DY 30: Poster II

Time: Thursday 16:00–18:00 Location: Poster D

DY 30.1 Thu 16:00 Poster D

Giant Diffusion in many particle systems — •Olga Zvyagolskaya[1], Stefan Bleil[1], Peter Reimann[2], and Clemens Bechinger[1] — [1]2. Physikalisches Institut, Universität Stuttgart, Germany — [2]Fakultät für Physik, Universität Bielefeld, Germany

The diffusion coefficient of a single particle in thermal equilibrium is reduced by the presence of an external (periodic) potential. When an additional constant driving force f is applied, the diffusion coefficient has been predicted to be largely enhanced and displays a maximum as a function vs. f. We have experimentally investigated this so-called giant diffusion by exposing a colloidal particle to a tilted periodic potential being created by means of optical tweezers. When measuring the diffusion coefficient with video microscopy we find good agreement with theoretical predictions. In addition to single particles, we also investigated the situation where many particles with repulsive interactions are present. We observe a strong enhancement of the diffusion coefficient as a function of the particle interaction strength for constant potential depth and driving force. In addition we observe the diffusion coefficient to depend on the ratio of particles and potential minima in the system.

P. Reimann, C. Van den Broeck, H. Linke, P. Hänggi, J.M. Rubi, and A. Pérez-Madrid; PRL 87, 010602 (2006)

DY 30.2 Thu 16:00 Poster D

Extending the Boltzmann equation to non-equilibrium: A novel method to determine external potentials. — •Valentin Blickle[1], Thomas Speck[2], Udo Seifert[2], and Clemens Bechinger[1] — [1]2. Physikalisches Institut, Universität Stuttgart — [2]II. Institut für Theoretische Physik, Universität Stuttgart

In tilted potentials the motion of a colloidal particle is an interplay between thermal diffusion and drift. Due to this superimposed motion the diffusion coefficient and the average particle velocity become non trivial functions of the driving force f. In our experiment we drive a colloidal particle along a toroidal three-dimensional laser trap using scanning optical laser tweezers. We use an electrooptical modulator to additionally impose a static laser potential V along the torus. To characterize the laser potential we introduce a novel method, based on a steady state non-equilibrium measurement. The method uses a modified Boltzmann equation which additionally considers the stationary current. We show that this method is independent of the driving force f und thus allows to determine the static potential V. Being not restricted to equilibrium fluctuations we can characterize potential depths up to several 100 k_BT.

DY 30.3 Thu 16:00 Poster D

Quantum Monte Carlo Investigation of Quantum Phase Transitions of Mixed Heisenberg Spin Chains — •Rainer Bischof[1], Peter Crompton[2], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Germany — [2]Center for Theoretical Physics, Massachusetts Institute of Technology, USA

By means of quantum Monte Carlo simulations at low temperatures, the quantum phase transitions in antiferromagnetic Heisenberg spin chains consisting of two different kinds of spin, S_a and S_b, that appear alternatingly in pairs, are investigated for the cases $S_\mathrm{a} = 1/2$ and $S_\mathrm{b} = 1$, $S_\mathrm{a} = 1/2$ and $S_\mathrm{b} = 3/2$ as well as $S_\mathrm{a} = 1$ and $S_\mathrm{b} = 3/2$. Transitions between qualitatively different ground states (quantum phases) are induced by varying the parameter α which is the relative coupling between unlike and like spins. In particular, the so-called twist order parameter as well as spatial and imaginary temporal correlation lengths are measured and analysed. Critical values of α, critical exponents and leading correction terms are extracted by finite-size scaling analysis.

