate a shear turbulence by using an active grid in a wind tunnel. This shear turbulence is homogeneous, so it has a constant gradient of the mean velocity. The active grid consist of rods with small flaps, where some rods are in horizontal and some in vertical direction. Each rod is connected to a step motor, and can rotate in a specified way. We are using a protocol which describe the time-dependent angle of each axis. We use the horizontal axis primary for a default blockage diterming the gradient, and the vertical to generate homogeneous turbulence by moving the flaps. With this approach we aim to remodel specific properties of the atmospheric layer.

DY 35: ISS Transport and Localization of interacting Bosons II

Time: Thursday 14:30–16:00 Location: BAR Schön

DY 35.1 Thu 14:30 BAR Schön

Interband dynamics in a many-body Wannier-Stark system — •Carlos Parra Murillo[1], Javier Madroñero[2], and Sandro Wimberger[1] — [1]Institut fuer theoretische Physik, Heidelberg University, D-69120, Heidelberg, Germany — [2]Physik Department, Technische Universitaet Muenchen, D-85747 Garching, Germany

In the last years the dynamics of ultracold atoms, in particular Bose condensates loaded into optical lattices, have become amply studied in view of interesting phenomena like Landau-Zener tunnelling, resonantly enhanced tunnelling (RET) and Bloch oscillations. Regular

and chaotic regimes can be reached by varying the parameters in the many-body description of ultracold bosons [1]. We present results obtained by studying the dynamical properties of a two-band Bose-Hubbard Hamiltonian for a one-dimensional tilted optical lattice [2]. We compare the interband dynamics for the single particle limit and for the fully interacting system, by computing the average occupation of the upper band. The spectral properties (avoided crossings) provide a comprehensive understanding of the dynamics close to RET as a control parameter is varied and the number of particles is increased. The dynamical correlations between the bands imply interesting perspectives for state-of-the-art experiments with ultracold bosons.

[1] A. Tomadin, R. Mannella, and S. Wimberger, Phys. Rev. Lett. 98, 130402 (2007). [2] P. Ploetz, J. Madroñero, and S. Wimberger, J. Phys. B 43, 081001(FTC) (2010).

DY 35.2 Thu 14:45 BAR Schön

Stability and decay of Bloch oscillations in Bose-Einstein condensates with time-dependent atom-atom interactions — •Christopher Gaul[1], Elena Díaz[1,2], Cord A. Müller[3], Rodrigo Lima[4], and Francisco Domínguez-Adame[1] — [1]GISC, Departamento de Física de Materiales, Universidad Complutense, E-28040 Madrid, Spain — [2]Institute for Materials Science, Technische Universität Dresden, D-01062 Dresden, Germany — [3]Centre for Quantum Technologies, National University of Singapore, Singapore 117543, Singapore — [4]Instituto de Física, Universidade Federal de Alagoas, Maceió AL 57072-970, Brazil

Bose-Einstein condensates in tilted optical lattices allow the observation of Bloch oscillations (BOs). Generically, the interaction leads to dephasing and to the decay of the wave packet. By means of Feshbach resonances, however, experimentalists can tune the s-wave scattering length to zero or modulate it in time. We investigate the effect of such time-managed interactions on BOs. Additionally to the noninteracting case and a solitonic solution, we find an infinite family of modulations that preserve the Bloch oscillating wave packet [1]. In these cases, the stability follows from a time-reversal argument. In the unstable cases, we employ a collective-coordinates ansatz and a stability analysis, in order to quantify the decay of the BOs. In particular we show that in presence of external perturbations, an additional modulation of the interaction can enhance the lifetime of the Bloch oscillation [2].

[1] Gaul et al. PRL 102, 255303 (2009)
[2] Díaz et al. PRA 81, 051607R (2010)

DY 35.3 Thu 15:00 BAR Schön

Wave packet surgery in driven optical lattices — •Stephan Arlinghaus and Martin Holthaus — Institut für Physik, Carl von Ossietzky Universität, D-26111 Oldenburg

The dynamics of particles in a periodic potential under the influence of homogeneous external forcing is governed by Bloch's acceleration theorem, provided the single-band approximation remains viable. However, interband transitions induced by strong time-periodic forces, which lie ouside the scope of this old approach, offer most interesting perspectives for coherent control. We show how a generalized acceleration theorem, based on the use of Floquet states, leads to novel control strategies, allowing one to selectively "cut out" certain parts from the particles' wave packets. Ultracold atoms in driven optical lattices provide experimentally accessible testing ground for these ideas.

DY 35.4 Thu 15:15 BAR Schön

Weak (anti-)localization of Bose-Einstein condensates in two-dimensional chaotic cavities: numerical results — •Timo Hartmann[1], Juan Diego Urbina[1], Klaus Richter[1], and Peter Schlagheck[2] — [1]Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany — [2]Département de Physique, Université de Liège, 4000 Liège, Belgium

The possibility to induce artificial magnetic gauge potentials for matter waves [1] and to create almost arbitrarily shaped confinement potentials [2] makes it now interesting and feasible to study coherent transport of Bose-Einstein condensates through various mesoscopic structures. Previous theoretical studies have focused on the question how coherent backscattering in disordered potentials is modified by the presence of the atom-atom interaction [3]. We now study the analogous scenario of weak localisation in ballistic billiard geometries which exhibit chaotic classical dynamics. To this end we numerically investigate the quasi-stationary propagation of a condensate through such structures within the mean-field approximation. The transmission is measured as a function of the magnetic gauge field and of the non-linearity. With increasing non-linearity an inversion of the weak-localisation peak is visible and its origin will be discussed.

[1] Y.-J. Lin et al., Phys. Rev. Lett. **102** 130401 (2009)
[2] K. Henderson et al., New J. Phys. **11**, 043030(2009)
[3] M. Hartung et al., Phys. Rev. Lett. **101**, 020603 (2008).

DY 35.5 Thu 15:30 BAR Schön

Destruction of localization in a nonlinear generalization of the quantum kicked rotor — •Goran Gligorić, Joshua Bodyfelt, and Sergej Flach — MPI für Physik komplexer Systeme

Quantum suppression of classically chaotic diffusion was first observed numerically in the quantum kicked rotor model. This phenomenon can be considered in many aspects as the dynamical version of Anderson localization in tight-binding disordered models [1]. In the case of the kicked rotor there is no true randomness and diffusion after an initial time interval appears, resulting from chaotic dynamics in the corresponding classical counterpart. The realization of Bose-Einstein condensates has opened a new opportunity for studying dynamical systems in the presence of many-body interactions. In the mean field approximation, these interactions can be represented by adding a quartic nonlinearity in the Schrödinger equation. Our aim is to utilize such a model, as introduced by Shepelyansky [2] in order to understand how nonlinearity generally affects the kicked rotor model. Particularly, we aim to understand the influence of nonlinearity on dynamical localization; of special concern is the possibility of a critical nonlinear strength above which localization is destroyed, and how this destruction comes about. Lastly, we will consider the corresponding anomalous subdiffusion law in this regime and test its universality.

[1] S. Fishman, D.R. Grempel and R.E. Prange, Phys. Rev. A 29 (1984) 1639
[2] D.L. Shepelyansky, Phys. Rev. Lett. 70 (1993) 1787

DY 35.6 Thu 15:45 BAR Schön

Localization of two interacting bosons in a random potential — •Dmitry Krimer[1,2], Ramaz Khomeriki[1,3], and Sergej Flach[1] — [1]Max Planck Institute for the Physics of Complex Systems, 01189 Dresden, Germany — [2]Institute for Theoretical Physics, University of Tuebingen, 72076 Tübingen — [3]Physics Department, Tbilisi State University, 0128 Tbilisi, Georgia

We study the dynamics of two interacting bosons in one-dimensional random lattices using the Bose-Hubbard model. In the absence of interaction all eigenstates are spatially localized and both particles follow the single particle dynamics corresponding to Anderson localization. Our study aims to clarify the interplay of disorder and interactions in few-body dynamics. In particular, we calculate the enhancement factor of the localization length l_2 in comparison to the single particle localization length l_1 for weak disorder performing rigorous numerical calculations. Previous studies based on the mapping of the two-particle problem onto a physically relevant matrix model contained different statements on this issue [1]. Our findings are in tact with predictions, which follow from the statistical properties of the overlap integrals of single particle eigenvectors [2].

[1] D.L. Shepelyansky, Phys. Rev. Lett. 73, 2607 (1994); K. Frahm, A. Müller-Groeling, J.-L. Pichard, D. Weinmann, Europhys. Lett., 31, 169 (1995)
[2] D.O. Krimer, S. Flach, Phys. Rev. E 82, 046221 (2010)

DY 36: Statistical Physics in Biological Systems IV (organised by BP)

Time: Thursday 14:00–16:45 Location: ZEU 260

DY 36.1 Thu 14:00 ZEU 260

Evolution of complex chemical mixtures: a problem linked to the origin of life — •Eva Wollrab[1], Sabrina Scherer[1], Christian Lay[1], Manuel Worst[1], Philipp Zimmer[2], Karsten Kruse[2], and Albrecht Ott[1] — [1]Universität des Saarlandes, Biologische Experimentalphysik, 66123 Saarbrücken — [2]Universität des Saarlandes, Theoretische Biologische Physik, 66123 Saarbrücken

How self-reproducing structures can form in a chemical mixture and how a steady increase in biochemical complexity of these cycles may occur is still unknown. We approach this question experimentally from two different directions.

In the first class of experiments highly reactive, primitive compounds are mixed. We track the temporal development of the mixture using mass spectroscopy for analysis. Tools from bioinformatics help us to develop ideas about the underlying chemical network.

The second class of experiments employs DNA. The DNA is designed to form autocatalytic reaction pathways. These experiments are designed to inductively find new conditions for self-reproducing chemical cycles. We suggest that this situation can be simulated in silico by autocatalytic reactions that exhibit fluctuations of the reaction pathways.

DY 36.2 Thu 14:15 ZEU 260

Complexity-stability relations in generalized food-web models with realistic parameters — •Sebastian Plitzko, Christian Guill, and Barbara Drossel — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt, Germany

We investigate conditions for positive complexity-stability relations in the niche model for food webs by evaluating the local stability of the fixed points of the system. We use a generalized method, where the fixed points are normalized to 1, which allows for an efficient numerical evaluation. We find that positive relations between local stability and complexity can be obtained if prey is not scarce, biomass loss due to predation is low and density-dependent mortality effects dominate over other contributions to mortality. Since these conditions are expressed in terms of the generalized parameters, we then determine the range of values of these parameters within locally stable niche model food webs with explicit dynamical equations. These equations include allometric scaling and parameter values that are realistic. We find that the values of the generalized parameters obtained from this explicit dynamical model depend on the trophic level. The range of these parameters is such that positive complexity-stability relations can be obtained.

DY 36.3 Thu 14:30 ZEU 260

Statistical topography of fitness landscapes — •Jasper Franke[1], Alexander Klözer[1], J. Arjan G. M. de Visser[2], and Joachim Krug[1] — [1]Cologne University, Cologne, Germany — [2]Wageningen University, Wageningen, Netherlands

The adaptive evolution of a population under the influence of mutations and selection is governed by the structure of the underlying fitness landscape. Previous theoretical studies of topographical quantities on fitness landscapes have mostly focused on local properties such as local maxima.

Here we investigate the global property of accessible paths traversing the complete genome configuration space towards the global optimum. Numerical and analytical studies and comparison to empirical data suggest a surprising unversality across almost all established theoretical models, indicating high accessibility of the globally optimal configuration in the biologically relevant limit of very long genome sequences.

DY 36.4 Thu 14:45 ZEU 260

Speed of Evolution in Spatially Extended Populations — •Erik A. Martens and Oskar Hallatschek — Group for Biophysics and Evolutionary Dynamics, Max Planck Institute for Dynamics and Self-Organization, 37073 Göttingen, Germany

How fast do species adapt to a given environment? This is one of the most fundamental questions in evolutionary biology. Many theoretical models are restricted to the case of well-mixed populations. To characterize the speed of evolution in spatially extended populations, it is necessary to consider the wave-like spread of evolutionary novelties. The presence of such wave-like sweeps reduces the speed of evolution for two reasons. First, the waves are slower than the exponential spread of beneficial mutations known from well-mixed populations. Second, because these sweeps are slower, spatially extended populations are more prone to be in a state where multiple beneficial mutations sweep simultaneously. This problem of clonal interference has been demonstrated in microbial experiments and has recently gained strong interest. We simulate the spread of mutations in spatial dimensions using computer simulations, where we include effects of recombination and long-range migration. We find that 1) the adaptation rate obeys robust power laws, which 2) are independent of the particular choice of selective fitness distributions ("universality"), 3) that spatial populations experience clonal interference over a broader range of parameters, and 4) that the effects of clonal interference can be mitigated by recombination and long-range migration. We therefore speculate that both processes are selectively favorable.

DY 36.5 Thu 15:00 ZEU 260

Predators, parasites and food web stability — •Lars Rudolf[1], Neo Martinez[2], and Thilo Gross[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [2]Pacific Ecoinformatics and Computational Ecology Lab, Berkley, USA

Predator-prey interactions and their influence on food web stability are a major topic of ecological research. The investigation of parasitic interactions, which are another fundamental part of the most ecological communities, has been less intensive. To close that gap, we used generalized modeling and studied several million replicates of food webs with different proportions of parasitic species. In this way we determine the impact of parasitism on different food web properties and how these properties affect food web stability. Specifically, we show that a moderate proportion of parasitic species enhances food web stability.

15 min. break

DY 36.6 Thu 15:30 ZEU 260

Dynamics of mutants in a stochastic compartment approach of hematopoiesis — •Benjamin Werner and Arne Traulsen — Research Group for Evolutionary Theory, Max Planck Institute for Evolutionary Biology, 24306 Plön

Cancer is typically caused by at most a handful of mutations that increase the reproductive fitness of a single cell. The probability of such a mutation, the dynamics of the resulting clone of cancer cells, and thus the effect to an organism is under intense investigation. First we present an established stochastic multicompartment model of hematopoiesis [1,2] (CML) as well as other blood disorders [3,4] can be embedded and analyzed in this framework. We show that there is a closed deterministic solution to the dynamics of mutants in this model that fits the averages of the stochastic process. This solution enables us to connect different model parameters directly to observed cell dynamics and thus gives in principle yet unknown information about disease progression and the impact of drug treatment.

Ref.:
[1] D. Dingli, A. Traulsen and J. M. Pacheco, PLoS ONE 2, e345 (2007).
[2] D. Dingli, A. Traulsen, T. Lenaerts and J. M. Pacheco, Genes & Cancer 1(4) 309-315 (2010).
[3] D. Dingli, J. M. Pacheco and A. Traulsen, Phys. Rev. E 77, 021915 (2008).
[4] A. Traulsen, J. M. Pacheco, L. Luzzatto and D. Dingli, BioEssays Vol.32 Issue 11 (2010).

DY 36.7 Thu 15:45 ZEU 260

Stochastic slowdown in evolutionary processes — •Philipp M. Altrock, Chaitanya S. Gokhale, and Arne Traulsen — Max-Planck-Institute for Evolutionary Biology, Plön

We examine birth–death processes with state dependent transition probabilities and at least one absorbing boundary. In evolution, this describes selection acting on two different types in a finite population where reproductive events occur successively. If the two types have equal fitness the system performs a random walk. If one type has a fitness advantage it is favored by selection, which introduces a bias (asymmetry) in the transition probabilities. How long does it take un-

til advantageous mutants have invaded and taken over? Surprisingly, we find that the average time of such a process can increase, even if the mutant type always has a fitness advantage. We discuss this finding for the Moran process and develop a simplified model which allows a more intuitive understanding. We show that this effect can occur for weak but non–vanishing bias (selection) in the state dependent transition rates and infer the scaling with system size. We also address the Wright–Fisher model commonly used in population genetics, which shows that this stochastic slowdown is not restricted to birth–death processes.

[1] Altrock, Gokhale, and Traulsen, Physical Review E 82, 011925 (2010)

DY 36.8 Thu 16:00 ZEU 260

Food Quality in Producer-Grazer Models — •Dirk Stiefs[1], George van Voorn[2], Bob Kooi[3], Ulrike Feudel[4], and Thilo Gross[1] — [1]Max-Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Wageningen University and Research Centre, Wageningen, The Netherlands — [3]Vrije Universiteit, Amsterdam, The Netherlands — [4]ICBM, Carl von Ossietzky Universität, Oldenburg, Germany

Stoichiometric constraints play a role in the dynamics of natural populations, but it is not yet resolved how stoichiometry should be integrated in population dynamical models, as different modeling approaches are found to yield qualitatively different results. We use the approach of generalized modeling to investigate the effects of stoichiometric constraints on producer-grazer systems. The stability of steady states can be analyzed by using a normalization technique to plot 3-dimensional bifurcation diagrams. Because we do not specify the functional form of the processes in the generalized model our results hold for a whole class of stoichiometric producer-grazer systems.

To understand the differences and commonalities between specific stoichiometric models we map the specific bifurcation diagrams into the generalized parameter space. On the one hand, these combined bifurcation diagrams show how the generic results of the generalized analysis are represented in the specific model. On the other hand, it becomes clear that some model features like the sequence of bifurcations observed during enrichment scenarios can be tied to specific modeling assumptions and are hence not structurally stable.

DY 36.9 Thu 16:15 ZEU 260

Evolutionary Game Theory in Growing Populations — •Anna Melbinger, Jonas Cremer, and Erwin Frey — Ludwig-Maximilians Universität, Munich, Germany

Existing theoretical models of evolution focus on the relative fitness advantages of different mutants in a population while the dynamic behavior of the population size is mostly left unconsidered. We here present a generic stochastic model which combines the growth dynamics of the population and its internal evolution. Our model thereby accounts for the fact that both evolutionary and growth dynamics are based on individual reproduction events and hence are highly coupled and stochastic in nature. We exemplify our approach by studying the dilemma of cooperation in growing populations and show that genuinely stochastic events can ease the dilemma by leading to a transient but robust increase in cooperation.

[1] Phys. Rev. Lett. 105, 178101 (2010)

DY 36.10 Thu 16:30 ZEU 260

A Non-Equillibrium Phase Transition in Expanding Populations — •Jan-Timm Kuhr and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München

Recently, expanding bacterial populations found much attention in both experimental and theoretical work [1]. These "range expansions" have interesting statistical properties, as constant genetic re-sampling from a small population at the expanding front induces strong fluctuations. The influence of non-neutral mutations on the dynamics is less well studied. Here, we introduce an extension of the Eden model [2], including mutations. Using Monte Carlo simulations, we analyze the interplay of kinetic surface roughening, mutations and selection at the front. While beneficial mutations always take over the front eventually, for detrimental mutations one finds two generic cases: if rare, mutant sectors are independent and wild types prevail. If mutants spawn more frequently, sectors coalesce and wild types are soon lost in the bulk. Between these regimes one finds self-affine patterns, and we identify a non-equilibrium phase transition. We measure critical exponents near this transition, and find universal scaling behavior for this model of evolution in expanding populations.

[1] O. Hallatschek and D. Nelson, Life at the front of an expanding population. Evolution, **64**, 193-206, (2010) – [2] M. Eden, A two-dimensional growth process, Proc. of the Fourth Berkeley Symposium on Mathematical Statistics and Probability, **4**, 223-239, (1960)

DY 37: Quantum Chaos II

Time: Thursday 16:00–17:15 Location: ZEU 118

DY 37.1 Thu 16:00 ZEU 118

Efficiency of quantum ratchets — •Fei Zhan, Sergey Denisov, Alexey V. Ponomarev, and Peter Hänggi — Insitute of Physics, University of Augsburg, Germany

Directed transport of matter-waves in optical periodic potentials can be initiated by modulation of the potential height, provided that the modulation protocol violates all relevant time and space symmetries. Quantum ratchets [1, 2] might be considered as a potentially new tool for the delivery of cold atoms to a desirable location. Unfortunately, the quantum transport is severely hampered by the diffusive spreading, which is enhanced by tunneling. The optimal regime is the one that maximizes net velocity and minimizes dispersion of the wave packet. We explore the impact of diffusion on the nonequlibrium quantum transport, focusing on the initially localized wave packets. By using a quantum version of the Péclet number, i.e. the ratio between the group velocity and the ballistic dispersion of a propagating matter-wave, we obtain the recipe for the optimization of quantum ratchet performance.

[1] S. Denisov, L. Morales-Molina, S. Flach, and P. Hänggi, Phys. Rev. A 75, 063424 (2007)

[2] T. Salger et al., Science 326, 1241 (2009)

[3] L. Machura et al., J. Phys. - Condensed Matter 17, S3741 (2005)

DY 37.2 Thu 16:15 ZEU 118

Transport in Rough Quasi-One-Dimensional Systems — •Otto Dietz[1], Ulrich Kuhl[1,2], Hans-Jürgen Stöckmann[1], Felix M Izrailev[3] und Nykolay M Makarov[3] — [1]Universität Marburg, Germany — [2]Université de Nice, France — [3]Universidad de Puebla, Mexico

Scattering at rough disordered boundaries strongly influence the conductance of nanowires. For rough silicon nanowires a much higher ratio of electric conductivity to thermal conductivity has been reported than expected from the Wiedemann-Franz law [1]. These findings have not been explained yet.

In the case of bulk disorder it is well known that correlations can drastically change conductance properties [2]. Similar effects have been predicted for rough nanowires [3] but drew little attention before their applicability to conductivity in silicon nanowires became evident.

We present a first experimental test of this theory in microwave waveguides with rough walls. Because of the strict analogy between the 2d Schrödinger equation and the Helmholtz equation, the results can be directly applied to electron transport in nano structures. Microwave techniques can be helpful because in contrast to real nanowires the surface roughness is both known and controllable. We could confirm that certain rough boundaries can block or enhance wave transport in given frequency windows.

[1] A. I. Hochbaum, et. al., Nature 451, 163 (2008).

[2] U. Kuhl, et.al., Appl. Phys. Lett. 77, 633 (2000).

[3] M. Rendón, et.al., Phys. Rev. B 75, 205404 (2007).

DY 37.3 Thu 16:30 ZEU 118

GOE-GUE transition catastrophe in many body systems — •Quirin Hummel, Juan Diego Urbina, Jack Kuipers, and Klaus Richter — Institute of Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

The quantum spectral fluctuations of classically chaotic systems un-

dergo a transition between the orthogonal (GOE) and unitary (GUE) universality classes when a weak magnetic field is applied. In the context of Random Matrix Theory, closed analytical expressions for measures of spectral fluctuations (as the spectral form factor) are known for the full transition, and a semiclassical understanding of such results for single particle systems has emerged during the last years. We study how the semiclassical analysis is affected by going from single particle dynamics to a many body system of identical particles. We report here the apparent existence of a catastrophe in the GOE to GUE regime, in the sense that the mathematical limit where the number of particles tends to infinity produces a transition which is either infinitely slow or infinitely fast with respect to the magnitude of the applied magnetic field. We investigate to what extent interactions play a role in the corresponding analysis.

DY 37.4 Thu 16:45 ZEU 118

Fractal Weyl law for three-dimensional chaotic hard-sphere scattering systems — •Alexander Eberspächer[1], Jörg Main[2], and Günter Wunner[2] — [1]Institut für Theoretische Physik, Otto-von-Guericke Universität, 39016 Magdeburg, Germany — [2]Institut für Theoretische Physik 1, Universität Stuttgart, 70550 Stuttgart, Germany

The fractal Weyl law [1] connects the asymptotic level number with the fractal dimension of the chaotic repeller. We provide the first test for the fractal Weyl law for a three-dimensional open scattering system.

For the four-sphere billiard, we investigate the chaotic repeller and discuss the semiclassical quantization of the system by the method of cycle expansion with symmetry decomposition. We test the fractal Weyl law for various symmetry subspaces and sphere-to-sphere separations [2].

[1] W. T. Lu, S. Sridhar, and M. Zworski, Phys. Rev. Lett. 91, 154101 (2003).

[2] A. Eberspächer, J. Main, G. Wunner, Phys. Rev. E 82, 046201 (2010)

DY 37.5 Thu 17:00 ZEU 118

From Fragile to Robust Pseudo-Hermitian Phase in Disordered PT-Symmetric Lattices — •Ragnar Fleischmann — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen

Non-hermitian Hamiltonians exhibiting PT-symmetry have sparked an extensive research effort in recent years due to their intriguing property of allowing for a pseudo-hermitian phase with an all real eigenvalue-spectrum [1]. This *PT-symmetric phase* in general will be spontaneously broken with the variation of a (gain/loss) parameter giving way to a *phase of brokenPT-symmetry* with a fully or partially complex spectrum. Theoretical work on *PT-systems* spans from quantum field theory to solid state physics. Most recently, however, with the first experimental realizations of such systems using optical wave guides [2] the center of interest shifted onto photonic systems. Here I will present our recent results on the influence of disorder on symmetry breaking and dynamics in PT-symmetric tight binding models [3] that can be used to describe light propagation in optical wave guide arrays.

[1] C. M. Bender, Rep. Prog. Phys. 70, 947-1018 (2007).

[2] A. Guoet al., Phys. Rev. Lett. 103, (2009); C.E. Rüter et al, Nat Phys (2010).

[3] O. Bendix, R. Fleischmann, T. Kottos, and B. Shapiro, Phys. Rev. Lett. **103**(3):030402 (2009); O. Bendix, R. Fleischmann, T. Kottos, und B. Shapiro, J. Phys. A: Math. Theor. 43, 265305 (2010); M.C. Zheng, D.N. Christodoulides, R. Fleischmann, and T. Kottos (2010) Phys. Rev. A **82**(1):010103(R).

DY 38: Data Analysis and Stochastic Modeling I (jointly with UP)

Time: Thursday 16:30–17:00 Location: ZEU 255

DY 38.1 Thu 16:30 ZEU 255

Analyzing the phase statistics of phenological records: fluctuations and correlations with temperature — •Diego Rybski, Anne Holsten, and Jürgen P. Kropp — Potsdam Institute for Climate Impact Research (PIK), P.O. Box 60 12 03, 14412 Potsdam, Germany

Phenological timing – i.e. the course of annually recurring development stages in nature – is of particular interest since it can be understood as a proxy for the climate at a specific region; moreover changes in the so called phenological phases can be a direct consequence of climate change. We analyze records of botanical phenology and study their fluctuations which we find to depend on the seasons. In contrast to previous studies, where typically trends in the phenology of individual species are estimated, we consider the ensemble of all available phases and propose a phenological index that characterizes the influence of climate on the multitude of botanical species.

DY 38.2 Thu 16:45 ZEU 255

An advanced method for the estimation of drift and diffusion coefficients from stochastic time series — •Christoph Honisch and Rudolf Friedrich — Institut für Theoretische Physik, Universität Münster, D-48149 Münster

We present a novel iterative method to estimate drift and diffusion coefficients from data of stationary univariate Markov processes $X(t)$. These coefficients are defined as $D^{(n)}(x) = \frac{1}{n!}\lim_{\tau\to 0}\frac{1}{\tau}\langle (X(t+\tau)-x)^n | x = X(t)\rangle$, where n=1,2 corresponds to drift and diffusion coefficients respectively. Our method overcomes the problem of performing the limit $\tau \to 0$ by taking advantage of a recently reported approach [1] to calculate exact finite sampling interval effects on the estimation of drift and diffusion. Therefore, good results are achieved in cases of sparsely sampled time series.