DY 30.4 Thu 16:00 Poster D

Pore scale model for carbonate rocks — •Bibudhananda Biswal[1], Paul-Eric Oren[2], Rudolf Held[3], Stig Bakke[2], and Rudolf Hilfer[1] — [1]ICP, Universitaet Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany — [2]Numerical Rocks AS, N-7041 Trondheim, Norway — [3]Statoil ASA, N-7005 Trondheim, Norway

A stochastic geometrical model for the diagenesis of carbonate rocks is proposed. It incorporates many crucial features of real carbonates: correlations with the primordial depositional textures, scale dependent intergranular porosity over many decades, vuggy porosity, a percolating pore space, a fully connected matrix space, strong dependence on the process of discretization and wide variability in the permeabilities etc. The continuum representation allows discretization of the microstructure at arbitrary resolutions. Pore scale geometries of two generic carbonate textures are successfully reconstructed using this model. Petrophysical parameters are measured on the discretized samples and compared with real samples. The model can be easily adapted to reconstruct the pore scale of a wide variety of carbonate rocks.

DY 30.5 Thu 16:00 Poster D

Voter model on lattices with a single antiferromagnetic bond — •Konstantin Klemm[1] and Takuya Yamano[2] — [1]Bioinformatics, Leipzig University, Haertelstr. 16-18, D-04107 Leipzig, Germany — [2]International Christian University, Social Science Research Institute, 3-10-2, Osawa, Mitaka-shi, Tokyo, 181-8585, Japan

Among the simplest types of spin kinetics is the voter model: In each update a pair (i, j) of neighboring sites is chosen and site i adopts the state of site j. Here we consider a version of the model where one of the lattice bonds is antiferromagetic and thus transmits the reverse spin state. Due to the lack of absorbing configurations the dynamics is vastly different from the original model. The density of interfaces shows a bimodal distribution, i.e. the system spends most of the time in strongly ordered and strongly disordered configurations while the time for switching between the two situations is short. The time-averaged density of interfaces decays algebraically with distance from the lattice defect, with an exponent $\approx 1/3$ in dimension $d = 2$. These numerical observations are in sharp contrast to the results for the Ising model on the same kind of perturbed lattice.

DY 30.6 Thu 16:00 Poster D

Colloidal Crystals in 2D: elasticity, structures and phase transitions — •Kerstin Franzrahe and Peter Nielaba — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Thin films on a substrate can be modelled by two dimensional colloidal systems. The influence of the substrate can be varied by adjusting e.g. the amplitude of an additional external laser field. We investigate the elastic and structural properties of such systems via Monte-Carlo simulations. Our model system consists of particles interacting via a hard-disk potential. For the field free case the influence of quenched impurities on the elastic properties of a mono-disperse system [1] is examined, while in the study of bi-disperse systems our focus is on the stability of crystalline structures for various size and mixing ratios. Modelling the effect of the substrate on the two dimensional crystal, we study the influence of a commensurable, spatially periodic, external laser field on a bi-disperse $S_1(AB)$ crystal. We observe laser induced freezing (LIF).

The fluctuations of the microscopic strains in a solid contain information on the elastic properties of the system. Generalising the approach by S. Sengupta et.al.[2], we analyse the strain correlation functions of a harmonic two dimensional system. The analysis shows that these correlations are highly anisotropic in the solid.

[1] K. Franzrahe et. al., Comp. Phys. Commun. **169**,pp 197-202 (2005)
[2] S. Sengupta, P. Nielaba, M. Rao and K. Binder,Phys. Rev. E **61**, pp. 1072 (2000)

DY 30.7 Thu 16:00 Poster D

An information distance and classical no-cloning theorem — •Takuya Yamano — International Christian University, SSRI, 3-10-2 Osawa, Mitaka-shi, Tokyo 181-8585, Japan

The conservation of the Kullback-Leibler (KL) information measure under the Liouville dynamics provides a classical counterpart of a quantum impossible process, i.e. the no-cloning theorem. We present the degree of the conflict in the distances of initial and final states in the copying process which is comprised of a tripartite (source, machine, and target) system whose probablity functions are factorized. We use a generalized KL measure obtained by operating the Jackson's symmetric q-derivative to a parametrized *overlap*. Some metrics (KL, Fubini-Study, and Wooters) on the Hilbert space provide equivalent values to the Euclidean one for two infinitesimally displaced states up to the second order in the shift. By investigating the metrics up to

higher oder, we study the difference among these metrics and intend to get insights into the theorem.