[1] St. J. Lade, Phys. Lett. A **373**, 3705 (2009)

DY 39: Data Analysis and Stochastic Modeling II (jointly with UP)

Time: Thursday 17:00–18:30 Location: ZEU 255

DY 39.1 Thu 17:00 ZEU 255

Changepoint detection in stochastic diffusion processes — •Andreas Ruttor[1], Florian Stimberg[1], Guido Sanguinetti[2], and Manfred Opper[1] — [1]Technische Universität Berlin — [2]University of Edinburgh, UK

While diffusion processes are often suitable for modelling the dynamics of a system driven by both deterministic and stochastic forces, their parameters may change suddenly at certain time points. Detecting such changepoints is possible by extending the model with a latent Markovian jump process. Each state of this unobserved process corresponds to one set of parameters for the diffusion process. Here the prior probabilities of jumps denote the expected frequency of changepoints. We derive partial differential equations describing the time evolution of the posterior probability distribution over system states, which can be used for exact inference in low-dimensional systems. We also present a Markov-Chain Monte Carlo algorithm suitable for larger models. In both cases only observations of the diffusion process at discrete points in time are used to estimate the position of the changepoints as well as the parameters of the model. Our results on both simulated and real data show that the approach is very successful in capturing latent dynamics and is suitable for a number of real data modelling tasks.

DY 39.2 Thu 17:15 ZEU 255

Can high-energy proton events in solar wind be predicted via classification of precursory structures? — •Sarah Hallerberg[1], Alexander Ruzmaikin[2], and Joan Feynman[2] — [1]Chemnitz University of Technology — [2]Jet Propulsion Laboratory, California Institute of Technology

Shock waves in the solar wind associated with solar coronal mass ejections produce fluxes of high-energy protons and ions with energies larger than 10 MeV. These fluxes present a danger to humans and electronic equipment in space, and also endanger passengers of over-pole

air flights. The approaches that have been exploited for the prediction of high-energy particle events so far consist in training artificial neural networks on catalogues of events. Our approach towards this task is based on the identification of precursory structures in the fluxes of particles. In contrast to artificial neural networks that function as a "black box" transforming data into predictions, this classification approach can additionally provide information on relevant precursory events and thus might help to improve the understanding of underlying mechanisms of particle acceleration.

DY 39.3 Thu 17:30 ZEU 255

How to measure low frequency signals with a sound card — •Thomas John and Dirk Pietschmann — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg

Modern sound cards as analog/digital-converter are cheap because of monolithic circuit design. They have a spectacular signal to noise ratio of more than 100 dB. A common disadvantage in usage as measurement instrument in laboratories is the low-pass filtering, with prevents exact measurements for frequencies below 100 Hz. We present a software based algorithm to bypass this disadvantage. All tested sound cards could be characterized by only two parameters for frequency behavior and one parameter for relative voltage scaling. These parameters can be easily determined with our algorithm. The achieved accuracy is approx 5 μV to 1 V in a frequency range from below 1 Hz up to 24 kHz with exact phase determination of the applied signal.

DY 39.4 Thu 17:45 ZEU 255

Continuous Time Data Assimilation And Ensemble Generation — •Jochen Bröcker[1] and Ivan G. Szendro[2] — [1]Max Planck Institut für Physik komplexer Systeme, Dresden, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Germany

Variational data assimilation in continuous time is revisited. Adopting techniques from the theory of optimal nonlinear control, we obtain a continuous time generalisation of what is known as weakly constrained four dimensional variational assimilation (WC–4D–VAR) in the geosciences. The technique allows to assimilate trajectories in the case of partial observations and in the presence of model error. Several mathematical aspects of the approach are studied. Computationally, it amounts to solving a two point boundary value problem. For imperfect models, the trade off between small dynamical error (i.e. the trajectory obeys the model dynamics) and small observational error (i.e. the trajectory closely follows the observations) is investigated. A minimum out of sample error is proposed as a criterion to settle this trade of, i.e. to select an optimal weighting between dynamical and observational error. Even if the model is perfect though, allowing for minute deviations from the perfect model is shown to have positive effects, namely to regularise the problem. Finally, we investigate the problem of generating ensemble forecasts by exploiting information obtained from the said boundary value problem.

DY 39.5 Thu 18:00 ZEU 255

Entwicklung eines effizienten Radarvorwärtsoperators für die Datenassimilation — •Dorit Epperlein[1], Yuefei Zeng[1] und Ulrich Blahak[2] — [1]Karlsruher Institut für Technologie (KIT) — [2]Deutscher Wetterdienst, Offenbach

Deutschlandweit liefern 16 Radargeräte des Deutschen Wetterdienstes (DWD) einzigartige, flächendeckend hochaufgelöste dreidimensionale Informationen über Wolkenstrukturen und Niederschlag. Bisher werden diese Radardaten jedoch kaum im numerischen Wettervorhersagemodell COSMO-DE des DWD verwendet. Die Entwicklung eines Radarvorwärtsoperators (RADVOP) soll hier im Rahmen eines neu angelaufenen Projekts erste Fortschritte bringen. Dieser berechnet aus den vom Modell auf einem diskreten Raumgitter prognostizierten Größen durch eine klassische Streustrahlungsrechnung „künstliche" Werte für die Radarmessgrößen Reflektivität, Radialwind sowie Polarisationsparameter, so wie sie in der simulierten Wettersituation von einem meteorologischen Radar gemessen worden wären. Hier müssen u.U. viele verschiedene physikalische Prozesse berücksichtigt werden, wie z.B. Dämpfung des Radarstrahls oder atmosphärische Refraktion.

Langfristiges Ziel ist einerseits die Anwendung von RADVOP für die Assimilation der Radarmessgrößen, andererseits sollen aber auch detaillierte Vergleiche von tatsächlich gemessenen und „simulierten" Radardaten zur Verbesserung der Wolkenphysikparametrisierungen und somit der kurzfristigen Niederschlagsvorhersage beitragen.

Ein erster einfacher Operator für Radialwind und Reflektivität wurde bereits entwickelt und dessen Ergebnisse werden vorgestellt.

DY 39.6 Thu 18:15 ZEU 255

Statistische Methoden in der Radioökologie: Zeitreihenanalyse künstlicher und natürlicher Radionuklide in Luft und Niederschlag — •Sabine Sickinger und Jochen Tschiersch — Helmholtz Zentrum München, Institut für Strahlenschutz, Neuherberg

Den Gegenstand der Untersuchungen bilden die Konzentrationen verschiedener Radionuklide wie z.B. ^{7}Be, ^{137}Cs und ^{210}Pb in der bodennahen Luft und im Niederschlag in München-Neuherberg. Im Rahmen der Umweltüberwachung werden die Nuklidkonzentrationen seit über 40 Jahren ermittelt und bilden in ihrem Umfang eine solide und herausragende Ausgangsbasis für statistische Analysen. Die Zeitreihen werden hinsichtlich verschiedener Trends und Periodizitäten einzeln und im Kollektiv untersucht. Die Analysen werden durch die Verwendung verschiedener meteorologischer Parameter erweitert.

Ziel der Arbeit ist es, verschiedene Ursachen von Trends und Schwankungen zu identifizieren, um die Exposition von Mensch und Umwelt durch die einzelnen Radionuklide besser abschätzen zu können.

DY 40: Posters II

Time: Thursday 17:00–19:00 Location: P3

DY 40.1 Thu 17:00 P3

Mobility and motion in a restricted geometry of liquid crystalline membranes — •Sebastian Baumgarten, Alexey Eremin, and Ralf Stannarius — Institut für Experimentelle Physik, Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

Flow phenomena in restricted geometries have been intensively studied in the last years with implications to different physical, chemical and biological systems. We report straightforward experiments where we observed the motion of inclusions in tilted free-standing films under gravity forces. Translational mobility of solid (silica beads) and liquid (water/glycerin droplets) microscopic inclusions in planar films of the smectic-A phase have been measured. The effects of the confinement (film size), and the role of the viscosity of the outer gas have been investigated. They will be discussed in terms of Saffman-Delbrück and Hughes-Pailthorpe-White (HPW) models.

DY 40.2 Thu 17:00 P3

Theoretical model for spontaneous imbibition of water in Vycor glass — •Zeinab Sadjadi and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany

We study theoretically the spontaneous imbibition, that is the capillary rise of water, in networks of hydrophilic silica pores with characteristic radii of 3-5 nm, which is realized by imbibition experiments with Vycor glass [1,2]. The latter is permeated by a network of interconnected pores which we model by a network of cylindrical pipes with random diameter and varying aspect ratio. We simulate the capillary rise of the liquid by solving the mass balance equations for ideal pipe flow at each node with the boundary pressure constraints given by the liquid reservoir on one side and the Laplace pressure at the moving menisci on the other side. We analyze the temporal evolution of the average height and width of the invasion front, as well as its morphological characteristics. Classical Lucas-Washburn law is expected for the time dependence of the height, varying theoretical predictions and experimental observations have been made for the tiem dependence of the front width, which we discuss in the light of our simulation results.

[1] Simon Grüner, Tommy Hofmann, Dirk Wallacher, Andriy Kityk and Patrick Huber, Phys. Rev. E 79, 067301 (2009).

[2] Simon Grüner and Patrick Huber, Phys.Rev. Lett 103, 174501 (2009).

DY 40.3 Thu 17:00 P3

Modelling a flexible sheet swimmer with stochastic rotation dynamics on graphic processing units — •Christian Schmeltzer and Holger Stark — TU Berlin

Artificial swimmers at low Reynolds numbers have attracted a lot of

attention in recent years. Concepts for the propulsion of planar flexible structures have been demonstrated [1]. Here, we present an artificial sheetlike swimmer in a viscous environment. The sheet is modelled using vertices connected by spring potentials. To prevent it from crumbling, we applied bending potentials at each vertex site. The flow fields around the sheet are calculated with stochastic rotation dynamics (SRD). SRD is a multi-particle collision method capable of simulating mesoscale hydrodynamic effects with thermal fluctuations while being easy to implement. We first investigated the diffusion of the sheet and found it to follow Zimm dynamics. We then applied external forces normal to the sheet surface at neighboring edges but with opposite directions. The sheet starts to rotate and develops a helical shape which propels the sheet forward. The simulations with SRD are optimized for parallel computation on a graphic processing unit (GPU), which reduces the calculation time considerably. I will explain how the sheet is coupled to the SRD fluid and how the simulation speed increases due to parallel computing on the GPU.

[1] Garstecki et al. Propulsion of flexible polymer structures in a rotation magnetic field. J. Phys.: Condens Matter 21 204110 1-8 (2009).

DY 40.4 Thu 17:00 P3

Colloidal dynamics induced by phasonic drifts — •Justus Kromer[1], Michael Schmiedeberg[2], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany

Phasons are unique to quasicrystals. These are non-periodic solids which nevertheless possess long-range positional and orientational order. Phasons correspond to global rearrangements of atoms in quasicrystals. Like phonons they are hydrodynamic modes since they do not increase the free energy in the long wavelength limit. The properties of phasons are still intensively discussed in the field [1].

We study the dynamics of a colloidal adsorbate induced by a phasonic drift in a quasicristalline substrate potential using Brownian dynamics simulations. The drift changes the potential landscape continuously where minima disappear and new ones are created. After the system has reached a non-equilibrium steady state, we find that the colloids perform a characteristic stick-slip motion. By slipping into new minimas, the colloids rearrange and thereby realize the phasonic drift in the adsorbate. Although individual particles move in different directions, the colloids exhibit a net drift that sensitively depends on the direction and velocity of the phasonic drift. Our observations help to get a deeper insight into the properties of phasonic displacements in colloidal as well as in atomic quasicrystals.

[1] C. L. Henley, M. de Boissieu, and W. Steurer, Philos. Mag. 86, 1131 (2006).

DY 40.5 Thu 17:00 P3

Das kapillare Brechungsproblem an einer stationären Wirbelschicht — •Walter Brett[1] und Wolfgang Ellermeier[2] — [1]TU Darmstadt — [2]TU Darmstadt

Das hier behandelte Problem entstammt der klassischen Hydrodynamik mit freien Oberflächen unter Schwerkraft- und Kapillaritätseinfluss. Zwei stationär unterschiedlich schnell strömende Flachwasserschichten bilden entlang ihrer Kontaktfläche eine Wirbelschicht (tangentiale Diskontinuität). Deren Stabilitäts-, Durchlass- und Reflexionsverhalten für Störungen kleiner Amplitude wird untersucht unter Einbeziehung der Analogien zwischen den entsprechenden Problemen der Strömung kompressibler Fluide und der Optik in bewegten Systemen. Ein Ausblick auf die nichtlinearen Aspekte wird gegeben.

DY 40.6 Thu 17:00 P3

Drawn meniscus in a precursor film model — •Mariano Galvagno and Uwe Thiele — Department of Mathematical Sciences, Loughborough University, Loughborough, LE11 3TU, UK

Dragging a flat plate out of a liquid bath may deposit a liquid film on it - a technique widely used in coating processes. To control the deposition one needs to understand the velocity-dependent shape of the meniscus. At high velocities U a macroscopic film is deposited – corresponding to the classical Landau-Levich problem [1]. For small U only a microscopic precursor film is deposited. Recent studies employ a slip model for contact line motion to discuss meniscus shapes and steady films of finite length [2].

We study the system with a precursor film model based on a Derjaguin pressure that describes partially wetting. As in [2] we find steady menisci at small U up to a saddle-node bifurcation at a limiting U_c. Depending on the inclination angle, in a small region below U_c, multiple steady solutions may exist. They correspond to menisci with a finite film-like 'foot'. The solution branches and the limits of the region of multiple steady solutions are traced employing numerical continuation [3].

We acknowledge support by the EU (PITN-GA-2008-214919).

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DY 40.7 Thu 17:00 P3

Onset of Instabilities in Cooled Binary Fluids — •Jan-Hendrik Trösemeier and Jürgen Vollmer — Max Planck Institute for Dynamics and Self-Organization, 37073 Göttingen

Slowly cooling a binary fluid into the miscibility gap induces concentration gradients in the direction perpendicular to an interface separating the coexisting phases. When these gradients are too large the system becomes unstable against formation of droplets and/or convection.

The evolution of the system can be described by an appropriately adapted version of model H [1], i.e. a modified Cahn-Hilliard equation for the nonlinear diffusion of concentration coupled to the Navier-Stokes equation. In this setting we investigate the onset of convective and diffusive instabilities. Linear stability theory provides the boundaries of the region with purely diffusive demixing, i.e. the threshold for the onset of nucleation [2] and for the onset of convection. Considering terms to quadratic order provides additional insight into the dynamics beyond the onset of stability.

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[2] J. Vollmer, *J Chem Phys* **129** (2008) 164502.

DY 40.8 Thu 17:00 P3

The Role of Convection in the Mpemba Effect — •Heiko Engelke and Jürgen Vollmer — Max Planck Institute for Dynamics and Self-Organization, 37073 Göttingen

Mpemba's cooling effect has long been a counter-intuitive puzzle [1]: Two identical samples of liquid are kept at different temperatures, then put into the freezer. The initally hotter sample is the one that freezes first.

Research in the late 20th century indicated that evaporative cooling and supercooling of the liquid contribute to this effect [2]. Surprisingly though, the role of convection for this effect has not thoroughly been addressed so far.

To fill in this gap we explore the flow patterns: After being put into the freezer the probe starts to cool inwards from the walls, a temperature gradient builds up, and convection arises. Depending on initial parameters, we see a transition between convective and diffusive cooling. This affects the temperature distribution at the arrest of the flow, and the freezing pattern.

For various viscosities, initial temperatures and geometric configurations the evolution of the temperature and the flow field are measured. The results are compared to numerical simulations.

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DY 40.9 Thu 17:00 P3

Quantitative analysis of numerical estimates for the permeability of porous media from lattice-Boltzmann simulations — •Thomas Zauner[1] and Rudolf Hilfer[1,2] — [1]Institute for Computational Physics, University of Stuttgart, 70569 Stuttgart, Germany — [2]Institute for Physics, University of Mainz, 55099 Mainz, Germany

A quantitative error assessment for numerically calculated permeabilities with different simulation setups, numerical approximations and different LB-implementations, such as single- and multirelaxation time schemes is carried out [1]. From the error analysis we derive an optimized simulation setup, efficient LB-implementations and appropriate numerical approximations. This simulation setup is used to calculate the permeability of a digitized Fontainebleau sandstone as a benchmark. The resulting permeabilities for this sample, a refined sample and the extrapolated results are compared to other numerical permeability measurements in the literature [2]. The presented work illustrates some pitfalls that can lead to unreliable numerical permeability calculations from LB simulations. Further, it shows that a resolution and relaxation time dependent analysis together with an extrapolation scheme is necessary when using LB simulations to calculate permeabilities of stochastic porous media.

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DY 40.10 Thu 17:00 P3

Percolation in two phase flow in porous media on macroscopic scales — •Florian Doster[1] and Rudolf Hilfer[1,2] — [1]Institute for Computational Physics, University of Stuttgart, 70569 Stuttgart, Germany — [2]Institute for Physics, University of Mainz, 55099 Mainz, Germany

The standard model for multiphase flow in porous media on scales of centimeters to hectometers shows several deficiencies when compared with experiments. Fundamental parameter functions are not unique due to hysteretic and dynamic effects. Residual saturations cannot be predicted but are injected as parameters into the standard model. A macroscopic mixture theory for immiscible two phase displacement in porous media aims to cope with these deficiencies by taking into account the differences in percolating and nonpercolating phases. Recently first numerical solutions to the theory have been published [2,3]. Here, analytical and quasi-analytical solutions of a hyperbolic limit of the theory are presented. The results show that the degeneracy of states of the traditional theory is resolved within the new one. The results show that hysteresis in relative permeabilities is indeed reproduced inherently by the new theory. It is further indicated that dynamic effects in saturations and residual saturations are contained and that the representation of irreducible fluids by constant parameters in the traditional theory is questionable.

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[2] R. Hilfer and F. Doster, Trans. Por. Med., 82 (3), 507-519 (2010)
[3] F. Doster et al., Phys. Rev. E, 81, 036307 (2010)

DY 40.11 Thu 17:00 P3

The behavior of deformable droplet in the Hele-Shaw cell — •Erfan Kadivar and Martin Brinkmann — Max Planck Institute for Dynamics and Self-Organization, Bunsenstr. 10, D-37073 Göttingen, Germany

Motivated by recent experiments in microchannels, we studied the behavior of liquid droplets flowing in a Hele-Shaw cell by numerical simulation. The continuity equation and Darcy's law in combination with the discontinuity of the pressure at the curved interface of the droplet are used to obtain an integral representation of the pressure inside and outside of the droplet. The boundary element method is used to numerically determine the velocity field in both liquid phases as function of mobility and pressure gradient at periodic boundaries and to evolve the shape and position of the droplet in the microchannel.

According to recent experimental works, we used two different geometries; The first one is a rectangular microfluidic channel with thin width and specific length which has been expended abruptly. The second one is the microfluidic channel with the sinusoidal boundaries. We focused on the case that the droplet size is comparable to minimum width of channel. Therefore, we studied the droplet deformation when is flowing in the microchannel.

DY 40.12 Thu 17:00 P3

Spatially Modulated Thermal Convection — •Georg Freund, Werner Pesch, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth

We study Rayleigh-Bénard convection (RBC) in a horizontal fluid layer heated from below and investigate theoretically different methods of imposing spatially periodic modulations.

It is well known that in (unmodulated) RBC a purely conductive state becomes unstable to convection, when the applied temperature gradient exceeds a critical value. The presence of spatial modulations breaks the translational symmetry leading to a convective state for any finite temperature difference between the top and bottom boundary. The spatial variation of such a 'forced' state follows the imposed modulation. However, these forced rolls are only stable for overcritical temperature gradients, if the wavenumber of the modulation lies in the vicinity of the critical wavenumber of unmodulated RBC. In this case one finds an imperfect-bifurcation scenario.

In recent experiments spatial modulations have been imposed by gluing block-shaped polymer stripes onto the lower boundary plate, while theoretical treatments exist for spatially varying temperature conditions on geometrically flat and to some extent on wavy-shaped boundary plates.

We solve the Oberbeck-Boussinesq equations directly and compare the various types of boundary conditions with each other. This allows for the first time a quantitatively consistent comparison to the experimental results.

DY 40.13 Thu 17:00 P3

Pattern evolution in a lifted Hele-Shaw cell — •Julia Nase[1,3], Didi Derks[2], and Anke Lindner[1] — [1]PMMH-ESPCI, 75231 Paris Cedex 5, France — [2]Graduate School of Engineering, Osaka University, Japan — [3]Fakutät Physik/DELTA, TU Dortmund, 44221 Dortmund

When a liquid is confined between two plates and the upper plate is lifted at constant speed, air penetrates into the liquid volume from the sides. For certain conditions, the contracting liquid does not form a stable circle, but air fingers develop. This instability is a variant of the Saffman-Taylor-instability and has the particularity to take place at changing control parameter. This situation is important for the understanding of debonding mechanisms in adhesion problems and might also give insight into growth mechanisms in biological systems.

We investigate the evolution of the finger pattern from the moment of destabilization to the final plate separation in a Newtonian liquid. At fixed time, the pattern is characterized by the number of fingers and the finger amplitude from tip to base. Starting from a variation of the parameters lifting speed v_0, initial gap width b_0, cell radius R_0, and fluid viscosity η, we investigate in depth the influence of these parameters on the pattern coarsening.

At each moment, we distinguish stagnant and growing fingers. We show that the number of growing fingers is well described by a purely linear theory. Surprisingly, this description is also valid at late times where the linear prediction usually is expected to fail. The total number of fingers and the amplitude, however, are determined by the exact experimental conditions, particularly by the cell geometry.

DY 40.14 Thu 17:00 P3

Statistical properties of turbulent Rayleigh-Bénard convection — •Johannes Lülff, Michael Wilczek, and Rudolf Friedrich — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster

We use PDF methods to analyze turbulent Rayleigh-Bénard convection. The equations governing the PDFs are derived, and occuring unclosed terms are estimated from DNS data. For this DNS, we developed an easy-to-implement numerical scheme using penalization techniques.

DY 40.15 Thu 17:00 P3

Adaptive de-trending and stochastic analyisis of wind time series. — •Allan Morales — Universität Oldenburg

Offshore horizontal wind speed time series are de-trended using an innovative so-called adaptive de-trending algorithm. The de-trended, turbulent fluctuating signal is analyzed and modelled with a one dimensional Langevian Equation. We show how this easy model is able to reproduce some basic statistical properties of the original turbulent signal.

DY 40.16 Thu 17:00 P3

Adaptive de-trending and stochastic analyisis of wind time series. — •Allan Morales — Universität Oldenburg

Offshore horizontal wind speed time series are de-trended using an innovative so-called adaptive de-trending algorithm. The de-trended, turbulent fluctuating signal is analyzed and modelled with a one dimensional Langevian Equation. We show how this easy model is able to reproduce some basic statistical properties of the original turbulent signal.

DY 40.17 Thu 17:00 P3

Resistance in percolating quasi 1D and 2D networks of nanofibers — •Milan Žeželj, Igor Stanković, and Aleksandar Belić — Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

The scaling laws describing the conductivity in random networks of straight conducting nanofibers are derived from percolation theory and verified in numerical simulations. The applicability of the scaling laws to complex structures of interconnected networks of carbon nanofiber films and thick 1D wires is investigated in mesoscopic simulations. The current transfer in composite materials is found to be strongly enhanced by self-organization of nanofibers. The electrical conductivity of nanofiber films varies by orders of magnitude depending on the aspect ratio of the nanofibers, density and their structural arrangement

in the material.

DY 40.18 Thu 17:00 P3

Shearing granular media: from elasticity to compaction — •Jean-Francois Metayer[1], Elie Wandersman[2], Martin Van Hecke[2], and Matthias Schroeter[1] — [1]MPI for Dynamics and Self-organization, Goettingen, Germany — [2]University of Leiden, Netherland

A granular system is able to behave like a solid (a sand pile for example) or like a liquid depending on the deformation imposed on the material.

Using rheometry measurements we investigate the response of a granular bed to an imposed deformation or an imposed stress as a function of its packing fraction. We observed different regimes: elastic, plastic behaviors, flow regime and finally compaction.

The dependence of these regimes on the packing fraction and on the pressure allows us to delineate the phase diagram of granular media.

DY 40.19 Thu 17:00 P3

Football in the rain - Rebound of balls from wetted ground — •Frank Gollwitzer[1], Kai Huang[1], Ingo Rehberg[1], and Christof A. Krülle[1,2] — [1]Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth, Germany — [2]Maschinenbau und Mechatronik, Hochschule Karlsruhe - Technik und Wirtschaft, D-76133 Karlsruhe, Germany

Considering the loss of energy when a solid particle hits hard on a flat surface and rebounds back into the air dates back to I. Newton who defined the coefficient of restitution for this inelastic collision as the ratio of the rebound vs. the impact velocity. Since the theoretical treatment of this complex phenomenon is difficult, experimental data are needed for comparison with elastomechanical models. It is known that the restitution coefficient depends on various parameters like impact velocity, size of the balls, materials involved, etc. Here we present results of an experimental investigation of the multiple collisions of a solid sphere hitting a hard surface wetted with liquid of various properties. For example, it is observed that the rebound occurs only above a critical approach velocity. From this, the energy needed to break the capillary bridge between ball and ground can be deduced.

DY 40.20 Thu 17:00 P3

Geometrical structure of spheres around Random Close Packing — •Frank Rietz[1,2], Charles Radin[3], Harry L. Swinney[3], and Matthias Schroeter[2] — [1]Univ. of Magdeburg — [2]MPI Dynamics & Self-Organization Goettingen — [3]Univ. of Texas at Austin

The name Random Close Packing refers to the experimental observation that some ways of packing of monodisperse beads (like vertical vibration or sedimentation) can't exceed a volume fraction of ≈64%. There are several competing theories trying to explain this phenomenon and it is still unclear how to correctly define the Random Close Packing density. The three-dimensional distribution of particles below and above Random Close Packing is investigated. We match the index of the surrounding liquid to provide access to the interior of the granular bed. We measured local packing densities and order parameter by means of Voronoi cells. This allows us to comment on the question if Random Close Packing is well defined.

DY 40.21 Thu 17:00 P3

The "Minimal Model 2.0": An accurate and efficient continuum description of sand dune formation — •Marc Lämmel, Daniel Rings, and Klaus Kroy — Institut für Theoretische Physik, Universität Leipzig, Germany

The so-called "minimal model" [1] is a continuum model of aeolian sand transport that can explain the formation and migration of sand dunes in the desert. What makes it conceptually and practically very appealing is that it captures the essential physical mechanisms while being computationally simple. Yet, recent research has demonstrated certain shortcomings of this popular model. Comparing the predicted dependence of the saturated sand flux on the wind speed with wind tunnel observations reveals a systematic deviation of that quantity: For stronger winds the model overestimates the flux significantly.

Here we show that a systematically improved version of the minimal model can be derived by considering two species of trajectories, similar to what has been proposed in Ref. [2]: low-energy reptating grains and high-energy saltating grains. The resulting predictions are in remarkable agreement with flux data from various wind tunnel measurements.

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[2] B. Andreotti (2004). A two-species model of aeolian sand transport. Journal of Fluid Mechanics 510, 4770.

DY 40.22 Thu 17:00 P3

3D particle tracking with a microwave radar setup — •Kai Huang[1,2] and Stephan Herminghaus[2] — [1]Experimentalphysik V, Universität Bayreuth, D-95440, Germany — [2]Max Planck Institute for Dynamics and Self-organization, Bunsenstr. 10, 37073 Göttingen, Germany

Granular matter is an agglomeration of macroscopic particles, which offers the opportunity to trace its dynamical behavior down to the mobility of individual particles. However, particle tracking in three dimensions, especially in an opaque medium such as a densely packed granular pile, is far from trivial. Here we introduce a microwave radar setup designed to trace a metallic particle in real time. The method is based on the phase shift between transmitted and reflected microwave signals, which are recorded by means of three receiver antennas. The tracing algorithms and first experiments to calibrate the setup will be presented.