DY 30.8 Thu 16:00 Poster D

Implications of mean field and non-mean field effects for a system of interacting particles — •Radha Banhatti, Klaus Funke, and Andreas Heuer — Universität Münster, Institut für Physikalische Chemie und SFB 458, Corrensstrasse 30, D-48149 Münster

Recently, a simple harmonic model (SHM) was formulated for an equilibrated system of mutually interacting N +1 particles to study the relaxation following the jump of a central particle at time t=0 [M. Kunow and A. Heuer, J. Chem. Phys. 119, 2338 (2003)]. The relaxation of the central particle (single-particle route) and that of the other N particles (multi-particle route) were cast in the form of rate equations. The SHM formalism was an attempt to enquire into the general validity of the rate equations formulated within jump relaxation models to understand the frequency-dependent conductivity in different classes of disordered materials including ionic crystals, conductors, inorganic glasses and ionic liquids. Using the formalism of the SHM, we show that it is possible to explicitly examine the effect of mean field (collective response) and non-mean field (distance-dependent response) nature of the neighborhood interactions with the central particle. The change in the shape of the trajectory of the central particle (the single-particle route) yields, for example, a direct correlation to the abrupt change of shape of the ion-conductivity spectra of a supercooled melt, calcium potassium nitrate of composition $0.4Ca(NO_3)_2 \cdot 0.6KNO_3$, around T = 375 K [K.Funke and R. D. Banhatti, Solid State Ionics, 177, 1551 (2006)]. A coherent description for the ion conduction in this regime is discussed.

DY 30.9 Thu 16:00 Poster D

Anomalous transport in disordered iterated maps — •Andreas Fichtner and Günter Radons — D-09107 Chemnitz, Germany

Anomalous transport is not only a phenomenon of systems with stochastic environmental forces. Also random walks in random environments can show such a behaviour. Sinai diffusion [1] characterises a class of random walks for which the so called Golosov phenomenon [2] was proven rigorously. We extend the Sinai model to random walks whose transitions are not restricted to nearest-neighbours. Thereby a vanishing global bias is guaranteed by a generalisation of binary disorder. [3,4]

For Sinai disorder exact results exist for the disorder averaged mean square displacement, the density of states of the propagator, and the size-dependence of the escape rate, or, the mean first passage time, respectively. For each of these quantities a characteristic exponent can be definded. We could show numerically that the characteristic exponents also exist for our extended model. At least for relatively small systems the characteristic exponents show a non-trivial dependence on system size and coincide. Perturbation theory, which is exact in the Sinai case, enables us to calculate escape rates for significantly larger systems. For our model we find as function of system size a transition from a large preasymptotic regime to the asymptotic behaviour.

[1] Ya.G.Sinai, Theor. Prob. Appl. 27 (1982) 247.
[2] A.Golosov, Commun. Math. Phys. 92 (1984) 491.
[3] A.Fichtner and G.Radons, New J. Phys. 7 (2005) 30.
[4] G.Radons, Physica D 187 (2004) 3.

DY 30.10 Thu 16:00 Poster D

Surface diffusion in potential landscapes — •Stephan Zschiegner[1,2], Stefanie Russ[3], Armin Bunde[1], Jörg Kärger[2], and Rustem Valiullin[2] — [1]Theoretische Physik III, JLU Giessen — [2]Experimentelle Physik, Universität Leipzig — [3]Theoretische Physik, FU Berlin

We study 2D surface diffusion with different types of potential landscapes. As test potentials we use Gaussian and power-law distributions with or without correlations. For these model surfaces we investigate diffusion properties that are the basis of understanding the inverse problem: Getting potential lanscapes from surface diffusion measurements. For this purpose, we determine a possible basis of potentials and their diffusion properties for a direct transformation from the experimental results to the underlying potential within the pore.