DY 40.23 Thu 17:00 P3

Granular Anisotropic Gases — •Kirsten Harth[1], Stephan Höme[2], Ulrike Kornek[1], Ulrike Strachauer[1], Torsten Trittel[1], Karl Will[3], and Ralf Stannarius[1] — [1]Institut für experimentelle Physik, Otto-von-Guericke Universität Magdeburg, Deutschland — [2]Institut für Automatisierungstechnik, Otto-von-Guericke Universität Magdeburg, Deutschland — [3]Institut für Elektronik, Signalverarbeitung und Kommunikationstechnologie, Otto-von-Guericke Universität Magdeburg, Deutschland

Granular materials accompany us from early childhood days - but they still retain lots of unsolved challenges for grown-up scientists and engineers. They can exhibit states similar to gases, fluids and solids. So far, most experiments and theoretical investigations focussed on spherical or irregularly shaped particles.

We study a granular gas of elongated cylindrical particles a few millimetres in length under microgravity conditions. Our fully automatic setup consists of a translucent box with shaking walls, which is monitored with digital cameras from two perspectives. We will present first results from our sounding rocket flight. From the video data, the three-dimensional motion of the particles can be reconstructed, to analyze typical statistical quantities of the granular dynamics.

DY 40.24 Thu 17:00 P3

Parallelization of 2D Contact Dynamics in the simulation of granular media — •Zahra Shojaaee, Mohammad Reza Shaebani, Lothar Brendel, János Török, and Dietrich Wolf — University of Duisburg-Essen, Duisburg, Germany

Contact Dynamics (CD) is an effective discrete element method to simulate systems consisting of a large number of particles with multiple contacts such as granular matter. We simulate non cohesive hard discs with coulomb friction. CD uses an iterative method to calculate the contact forces, which fulfill the convergence criteria. To preserve reasonable computational time specially for large dense systems we have parallelized our CD code using open MPI. In contrast to the parallel MD method a large amount of communication between the processors is needed to calculate the contact forces in CD method. That is an important reason to pay more attention to the domain decomposition method. We have used a topological hierarchical domain decomposition method and an adaptive load balancing scheme, which aim to minimize the standard deviation of the real CPU time of all processors. The main challenge is to handle the iterative force calculation process in an optimal way. We investigate the performance of the iterative force calculation scheme, as well as the overall performance of the parallel code. Optimizing the communications between the processors results in a code which fulfills a good linear scaling also for a large number of processors. The solution remains stable until a critical number of processors depending on the system size, which deals with the weak point of CD method not bearing a parallel updating of contact forces.

DY 40.25 Thu 17:00 P3

Transition from attractive to repulsive Casimir-like forces in granular media — •reza shaebani[1], jalal sarabadani[2], and dietrich wolf[1] — [1]Department of Theoretical Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Department of

Physics, University of Isfahan, Isfahan 81746, Iran

We investigate the effective long-range interactions between intruder particles immersed in a randomly driven granular fluid. The effective force between two intruders, induced by the fluctuations of the hydrodynamic fields, is attractive when the volume fraction of the granular fluid is sufficiently high. However, a crossover from attraction to repulsion occurs as the volume fraction decreases. This behavior can be explained by two competing dynamical effects, resulting in a non-uniform collision distribution around the intruders. We present the phase diagram of the transition with three control parameters: the volume fraction, the distance between the intruders, and the restitution coefficient. Our results reveal that the force is proportional to the steady-state temperature and grows logarithmically with increasing the system size in two dimensions. Moreover, by increasing the number of intruders, we verify that the fluctuation-induced interaction is not derived from a pair-potential. These results shed new light on the mechanisms of segregation in granular media.

DY 40.26 Thu 17:00 P3

Influence of polydispersity on the static properties of granular materials — •Reza Shaebani[1], Mahyar Madadi[2], Stefan Luding[3], and Dietrich Wolf[1] — [1]Department of Theoretical Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Department of Applied Mathematics, The Research School of Physics and Engineering, The Australian National University, Canberra 0200, Australia — [3]Multi Scale Mechanics (MSM), TS, CTW, Universiteit Twente , P.O. Box 217, 7500 AE Enschede, Netherlands

We study the effect of polydispersity on the macroscopic physical properties of granular packings in two and three dimensions. A mean-field approach is developed to approximate the micro-scale quantities that are linked to the macroscopic ones. We show that the trace of the fabric and stress tensors are proportional to the mean packing properties (e.g. packing fraction, average coordination number and average normal force) and correction factors which depend only on the moments of particle size distribution. Similar results are obtained for the elements of the stiffness tensor in the linear response regime. In order to compare the analytical results with numerical simulations, static homogeneous packings of particles are generated by means of the contact dynamics method. Our theoretical predictions are in good agreement with the simulation results.

DY 40.27 Thu 17:00 P3

Coarsening in granular segregation, an entropic approach — •Tilo Finger[1], Matthias Schröter[2], and Ralf Stannarius[1] — [1]Otto-von-Guericke-University-Magdeburg — [2]MPI for Dynamics and Self-organization Göttingen

When one fills a binary mixture in a cylindrical drum, one observe size segregation after agitation by horizontal rotation. This experiment has become a classic in granular physics. Segregation takes place on different time scales. At first, a radial segregation of the large and small particles is observed. This process is often followed by an axial segregation into band patterns. Gradual merging of the bands leads to an almost complete demixing on long time scales [1]. So far, the nature of this coarsening process is not understood. Here we present an X-ray tomography study where we visualize the tree-dimensional particle distribution in the cylinder. Our experiments aim at the confirmation of an increase of configurational entropy [2] during the coarsening process.

[1] T. Finger et al., PRE 74, 031312 (2006)
[2] S.F. Edwards & R.B.S. Oakeshott, Physica A 157, 1080 (1989)

DY 40.28 Thu 17:00 P3

A contact model for the yielding of caked granular materials — •János Török[1], Lothar Brendel[1], Roman Kirsch[2], and Ulrich Bröckel[2] — [1]Facultät für Physik, Universität Duisburg-Essen, Duisburg, Deutschland — [2]Fachhochschule Trier, Umwelt-Campus Birkenfeld, Deutschland

We present a visco-elastic coupling model between caked spheres, suitable for DEM simulations, which incorporates the different loading mechanisms (tension, shear, bending, torsion) in a combined manner and allows for a derivation of elastic and failure properties on a common basis. In pull, shear, and torsion failure tests with agglomerates of up to 10000 particles, we compare the failure criterion to different approximative variants of it, with respect to accuracy and computational cost. The macroscopic elastic behavior and failure properties of the agglomerates can be derived from the microscopic quantities which allows the scaling of all simulation results. The used method also gives also insight into the relative relevance of the different contact load modes.

DY 40.29 Thu 17:00 P3

Anisotropic elasticity in a frictional packing of disks — •Jens Boberski[1], Reza Shaebani[1], Tamás Unger[2], and Dietrich Wolf[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]Institute of Physics, Budapest University of Technology and Economics, 1111 Budapest, Hungary

Granular materials, when sheared, can evolve anisotropies due to the opening of contacts in a preferred direction. The opening of contacts leads to a change of the fabric and thus in the constitutive relation. The evolution of the contact distribution as well as the distribution of sliding contacts is predicted by assuming affine displacements of the disks. In a mean-field like approach the three elastic constants (bulk, shear and anisotropy moduli) are obtained by averaging over these distributions while assuming affinity. These predicted moduli are strain dependent and compared with results of DEM Simulations.

DY 40.30 Thu 17:00 P3

Capillary interaction between spherical particles: multi-body interactions and the effect of contact angle hysteresis — Ciro Semprebon, Stephan Herminghaus, and •Martin Brinkmann — Max Planck Institute for Dynamics and Self-Organization, Bunsenstr. 10, 37073 Göttingen, Germany

The mechanics of mixtures of sub-millimetric grains and liquids play an important role in process engineering and in the industrial scale production of many materials. At low liquid saturations, the cohesion in a granular assembly of spherical gains can be well explained by capillary forces induced by individual liquid bridges between neighboring beads. To account for the presence of larger liquid clusters, we numerically computed the capillary forces between three and more beads in contact to certain types of liquid clusters along with their interfacial energy and Laplace pressure. Besides these 'multi-body' interactions, we considered effects of contact angle hysteresis on the capillary interaction between two spherical particles. Both effects have an impact on the collective mechanical behavior of large particle assemblies and can be easily implemented in three dimensional contact dynamic simulations of frictional particles.

DY 40.31 Thu 17:00 P3

Monte Carlo Study of Mixed-Spin S=(1/2,1) Ising Ferrimagnets — •Walter Selke[1] and Jaan Oitmaa[2] — [1]Institut für Theoretische Physik der Phasenübergänge, RWTH Aachen, Germany — [2]School of Physics, University of New South Wales, Sydney, Australia

We investigate classical Ising ferrimagnets on square and simple–cubic lattices with exchange couplings between spins of values S=1/2 and S=1 on neighbouring sites and an additional single–site anisotropy term on the S=1 sites [1]. Based mainly on a careful and comprehensive Monte Carlo study, we conclude that there is no tricritical point in the two–dimensional case, in contradiction to mean-field predictions and recent series results. However, evidence for a tricritical point is found in the three–dimensional case. In addition, a line of compensation points is found for the simple–cubic, but not for the square lattice.

[1] W.Selke and J. Oitmaa, J. Phys. C: Condensed Matter 22, 076004 (2010)

DY 40.32 Thu 17:00 P3

The order parameter distribution of the 2D Ising model: A flat histogram Monte Carlo — •Anjan Prasad Gantapara[1] and Rudolf Hilfer[1,2] — [1]Institute for Computational Physics, University of Stuttgart, 70569 Stuttgart, Germany — [2]Institute for Physics, University of Mainz, 55099 Mainz, Germany

A high precision flat histogram Monte Carlo method is employed to calculate the order parameter distribution $p(m)$ of the 2D Ising model for a specified lattice size L and temperature T. Periodic, free and fixed boundary conditions are considered in our simulations. Universal forms of the $p(m)$ at temperatures below, above and at the ciritical point T_c are extracted and analyzed from the finite lattice simulations. The critical order parameter distribution is a function of the boundary condition unlike the $p(m)$ at temperatures away from T_c. Fat stretched exponential tails are seen in $p(m)$ for all the three boundary conditions at T_c corroborating previous analytical predictions [1]. The simulations provide the best converged critical order parameter universal scaling functions for periodic, free and fixed boundary conditions

available at present.
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DY 40.33 Thu 17:00 P3

Examining the SLE properties of paths in the negative-weight percolation model — •Christoph Norrenbrock, Oliver Melchert, and Alexander K. Hartmann — Institut für Physik, Carl-von-Ossietzky Universität Oldenburg, Oldenburg (Germany)

We consider lattice spanning paths of total negative weight on two-dimensional lattice graphs, where edge weights are drawn from a distribution that allows for positive and negative weights. Each realization of the disorder consists of a random fraction $(1-\varphi)$ of bonds with unit strength and a fraction φ of bonds drawn from a Gaussian distribution with zero mean and unit width. This negative-weight percolation (NWP) problem is fundamentally different from conventional percolation [1]. To investigate this percolation problem by means of numerical simulations [2], one has to perform a non-trivial transformation of the original graph and apply sophisticated matching algorithms.

Here we study whether the geometry of these paths can be described in terms of Schramm-Loewner evolution. We exhibit that the paths do not verify the prediction of Schramm's "left passage formula" [3].
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[2] Hartmann, A. K., Practical guide to computer simulations (World Scientific, 2009)
[3] Schramm, O., Electr. Comm. Prob. 6 (2001)

DY 40.34 Thu 17:00 P3

Parallelising the transfer-matrix method in disordered systems using graphics processors — •Thomas Edwards and Rudolf Römer — University of Warwick, Coventry, United Kingdom

We study the disorder-induced Anderson localisation of a d-dimensional solid and compute the localisation lengths using the transfer matrix method (TMM), seeking a parallel implementation to run on graphics processing units (GPU's). In the TMM, a quasi one-dimensional bar of length $L \gg M$ is split into slices of size M^{d-1}. The Schrödinger equation is recursively applied such that the wave function at the future slice ψ_{i+1} is computed from the past and present slices, ψ_i and ψ_{i-1}. Reformulating the Schrödinger equation into a transfer matrix and repeating multiplications of these matrices at each slice gives the 'global transfer matrix', which maps the wave functions from one side of the bar to the other. The minimum eigenvalue computed from this matrix gives the localisation length. To obtain the minimum eigenvalue and prevent numerical instabilities resulting from the exponential increase in the eigenvalues, the eigenvectors must be re-orthonormalised after every few matrix multiplications. This takes a considerable amount of time, as does computing the transfer matrices themselves, making it crucial to efficiently parallelise the TMM code. To do this we use CUDA, NVIDIA's proprietary GPU programming language. The speed-up gained from running the code on NVIDIA GPU's is then analysed using the Karp-Flapp metric.

DY 40.35 Thu 17:00 P3

Worm algorithm in ordered and disordered media — •Martin Marenz and Wolfhard Janke — Institut für theoretische Physik, Universität Leipzig, Germany

The Worm algorithm is a Monte Carlo method that uses the high-temperature expansion series for simulating spin systems. It was introduced by Prokof'ev and Svistinov in 2001.

This work and a few other papers suggest that this algorithm does not suffer from critical slowing down. We investigated the critical behavior of the algorithm, which means we have calculated the dynamic critical exponents. This procedure has also been repeated for bond-disordered and site-diluted systems, therefore we expanded the algorithm to such systems and introduced several estimators for common observables. We could affirm that the critical slowing down has no practical influence for the Worm algorithm, this also holds true for disordered and diluted systems. Furthermore, we have introduced a reweighting method.

DY 40.36 Thu 17:00 P3

A new technique for complete enumeration of self-avoiding walks (SAWs) on percolation clusters — •Niklas Fricke and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Germany

The critical behavior of SAWs on disordered lattices has been studied extensively in recent decades. Of particular interest is the situation at the percolation threshold where the fractal dimension changes. Unfortunately, the strong disorder poses a problem for Monte Carlo methods. Straightforward enumeration may benefit from the reduction of the number of paths at criticality, but the exponential increase still prohibits the study of longer chains. Here, a more effective enumeration scheme is presented. Exploiting the structural properties of the critical percolation cluster, it essentially removes the exponential increase in complexity. This permits studying walks of several hundred steps (involving effective enumeration of over 2^{100} chains) at or close to the percolation threshold.