DY 30.11 Thu 16:00 Poster D

Nonlinear integral equations for the thermodynamics of the Uimin-Sutherland model — •Jens Damerau and Andreas Kluemper — Fachbereich C – Physik, Bergische Universität Wuppertal, 42097 Wuppertal, Germany

We investigate the thermodynamical properties of integrable one-dimensional spin-chains of Uimin-Sutherland type. This class includes several interesting models like the spin-1/2 Heisenberg model, the $t-J$ model, the $SU(4)$-symmetric spin-orbital model and certain spin-ladder systems. We derive well-posed finite sets of nonlinear integral equations (NLIE) which allow for the numerical evaluation at arbitrary finite temperature. Analytical solutions are possible in the high- and low-temperature limits. In the low-temperature regime, we find divergences of the magnetic susceptibilities at critical fields and logarithmic singularities for zero magnetic field. In comparison to other recently derived NLIE, the evaluation at low temperature poses no problem in our formulation.

DY 30.12 Thu 16:00 Poster D

The target decay on irregular networks — •mircea galiceanu and alexander blumen — Theoretische Polymerphysik, Universität Freiburg, Hermann-Herder-Straße 3, D-79104 Freiburg, Germany

We investigate the survival probability of immobile targets, which get annihilated by random walkers at first encounter. As irregular lattices we focus on scale free networks [1] and on small world networks [1], [2]. For scale free networks we consider two kinds of degree distributions (number of nearest neighbors) with long time-tails. In the first case we start the degree distribution from degree 1, while in the second case from degree 2. It turns out that the survival probability and the quality of its description through the average number of distinct sites visited, S_n, depend on the details of the degree distribution: networks which are more ramified (the first situation) have survival probabilities which are more regular, whereas the scale free networks with long chain-like segments (the second case) display decay laws similar to those of small world networks, where a description only in terms of S_n is rather poor.

[1] Galiceanu M and Blumen A, *J. Phys. A*, in press
[2] Jasch F and Blumen A *J. Chem. Phys.* **117**, 2474, (2002)

DY 30.13 Thu 16:00 Poster D

Evolution of Canalizing Boolean Networks — •Agnes Szejka and Barbara Drossel — Institut für Festkörperphysik, Technische Universität Darmstadt, Deutschland

Canalizing Boolean networks are used to model gene regulatory networks. To get insight into how evolutionary forces may shape such structures, we simulate the evolution of a canalizing Boolean network by means of an adaptive walk. The mutations considered concern the functions and the connections of the nodes. The fitness criterion is robustness against small perturbations. As the adaptive walk leads to a local maximum in the fitness landscape it can deliver insight into the fitness landscape of a system. We find that all networks always reach maximum fitness and that there is a huge neutral plateau at this value that allows for further evolution. The evolved networks, although robust, show many properties characteristic for chaotic networks.

DY 30.14 Thu 16:00 Poster D

Multicomponent reaction-diffusion processes on complex networks — •Sebastian Weber and Markus Porto — Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt, Germany

We study the reaction-diffusion process $A + B \to \emptyset$ on uncorrelated scale-free networks analytically [1]. By a mean-field ansatz we derive analytical expressions for the particle pair-correlations and the particle density. Expressing the time evolution of the particle density in terms of the instantaneous particle pair-correlations, we determine analytically the 'jamming' effect which arises in the case of multicomponent, pair-wise reactions. Comparing the relevant terms within the differential equation for the particle density, we find that the 'jamming' effect diminishes in the long-time, low-density limit. This even holds true for the hubs of the network, despite that the hubs dynamically attract the particles.

[1] S. Weber and M. Porto, Phys. Rev. E **74**, 046108 (2006).