DY 40.37 Thu 17:00 P3

Loop length distribution in higher dimensional negative weight percolation — •Gunnar Claussen, Oliver Melchert, and Alexander K. Hartmann — Institut für Physik, Carl-von-Ossietzky-Universität Oldenburg

We consider the negative weight percolation (NWP) problem [1] on large square and cubic lattice graphs, using disorder distributions that allow for edge weights of either sign. We examine loops with negative weight, i.e. percolating and "small" loops, and vary the concentration ρ of negative edge weights. The NWP problem is fundamentally different from conventional percolation problems, e.g. it shows no transitivity, hence there is no simple definition of clusters. Thus, numerical studies on this loop model require a non-trivial transformation of the original graph and the application of sophisticated matching algorithms.

Here, we study the problem by numerical methods [2]. The phenomenon is examined for $\rho \leq \rho_c$, the critical point. We characterize the ensemble of "small" loops by the Fisher exponent τ, which describes the distribution of loop lengths at ρ through $n_\rho(l) \sim l^{-\tau} e^{-T_L l}$, and by the loop-size cut-off exponent σ, which determines the line tension T_L by $T_L \sim |\rho - \rho_c|^{1/\sigma}$. We compare our results to previous finite-size scaling analyses [3].
[1] O. Melchert and A.K. Hartmann, New J. Phys. 10 (2008) 043039
[2] A.K. Hartmann, *Practical Guide to Computer Simulations*, World Scientific (2009)
[3] O. Melchert, L. Apolo and A.K. Hartmann, Phys. Rev. E 81 (2010) 051108

DY 40.38 Thu 17:00 P3

The two-dimensional Ising spin glass at zero temperature — •Hamid Khoshbakht and Martin Weigel — Institut für Physik, KOMET 331, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55127 Mainz

Ground states for the Ising spin glass in two dimensions can be determined in polynomial time as long as periodic boundary conditions are applied in at most one direction. Using a recently proposed mapping to an auxiliary graph decorated with Kasteleyn cities, we determine ground states for systems with open-periodic boundary conditions for lattices of linear sizes up to $L = 9000$ and calculate defect energies as well as domain-wall lengths. Although the matching approach does not work for periodic-periodic boundaries, where less finite-size corrections are expected, using a windowing technique allows to determine quasi-exact ground-states for lattices up to $L = 3000$. For the case of bimodal couplings, a controlled perturbation method allows the matching approach to sample from the manifold of degenerate ground states without bias. Using the combination of these techniques, we arrive at high-precision estimates of the spin-stiffness exponent and domain-wall fractal dimension for Gaussian couplings, which are compared to a scaling relation conjectured from stochastic Loewner evolution. For bimodal couplings, our results allow for a first-time determination of the fractal dimension of domain walls.

DY 40.39 Thu 17:00 P3

Multicanonical and Wang-Landau simulations on GPU — •Taras Yavors'kii and Martin Weigel — Institut für Physik, KOMET 331, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55127 Mainz

Over the last couple of years it has been realized that the vast computational power of graphics processing units (GPUs) could be harvested for purposes other than the video game industry. This power, which is advertised to exceed that of current CPUs by a large factor, results from the relative simplicity of the GPU architectures as compared to CPUs, combined with a large number of parallel processing units on a

single chip. To benefit from this setup for general computing purposes, the problems at hand need to be prepared in a way to profit from the inherent parallelism and hierarchical structure of memory accesses. In this contribution, we discuss how suited this massively parallel setup is for simulations of the multicanonical or Wang-Landau type, which have proven useful for the study of systems with complex energy landscapes and first-order phase transitions. In contrast to canonical simulations, such approaches appear to require knowledge of the current value of a global reaction coordinate such as energy or magnetization prior to each spin flip. This seems to preclude their efficient implementation on GPUs. We assess the performance potential of different parallel implementations of such algorithms on GPU and compare to the speedups previously gained for simulations in the canonical ensemble.

DY 40.40 Thu 17:00 P3

Quantum Criticality in the 3d Gross-Neveu Model from the Functional Renormalization Group — Jens Braun, Holger Gies, and •Daniel David Scherer — Theoretisch-Physikalisches Institut, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena, Germany

Using the functional renormalization group, we study the fixed-point structure of the three dimensional Gross-Neveu model describing planar Dirac fermions interacting in a scalar-scalar channel. We employ both a purely fermionic as well as a partially bosonized language. We find non-Gaußian fixed points responsible for gap generation by a second order quantum phase transition in both formulations, the universal critical exponents of which we determine quantitatively as a function of flavor number N_f. We also make contact to the large-N_f expansion. In this limit, the fixed-point action as well as all universal critical exponents can be computed analytically.

DY 40.41 Thu 17:00 P3

Cutting-Plane Approach for Vertex Covering of Random Graphs — •Timo Dewenter and Alexander K. Hartmann — Institut für Physik, Universität Oldenburg, 26111 Oldenburg

The NP-complete vertex cover problem (VC) on Erdős-Rényi (ER) random graphs with finite connectivity c is well studied [1]. Within numerical simulations, usually the minimum-size cover is calculated via branch-and-bound algorithms.

Here, we apply the translation of VC to a linear programming problem (LP), where the nodes of the graph are represented by variables $x_i \in [0,1]$. Each edge $\{j,k\}$ of the graph corresponds to a constraint $x_j + x_k \geq 1$. The simplex algorithm is used to solve this LP, but for larger c less solutions of the desired form $x_i \in \{0,1\}$ are found. So we use two heuristics to obtain better results. First, a node-heuristic is implemented, which generates an upper bound of the minimum cover. Further, a cutting plane approach is used, that adds constraints to the LP based on loops in the graph with odd length leading to exact solutions or lower bounds. We study the behaviour of these algorithms for ER random graphs as a function of c. After performing a statistical analysis [2] for different system sizes, we compare with the phase diagram for the critical fraction x_c of covered vertices.

[1] M. Weigth and A.K. Hartmann: *Number of Guards Needed by a Museum: A Phase Transition in Vertex Covering of Random Graphs*, Phys. Rev. Letters **84**, 26 (2000)

[2] A.K. Hartmann: *Practical Guide to Computer Simulations*, World-Scientific, 2009

DY 40.42 Thu 17:00 P3

Phasenübergänge zweidimensionaler Modellkolloide in äusseren periodischen Feldern — •Theda Brokamp und Peter Nielaba — Universität Konstanz, Deutschland

2D-Kolloide in eindimesional periodischen Feldern dienen als Modell für Phasenübergänge in zwei Dimensionen. Das eindimensionale Sinuspotential hat eine Wellenlänge, die $1/p$ der Braggebenen im Kolloidkristall entspricht (p=Kommensurabilitätsverhältnis). Hier werden erstmals Ergebnisse aus Monte Carlo Simulationen mit finite size scaling-Analysen gezeigt für Kommensurabilitätsverhältnisse $p = 3$ und $p = 4$. Dabei wurden Dichte und Potential variert. Die resultierenden Phasendiagramme zeigen modulated liquid, locked smectic und locked floating solid Phasen.

DY 41: Brownian Motion, Stochastic Processes, Transport II

Time: Friday 10:15–13:15 Location: HÜL 186

DY 41.1 Fri 10:15 HÜL 186

Effective temperatures in hot Brownian motion — •Daniel Rings[1], Dipanjan Chakraborty[1], Markus Selmke[2], Frank Cichos[2], and Klaus Kroy[1] — [1]ITP, University of Leipzig, Germany — [2]EXP1, University of Leipzig, Germany

Recently, we have introduced a theoretical model for the Brownian motion of heated nanoparticles in suspension [1], which successfully passed its first test in photothermal spectroscopy experiments [2].

Now, we wish to shed light on various aspects of the non-equilibrium phenomenon of hot Brownian motion, in particular the implications of the generalized concept of temperature with respect to translational and rotational diffusion, and dynamic effects. Different temperatures must be assigned to different modes of motion in this non-equilibrium system. I shall present results based on both the analytical theory of fluctuating hydrodynamics and molecular dynamics simulations.

[1] D. Rings, R. Schachoff, M. Selmke, F. Cichos, and K. Kroy, Phys. Rev. Lett., 105 (9), 090604 (2010)

[2] R. Radünz, D. Rings, K. Kroy, and F. Cichos, J. Phys. Chem. A 113 (9), 1674-1677 (2009)

DY 41.2 Fri 10:30 HÜL 186

Exact low-density expansion of the dynamics in the Lorentz gas — •Thomas Franosch[1], Felix Höfling[2], Teresa Bauer[3], and Erwin Frey[3] — [1]Institut für Theoretische Physik, FAU Erlangen, Erlangen, Germany — [2]Max-Planck-Institut für Metallforschung, Stuttgart, and Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Stuttgart, Germany — [3]Arnold Sommerfeld Center for Theoretical Physics, LMU München, München, Germany

We provide an analytic solution for the dynamics of a tracer for a dilute planar Lorentz gas [1] employing the many-body T-matrix formalism. In particular, we show that for particles performing Brownian motion in a frozen array of obstacles long-time correlations emerge in the mean-square displacement. Defining the velocity autocorrelation function (VACF) via the second time-derivative of the mean-square displacement, power-law tails govern the long-time dynamics similar to the case of ballistic motion. The physical origin of the persistent memory is due to repeated encounters with the same obstacle which occurs naturally in Brownian dynamics without involving other scattering centers. This observation suggests that in this case the VACF exhibits these anomalies already at first order in the scattering density.

Our result support the idea that quenched disorder provides a generic mechanism for persistent correlations irrespective of the microdynamics of the tracer particle. Our analytic approach is corroborated by computer simulations with a surprisingly large range of validity.

[1] T. Franosch, F. Höfling, T. Bauer, and E. Frey, Chem. Phys. **375** (2010) 540

DY 41.3 Fri 10:45 HÜL 186

Asymmetric Brownian Particles — •Martin Reichelsdorfer and Klaus Mecke — Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudstr. 7, 91058 Erlangen

We study the influence of the shape of Brownian particles on their dynamics. Under nonequilibrium conditions, asymmetric particles are found to be able to conduct directed average motion. A simple generic three-state model is proposed, which already exhibits crucial features and which reveals how the system relaxes to equilibrium from a symmetric nonequilibrium velocity distribution through asymmetric intermediate states. However, the differences in the behaviour of symmetric and asymmetric particles are not restricted to nonequilibrium. For instance, additional time-scales appear in the equilibrium velocity autocorrelation function and the latter may now also oscillate and adopt negative values.

In terms of an application, asymmetric Brownian particles can be used for constructing molecular motors that work even in spatially symmetric environments (e.g., no temperature gradients, no tilted or asymmetric potentials). Inspired by biology, we present a model where nonequilibrium is sustained by periodically stopping the motor at bind-

ing sites along a rail.

DY 41.4 Fri 11:00 HÜL 186

Fluctuation relations for anomalous dynamics — Aleksei V. Chechkin[1] and •Rainer Klages[2] — [1]Institute for Theoretical Physics NSC KIPT, Kharkov, Ukraine — [2]Queen Mary University of London, School of Mathematical Sciences, London, UK

We consider work fluctuation relations (FRs) for generic types of dynamics generating anomalous diffusion: Levy flights, long-correlated Gaussian processes and time-fractional kinetics. By combining Langevin and kinetic approaches we calculate the probability distributions of mechanical and thermodynamical work in two paradigmatic nonequilibrium situations, respectively: a particle subject to a constant force and a particle in a harmonic potential dragged by a constant force. We check the transient FR for two models exhibiting superdiffusion, where a fluctuation-dissipation relation does not exist, and for two other models displaying subdiffusion, where there is a fluctuation-dissipation relation. In the two former cases the conventional transient FR is not recovered, whereas in the latter two it holds either exactly or in the long-time limit [1].

[1] A.V.Chechkin, R.Klages, J.Stat.Mech. L03002 (2009)

DY 41.5 Fri 11:15 HÜL 186

Markovian embedding and origin of hyperdiffusion in generalized Brownian motion — Peter Siegle, •Igor Goychuk, and Peter Hänggi — University of Augsburg

The Fractional Langevin Equation (FLE) describes a non-Markovian Generalized Brownian Motion with long time persistence (superdiffusion), or anti-persistence (subdiffusion) of both velocity-velocity correlations, and position increments. It presents a case of the Generalized Langevin Equation (GLE) with a singular power law memory kernel. We propose and numerically realize a numerically efficient and reliable Markovian embedding of this superdiffusive GLE [1], which accurately approximates the FLE over many, about r=N lg b -2, time decades, where N denotes the number of exponentials used to approximate the power law kernel, and b>1 is a scaling parameter for the hierarchy of relaxation constants leading to this power law. Besides its relation to the FLE, our approach presents an independent and very flexible route to model anomalous diffusion. In particular, it contains as a special case the minimal three-dimensional embedding of ballistic superdiffusion [2]. Studying such a superdiffusion in tilted washboard potentials, we demonstrate the phenomenon of transient hyperdiffusion which emerges due to transient kinetic heating effects.

[1] P. Siegle, I. Goychuk, P. Hänggi, arXiv:1011.2848 [cond-mat.stat-mech] (2010).

[2] P. Siegle, I. Goychuk, P. Hänggi, Phys. Rev. Lett. 105, 100602 (2010).

DY 41.6 Fri 11:30 HÜL 186

Random walks in active media: perturbation spreading in many-body systems — Vasily Zaburdaev[1], •Sergey Denisov[2], and Peter Hanggi[2] — [1]School of Engineering and Applied Science, Harvard University, 29 Oxford Str., Cambridge, MA 02138 USA — [2]Institut fur Physik, Universitat Augsburg, Univeritatsstr. 1, 86135 Augsburg

Propagation of an initially localized perturbation through a many-particle Hamiltonian system can be viewed as a diffusion process,due to the conservation of perturbation energy. Remarkably, conventional diffusion equations are not suitable for the description of this process. We argue that the perturbation spreading can be evaluated by use of a Levy walk formalism, and develop a model that describes the dynamics of a cloud of walkers spreading through an active medium. By using two renowned many-particle systems, that is (i) a hard-point gas and (ii) a Fermi-Pasta-Ulam chain, we demonstrate that the perturbation profiles of both systems coincide with the diffusion profiles of the generalized Levy walk process. Parameters of the model are related to the physical parameters of the corresponding testing systems by simple algebraic expressions. Finally we discuss possible practical applications of our findings.

15 min. break.

DY 41.7 Fri 12:00 HÜL 186

Gas-induced metal-insulator transition in nanoporous crystalline multilayered metal oxide systems — •Julia Dräger[1,2], Stefanie Russ[2], Claus-Dieter Kohl[3], and Armin Bunde[1] — [1]Inst. f. Theoret. Physik III, Justus-Liebig-Universität Giessen, Germany — [2]Inst. f. Theoret. Physik, Freie Universität Berlin, Germany — [3]Inst. f. Angew. Physik, Justus-Liebig-Universität Giessen, Germany

We use a site-bond percolation model to study, both numerically and analytically, the gas-induced metal-insulator transition in thin layers of nanoporous crystalline metal oxides. While below a critical gas concentration Nc the nanoporous structure is insulating due to the absence of a percolating path, which consists of conducting grains (sites) and intergranular contacts (bonds), above Nc the conductance increases rapidly. We find two different scenarios: (i) For systems of high porosity, the transition arises from missing conducting grains, leading to site percolation effects. (ii) For systems of low porosity, the underlying conduction mechanism changes with increasing mean grain-size <D>: For large <D> the transition occurs due to bond- and for small <D> due site percolation effects. While for bond percolation Nc grows linearly with <D>, for site percolation a nonlinear behavior of Nc shows up for very small <D>. Our findings explain the linear dependence of Nc on <D> found in former works, which had not been fully understood before and suggest how the different conduction mechanisms possibly show up in experiments. We furthermore explore how the distribution of grain-sizes influences the shape of the characteristics.

DY 41.8 Fri 12:15 HÜL 186

The entropy production paradox in the space-fractional diffusion equation case — •Janett Prehl[1], Karl Heinz Hoffmann[1], and Chris Essex[2] — [1]Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Deutschland — [2]Department of Applied Mathematics, The University of Western Ontario, London, Canada N6A 5B7

Contrary to intuition, entropy production rates grow as reversible, wave-like behavior is approached. This paradox was discovered in time-fractional diffusion equations. It was found to persist for extended entropies and for space-fractional diffusion as well. This paper completes the possibilities by showing that the paradox persists for Tsallis and Rényi entropies in the space-fractional case. Complications arising due to the heavy tail solutions of space-fractional diffusion equations are discussed in detail.

[1] J. Prehl, C. Essex, K. H. Hoffmann, *Physica A* (2010) **389**: 215–224

DY 41.9 Fri 12:30 HÜL 186

Subdiffusive transport on the infinite cluster of the Lorentz Model — •Markus Spanner[1], Felix Höfling[2], Gerd Schröder-Turk[1], Klaus Mecke[1], and Thomas Franosch[1] — [1]Theoretische Physik 1, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen — [2]MPI für Metallforschung, Heisenbergstr. 3, und Institut für Theoretische und Angewandte Physik, Pfaffenwaldring 57, 70569 Stuttgart

The Lorentz model is a model for transport in porous materials, where a point-like tracer moves through an array of quenched spherical obstacles. Extensive simulations of this model were performed recently, and revealed anomalous transport at the void-space percolation transition. These studies considered all-cluster-averaged quantities, yet for deeper insight one would like to resolve the motion on the various clusters.

We conducted simulations of particles confined to the 'infinite' cluster, i.e. the fraction of void space that percolates through the system of obstacles, identified using a Voronoi tessellation. We find that the motion stays subdiffusive $\delta r^2_\infty(t) \sim t^{2/d_w}$ with a new exponent $d_w = 4.81$ known as walk dimension in the context of random walks in lattice percolation. Besides measuring the volume of the infinite cluster as a function of the obstacle density for systems of overlapping spheres, a detailed analysis of transport on this infinite cluster was carried out, including the vanishing of the diffusion coefficient near the transition, the non-gaussian parameter, the influence of finite system sizes and an extrapolation of the critical density from the dynamics. In contrast to the all-cluster-averaged dynamics, we observe a gaussian behavior for long times for densities below the localization threshold.

DY 41.10 Fri 12:45 HÜL 186

Modeling non-Gaussian 1/f noise using stochastic differential equations and by sequences of stochastic pulses — •Bronislovas Kaulakys, Miglius Alaburda, and Julius Ruseckas — Institute of Theoretical Physics and Astronomy, Vilnius University, A. Gostauto 12, LT-01108 Vilnius, Lithuania

We present and analyze models of $1/f$ noise, which can be relevant

for the understanding of the origin, main properties and parameter dependencies of the flicker noise. Signals represented as sequences of the random pulses [1] and models based on the stochastic differential equation with different relaxation rates [2, 3] are analyzed. The models generate signals with the Gaussian and non-Gaussian power-law distributions and $1/f^{\beta}$ power spectrum.

[1] J. Ruseckas, B. Kaulakys and M. Alaburda, Lith. J. Phys. **43**, 223 (2003); arXiv:0812.4674.

[2] B. Kaulakys, V. Gontis, and M. Alaburda, Phys. Rev. E **71**, 051105 (2005).

[3] B. Kaulakys, M. Alaburda and J. Ruseckas, AIP Conf. Proc. **922**, 439 (2007); arXiv:1001.2635v1.

DY 41.11 Fri 13:00 HÜL 186

Exact solution of a stochastic birth and death process with delayed death — •Luis F. Lafuerza and Raul Toral — Intitute for Cross-Disciplinary Physics and Complex Systems

Motivated by protein dynamics where degradation can occur with a time delay, we study a stochastic birth and death process with delayed-degradation. This is one of the simplest rocesses in which the interplay between stochasticity and delay can be studied.

In this work we develop a rigorous derivation of the stochastic description of a birth and death process that includes delay and solve it exactly. We find that the exact solution for the probabilities leads to equations for the mean values that do not comply with simple intuitive arguments and that oscillatory behavior does not exist (while it is usually assumed to be present in this type of system). This warns about the derivation of dynamical equations describing the evolution of the concentrations in cases in which delay plays a role.

DY 42: Critical Phenomena and Phase Transitions

Time: Friday 10:15–12:45 Location: ZEU 255

DY 42.1 Fri 10:15 ZEU 255

Ground states of random-field Ising magnets with correlated disorder — •Björn Ahrens and Alexander K. Hartmann — Universität Oldenburg

We consider the random-field Ising magnet (RFIM) in $d = 3$ with correlated disorder. The RFIM consists of ferromagnetically coupled Ising spins with an additional quenched local random field. To ensure unique ground states the random field is chosen to be distributed according to a Gaussian with zero mean and a tunable standard deviation. Using Fourier transforms, we generate correlated random fields which exhibit a power-law shaped two-point correlation function. This well known method conserves the Gaussian distribution of the random field.
To obtain the ground state for each realisation of the disorder numerically, we map the random field to a graph with suitable chosen edge capacities [Picard and Ratliff, Networks 5, 357 (1975)]. For these graphs we calculate the maximum flow using a fast polynomial max-flow/min-cut algorithm, recently developed in algorithmic graph theory. Therein the minimum cut corresponds to a ground state configuration of the system. This allows to calculate exact ground states of systems up to $N = 100^3$ spins.
Similar to the RFIM with uncorrelated Gaussian disorder we find phase transitions for different two-point correlation functions. We obtain critical scaling exponents to analyse the transitions, using finite-size scaling.

DY 42.2 Fri 10:30 ZEU 255

Delocalized-localized transition of disordered phonons — •Sebastian Pinski and Rudolf Römer — Department of Physics and Centre for Scientific Computing, University of Warwick, Coventry, CV4 7AL, United Kingdom

The Anderson model (AM) of localization has been a major topic of research for over 50 years. The resemblance of this model with that of the 'scalar' model of phonon localization (SMPL) due to disorder has been noted, yet only probed in 1D systems. Past research on the SMPL has been heavily directed towards the vibrational density of states and unearthing the origins of the boson-peak, with the delocalized-localized transition assumed to be close to the upper band edge. We present work on a equivalence relation between the AM and the SMPL that has enabled direct translation of the electron phase diagram with on-site potential disorder to that of a phonon phase diagram with mass disorder. This has been verified with high accuracy transfer matrix method (TMM) calculations. Phononic phase diagrams for both mass and force-constant disorder in the SMPL are presented for the first time and the implications of these diagrams are discussed. Finally, finite size scaling of the results obtained from TMM indicates that the critical exponent of phononic systems is similar to that of electronic systems.

DY 42.3 Fri 10:45 ZEU 255

Migdal-Kadanoff approximation to the diluted negative-weight percolation problem — •Oliver Melchert[1], Stefan Boettcher[2], and Alexander K. Hartmann[1] — [1]Institut für Physik, Carl-von-Ossietzky Universität Oldenburg, Oldenburg (Germany) — [2]Department of Physics, Emory University, Atlanta (USA)

We consider the diluted negative weight percolation (NWP) problem [1] on lattice graphs, wherein edge weights are drawn from disorder distributions that allow for weights of either sign. We are interested whether there are system-spanning paths or loops of total negative weight. So as to study the model on hypercubic lattice graphs numerically, one has to perform a non-trivial transformation of the original graph and apply sophisticated matching algorithms.

Here, we consider the NWP model on hierarchical lattice graphs, where a Migdal-Kadanoff (MK) approximation can be used to gain insight on the topology of the phase diagram. For a very basic disorder distribution we set up a renormalization group (RG) transformation and study the RG flow in the disorder-dilution plane in order to find fixed points and critical indices for the linearized model. We further implement the "pool" method [2] to yield the phase diagram and critical exponents upon decimation of huge graphs and we compare our findings to previous results from finite-size scaling analyses [1,3].

[1] L. Apolo, OM, and A.K. Hartmann, Phys. Rev. E 79 (2009) 031103

[2] S. Boettcher, Eur. Phys. J. B 33 (2003) 439

[3] OM, L. Apolo, and A.K. Hartmann, Phys. Rev. E 81 (2010) 051108

DY 42.4 Fri 11:00 ZEU 255

A numerical study of self-avoiding walks (SAWs) on disordered two-dimensional lattices — •Niklas Fricke and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Germany

We revisit the long-standing problem of SAWs on diluted two-dimensional lattices at and above the percolation threshold, employing a Monte Carlo algorithm as well as a newly developed complete enumeration technique.

Some of the results are quite surprising, as they are in conflict with the Meir-Harris model [1], which is generally assumed to provide the qualitatively correct description for the scaling behaviour of SAWs on disordered lattices.

The widely held conviction that the exponents on the backbone are the same as on the full percolation cluster is also put under scrutiny.

[1] Y. Meir and A. B. Harris, Phys. Rev. Lett. 63, 26 (1989)

DY 42.5 Fri 11:15 ZEU 255

Speeding up critical system dynamics through optimized evolution — •Tommaso Caneva[1], Tommaso Calarco[1], Rosario Fazio[3], Giuseppe E. Santoro[2,4,5], and Simone Montangero[1] — [1]Institut für Quanteninformationsverarbeitung, Universität Ulm, D-89069 Ulm, Germany — [2]International School for Advanced Studies (SISSA), Via Beirut 2-4, I-34014 Trieste, Italy — [3]NEST, Scuola Normale Superiore & Istituto di Nanoscienze - CNR, Piazza dei Cavalieri 7, I-56126 Pisa, Italy — [4]CNR-INFM Democritos National Simulation Center, Via Beirut 2-4, I-34014 Trieste, Italy — [5]nternational Centre for Theoretical Physics (ICTP), P.O.Box 586, I-34014 Trieste, Italy

The number of defects which are generated on crossing a quantum phase transition can be minimized by choosing properly designed time-dependent pulses. In this talk we show what are the ultimate limits of this optimization. We discuss under which conditions the production of defects across the phase transition is vanishing small. Furthermore we

show that the minimum time required to enter this regime is $T = \pi/\Delta$, where Δ is the minimum spectral gap, unveiling an intimate connection between an optimized unitary dynamics and the intrinsic measure of the Hilbert space for pure states. Surprisingly, the dynamics is non-adiabatic; this result can be understood by assuming a simple two-level dynamics for the many-body system.

DY 42.6 Fri 11:30 ZEU 255

Critical Parameters from a Generalized Multifractal Analysis at the Anderson Transition — Alberto Rodriguez[1], Louella J Vasquez[1], Keith Slevin[2], and •Rudolf A Römer[1] — [1]Dept. of Physics and Ctr for Scientific Computing, University of Warwck, Coventry, CV4 7AL, UK — [2]Department of Physics, Osaka University, 1-1 Machikaneyama, Toyonaka, Osaka 560-0043, Japan

We propose a generalization of multifractal analysis that is applicable to the critical regime of the Anderson localization-delocalization transition. The approach reveals that the behavior of the probability distribution of wave function amplitudes is sufficient to characterize the transition. In combination with finite-size scaling, this formalism permits the critical parameters to be estimated without the need for conductance or other transport measurements. Applying this method to high-precision data for wave function statistics obtained by exact diagonalization of the three-dimensional Anderson model, we estimate the critical exponent $\nu = 1.58 \pm 0.03$.

DY 42.7 Fri 11:45 ZEU 255

The infinite-component spin glass revisited — •Frank Beyer and Martin Weigel — Institut für Physik, KOMET 331, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55127 Mainz

Starting from the Sherrington-Kirkpatrick (SK) mean-field spin-glass model with a broken replica symmetry, an expansion towards finite (spatial) dimensions ($d = 2, 3, \ldots$) breaks down at the upper critical dimension. One way of bypassing these problems might be to consider the replica-symmetric m-component vector spin glass in the limit $m \to \infty$ and attempt an expansion towards the finite-m cases including the XY and Heisenberg spin glass. In this contribution, we study vector spin glasses in the $m \to \infty$ limit using ground-state calculations at zero temperature and a saddle-point approximation at finite temperatures. For the SK model, we show the existence of a finite order parameter in the ordered phase and critical scaling behavior consistent with an upper critical dimension equal to eight. Using ground-state calculations, we determine the lower critical dimension to be $5 \leq d_l \leq 6$ when the limit $m \to \infty$ is taken before the thermodynamic limit $N \to \infty$, while we find indications for $d_l = 3$ for the opposite (physical) order of taking limits. Complementing these results, we studied a one-dimensional chain with power-law decay of interactions that can be continuously tuned from the mean-field to the short-range regime.

DY 42.8 Fri 12:00 ZEU 255

Aspect ratio dependence of critical Casimir forces — •Alfred Hucht, Daniel Grüneberg, and Felix Schmidt — Fakultät für Physik, Universität Duisburg-Essen

We consider three-dimensional Ising models in a $L_\perp \times L_\parallel \times L_\parallel$ cuboid geometry with finite aspect ratio $\rho = L_\perp/L_\parallel$ and periodic boundary conditions along all directions. For these models the universal finite-size scaling function of the thermodynamic Casimir force is evaluated numerically by means of Monte Carlo simulations employing the method recently presented in [1]. The Monte Carlo results are compared to recent field theoretical results for the Ising universality class for temperatures below and above the bulk critical temperature T_c [2], and to the finite-size scaling functions of the thermodynamic Casimir force derived in [3] for the $O(n)$-symmetrical case and temperatures $T \geq T_c$ in the framework of the renormalization group-improved perturbation theory to two-loop order. The MC data are found to be in good agreement with these field theoretical results. Furthermore, the Casimir force scaling function for the two dimensional Ising model as function of ρ is calculated exactly and compared to the three dimensional case.

[1] A. Hucht, Phys. Rev. Lett. 99, 185301 (2007). [2] V. Dohm, Europhys. Lett. 86, 20001 (2009). [3] D. Grüneberg and H. W. Diehl, Phys. Rev. B, 77, 115409 (2008).

DY 42.9 Fri 12:15 ZEU 255

Critical Casimir forces in the presence of a chemically structured substrate — •Francesco Parisen Toldin[1] and Siegfried Dietrich[2,3] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany — [2]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart, Germany — [3]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, D-70569 Stuttgart, Germany

Motivated by recent experiments on a binary liquid mixture, we study the critical properties of a system in the Ising universality class, in a film geometry in the presence of a chemically structured substrate, with alternating adsorption preference. By means of Monte Carlo simulations of an improved Hamiltonian, so that the leading scaling corrections are suppressed, numerical integration, and finite-size scaling analysis we determine the critical Casimir force and its universal scaling function.

DY 42.10 Fri 12:30 ZEU 255

Optimizing Wilson's Momentum Shell Renormalization Group — •Andreas Troester — Johannes Gutenberg University, Mainz, Germany

Previous attempts to accurately compute critical exponents from Wilson's momentum shell renormalization prescription suffered from the difficulties posed by the presence of an infinite number of irrelevant couplings. Taking the example of the 1d long-ranged Ising model [A. Tröster, PRE **79**, 036707 (2009)], we calculate the momentum shell renormalization flow in the plane spanned by the coupling constants (u_0, r_0) by a simulation method based on our recently developed Fourier Monte Carlo algorithm [A. Tröster, PRB **76**, 012402 (2007); PRL **100**, 140602 (2008); Comput. Phys. Comm. **179**, 30 (2008)]. Carrying out such simulations for different values of the momentum shell thickness parameter b, we report strong anomalies in the b-dependence of the fixed point couplings and the resulting exponents y_τ and ω in the vicinity of a shell parameter $b^* < 1$ characterizing a thin but finite momentum shell. Evaluation of the exponents for this "optimized" value b^* of b yields a dramatic improvement of their numerical accuracy, indicating a strong damping of the influence of irrelevant couplings [A. Tröster, Phys. Rev. B **81**, 125135 (2010); Comput. Phys. Comm., accepted for publication (2010)].

DY 43: Soft Matter

Time: Friday 10:15–12:30 Location: ZEU 118

DY 43.1 Fri 10:15 ZEU 118

Mobility and Diffusion of a Tagged Particle in a Driven Colloidal Suspension — •Boris Lander[1], Udo Seifert[1], and Thomas Speck[2,3] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [2]Department of Chemistry, University of California, Berkeley, California 94720, USA — [3]Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

Mobility and diffusion of single particles play a key role in the understanding of colloidal suspensions. While beyond linear response, diffusion coefficients can still be obtained by a Green-Kubo relation, determining the mobility is challenging. A novel method enables us to compute the time-dependent response function for a single tagged particle perturbed by a small force and thus the mobility in a Brownian dynamics simulation [1]. For a suspension driven into a nonequilibrium steady state by simple shear flow, both mobility and diffusion constant of the tagged particle increase with shear. Our data can be approximated by an expansion, where the mobility becomes proportional to the square root of the strain rate. Somewhat surprisingly, the initial decay of the velocity autocorrelation function can be mapped onto a corresponding response function by a time-independent scaling factor, allowing for an interpretation in terms of an 'effective temperature'. Such a phenomenological effective temperature recovers the Einstein relation in nonequilibrium.

[1] B. Lander, U. Seifert, T. Speck, EPL, in press.

DY 43.2 Fri 10:30 ZEU 118

Entanglements in globular polymer phases: A Monte Carlo study — •Daniel Reith and Peter Virnau — Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz

Bridging algorithms are global Monte Carlo moves which allow for simulation of globular phases of single polymers [1]. These moves ensure an efficient sampling of the topological degrees of freedom, which is usually hindered by the high monomer density and self-entanglements, by destroying and recreating bonds. In this context, the determination of knots provides a measure for entanglement which allows us to gauge the efficiency of the move sets.
The second part will focus on the application of these bridging moves to problems related to single chain polymers in globular phases. To this end we discuss single polystyrene chains in miniemulsion droplets, the influence of chain stiffness on self-entanglements of a single polymer chain in a spherical capsid and the influence of sequence on the knotting of globular heteropolymers.
[1] D. Reith, P. Virnau, Comput Phys Commun **181**, 800 (2010)

DY 43.3 Fri 10:45 ZEU 118

Friction controlled bending solitons as folding pathway toward colloidal clusters — •Nebojsa Casic[1], Steffen Schreiber[2], Pietro Tierno[3], Walter Zimmermann[2], and Thomas M. Fischer[1] — [1]EP V, Uni Bayreuth, Germany — [2]TP 1, Uni Bayreuth, Germany — [3]Departament de Química Física, Universitat de Barcelona, Spain

We study the conformational transition of an ensemble of magnetic particles from a linear chain to a compact cluster when subjected to an external magnetic field modulation. We show that the transient dynamics induced by switching the field from static to rotating is governed by the relative friction of adjacent particles in the chain. Solid particles show bending solitons counter-propagating along the chain while buckling of the chain is the mechanism preferred by ferrofluid droplets. By combining real-space experiments with numerical simulations we unveil the underlying mechanism of folding pathways in driven colloidal systems. EPL, 90 (2010) 58001

DY 43.4 Fri 11:00 ZEU 118

Switching A Gelified Liquid Crystal — •Thomas Müller[1], Maxim Khazimullin[2], Ingo Rehberg[1], Wolfgang Schöpf[1], Alexei Krekhov[3], Robin Pettau[4], and Klaus Kreger[4] — [1]Experimental Physics V, University of Bayreuth, 95440 Bayreuth, Germany — [2]Institute of Molecule and Crystal Physics, Russian Academy of Science, Ufa, Russia — [3]Theoretical Physics I, University of Bayreuth, 95440 Bayreuth, Germany — [4]Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany

Liquid crystal displays make use of the electrooptical effect, caused by the orientation of the liquid crystals in an external electrical field above a certain threshold voltage (Fréedericksz effect). We investigate this effect in a new class of liquid crystal material, namely a diluted solution of an ABA-triblock copolymer in the nematic liquid crystal 5CB. The motivation of our studies is to obtain the physical parameters of this novel material with special emphasis on its dynamical behavior. In our experiments we use polarizing microscopy to detect the electrically controlled birefringence in homogeneous cells. We measure the temporal evolution of the light intensity when switching the electrical field above and below the threshold. It provides information about relaxation times of the director orientation, which can be used to determine the Fréedericksz threshold voltage and the elasticity of the gelified liquid crystal. Moreover, the relaxation times yield the rotational viscosity which contains information about the interaction between polymer molecules and liquid crystals.

DY 43.5 Fri 11:15 ZEU 118

Phase diagram and orientational dynamics of nematic liquid crystals under shear flow: A numerical bifurcation analysis. — •David A. Strehober and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We study the nonequilibrium dynamics of rodlike nematic polymers under shear flow. Starting from a mesoscopic description involving the alignment tensor [1][2], we investigate the rheological phase diagram with respect to the shear rate and tumbling parameter. The dynamics of the alignment tensor is described by five coupled differential equations. We employ numerical continuation methods, specifically the freely available software package MATCONT [3], to find the boundaries between different dynamic states. We recover the results that were obtained via direct integration [4] of the set of differential equations for the alignment tensor. On top of that, we are able to make statements about the nature of the bifurcations, and how orientational modes, i.e. Kayaking Wagging or Tumbling, are born. We conclude the talk with a discussion of the role of temperature.
[1] S. Hess, Z.Naturforsch. A **31a**, 1034 (1976)
[2] M. Doi, J.Polym. Sci., Polym. Phys. Ed. **19**, 229 (1981)
[3] A. Dhooge, W. Govaerts, and Yu. A. Kuznetsov., ACM Trans. Math. Softw. **29**, (2003)
[4] S. Grandner, S. Heidenreich, S. Hess and S. H. L. Klapp, Eur.Phys.J. E **24**, 353 (2007)

DY 43.6 Fri 11:30 ZEU 118

Helical crystals of charged colloids in cylindrical confinement — •Erdal Celal Oguz, René Messina, and Harmut Löwen — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany

By lattice sum calculations we explore the ground state phase diagram of screened Coulomb particles in a cylindrical confinement. We obtain several chiral as well as achiral helical phases. Similar systems were studied with dusty plasmas [1] and hard spheres [2]. We also compare our results to computer simulations and experiments with highly screened particles [2,3].
[1] V. N. Tsytovich, G. E. Morfill, V. E. Fortov, N. G. Gusein-Zade, B. A. Klumov and S. V. Vladimirov, New Journal of Physics **9**, 2007
[2] G. T. Pickett, M. Gross and H. Okuyama, Phys. Rev. Lett. **85**, 2000
[3] M. Tymczenko, L. F. Marsal, T. Trifonov, I. Rodriguez, F. Ramiro-Manzano, J. Pallares, A. Rodriguez, R. Alcubilla and F. Meseguer, Adv. Mater. **20**, 2008

DY 43.7 Fri 11:45 ZEU 118

Binary non-additive hard sphere mixtures: Fluid demixing, asymptotic decay of correlations and free fluid interfaces — •Matthias Schmidt[1,2] and Paul Hopkins[2] — [1]Theoretische Physik II, Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany — [2]H.H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK

Using a fundamental measure density functional theory we investigate both bulk and inhomogeneous systems of the binary non-additive hard sphere model. For sufficiently large (positive) non-additivity the mixture phase separates into two fluid phases with different compositions. We calculate bulk fluid-fluid coexistence curves for a range of size ratios and non-additivity parameters and find that they compare well to simulation results from the literature. Using the Ornstein-Zernike equation, we investigate the asymptotic decay of the partial pair correlation functions. At low densities a structural crossover occurs in the asymptotic decay between two different damped oscillatory modes with different wavelengths corresponding to the two intra-species hard-core diameters. On approaching the fluid-fluid critical point there is a Fisher-Widom crossover from exponentially damped oscillatory to monotonic asymptotic decay. Using the density functional we calculate the density profiles for the planar free fluid-fluid interface between coexisting fluid phases. We show that the type of asymptotic decay of the pair correlation functions not only determines the asymptotic decay of the interface profiles, but is also relevant for intermediate and even short-ranged behaviour.

DY 43.8 Fri 12:00 ZEU 118

Conformational studies of bottle-brush polymers absorbed on a flat solid surface under good solvent conditions — •Hsiao-Ping Hsu[1], Wolfgang Paul[2], and Kurt Binder[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Mainz, Germany — [2]Theoretische Physik, Martin Luther Universität Halle-Wittenberg, Halle, Germany

The adsorption of a bottle-brush polymer end-grafted with one chain end of its backbone to a flat substrate surface is studied extensively by Monte Carlo simulations. The bond fluctuation model on the simple cubic lattice, is used here [1]. Varying the backbone chain length and the side chain length, and fixing the grafting density to 1, our simulations cover the range which is accessible for the comparison of experimental data and the theoretically scaling predictions. When the adsorption energy strength is varied, we find that the adsorption transition roughly occurs at the same value as for ordinary linear chains. For longer side chains we show that the adsorption of bottle-brushes is a two step process, the decrease of the perpendicular linear dimen-

sion of side chains with adsorption energy strength can even be non-monotonic [2]. As the bottle-brush polymer is deeply adsorbed to the surface, the evidence for a quasi-two-dimensional scaling is presented.

[1] H.-P. Hsu, W. Paul, and K. Binder, Macromolecules **43**, 3094 (2010).

[2] H.-P. Hsu, W. Paul, and K. Binder, J. Chem. Phys. **133**, 134902 (2010)

DY 43.9 Fri 12:15 ZEU 118

Quantum-classical adaptive simulation of liquid para-hydrogen — •Adolfo Poma and Luigi Delle Site — Max-Planck-Institute for Polymer Research, Ackermannweg 10, D-55021 Mainz, Germany

Adaptive resolution simulations for classical systems are currently made within a reasonably consistent theoretical framework. Recently we have extended this approach to the quantum-classical coupling by mapping the quantum nature of an atom onto a classical polymer ring representation within the path integral approach. In this way the process of interfacing adaptively a quantum representation to a classical one corresponds to problem of interfacing two regions with a different number of effective "classical" degrees of freedom; thus the classical formulation of the adaptive algorithm applies straightforwardly to the quantum-classical problem. In this work we show the robustness of such an approach for a liquid of para-hydrogen at low temperature. This system represents a highly challenging conceptual and technical test for the adaptive approach due to the extreme thermodynamical conditions where quantum effects play a central role.