DY 30.15 Thu 16:00 Poster D

Random Boolean Networks with noise — •Christoph Fretter and Barbara Drossel — Institut für Festkörperphysik, Technische Universität Darmstadt, Deutschland

Boolean networks are used as a model for gene regulation networks, where stochastic fluctuations are ubiquitous due to small molecule concentrations. We investigate the influence of stochastic noise on the dynamics of Boolean networks. Noise is implemented in terms of a "temperature", i.e., a probability that a node is assigned a random

state instead of following the deterministic update rule. We measure the robustness of the network dynamics against noise by evaluating the probability of returning to the same attractor after the noise has acted for a finite time. The parameters to be varied are the noise strength, the network size and network topology, and the set of update functions used. We show that under weak noise even simple networks display nontrivial behaviour. We use the theory of relevant components to extrapolate the results to large networks. The methods used are numerical simulations as well as analytical calculations.

DY 30.16 Thu 16:00 Poster D

Ising model on hierarchical scale-free networks — •Sebastian Komosa and Janusz Hołyst — Faculty of Physics and Center of Excellence for Complex Systems Research, Warsaw University of Technology, Koszykowa 75, 00-662 Warsaw, Poland

We studied behavior of a Ising spin model on different hierarchical scale-free networks using Monte Carlo simulations. We observed a phase transition from ferromagnetism to paramagnetism and a power-law behavior of critical temperature with network size. Two different order parameters were used: a standard average network spin and a weighted average network spin. The critical temperature is a power-law function of the ratio $\langle k^2\rangle/\langle k\rangle$.

DY 30.17 Thu 16:00 Poster D

Topographical Stability of Self-Organizing Neural Maps: The case of nonlinear Concave/Convex learning — Fabien Molle[1,2] and •Jens Christian Claussen[2] — [1]Theoretical Physics, Göteborg Universitetet, Sweden — [2]Theoretical Physics, Univ. Kiel, Germany

The apparant self-organizing dynamics of biological topographic feature maps has, apart from the biological modeling, provided various methods of Neural Vector Quantizers as Kohonen's Self-Organizing Map and Martinetz' Neural Gas. The invariant density of the attractor states has been studied extensively the last two decades. In most cases the neural output density adapts the input data density by a power law, which in many cases can be calculated analytically, and even be influenced systematically by modifications in the learning rule [1,2]. Here, we consider a nonlinear learning rule investigated in [2], which is capable to generate information-theoretically optimal maps at least in the 1D case [2]. However, much less is known for the learning dynamics. We introduce a simple crossproduct based stability measure to detect topological defects of the representation when the learning rate is increased [3]. The stability border shows a similar shape for all considered cases, but with different maximal learning rate. The exploration of these stability properties is relevant for applications of neural vector quantizers.

[1] J.C.Claussen, Complexity 8(4),15(2003); Neural Computation 17,996(2005), Claussen & T.Villmann, Neurocomputing 63,124(2005)
[2] T. Villmann & J.C.Claussen, Neural Computation 18, 446 (2006)
[3] F. Molle & J.C. Claussen, Lect. Notes Comp. Sci. 4131, 208 (2006)

DY 30.18 Thu 16:00 Poster D

Resilience of public transport networks against attacks — •Christian von Ferber[1,2], Taras Holovatch[3], Yurij Holovatch[4,5], and Vasyl Palchykov[4] — [1]Applied Mathematics Research Centre, Coventry University, UK — [2]Theoretische Polymerphysik, Universität Freiburg — [3]Ivan Franko University of Lviv, Ukraine — [4]Institute for Condensed Matter Physics, National Academy of Sciences Ukraine, Lviv — [5]Institut für Theoretische Physik, Universität Linz, Österreich

In a recent study of metropolis public transport networks (PTN) we show that these - like many other complex networks - may exhibit scale free behavior [physics/0608125]. In particular, the number of neighboring stations k of a given station is often found to be distributed as $P(k) \sim k^{-\lambda}$, For ideal scale free networks the exponent λ determines the percolation properties, i.e. if $\lambda < 3$ no percolation threshold exists and a giant connected component persists no matter how many nodes are removed. Here, we analyse a number of PTNs of metropolitan areas and extract correlations between the resilience threshold against targeted attacks and their architecture as measured by network characteristics that we find to vary considerably among cities. We develop and simulate an evolutionary model of PTNs that reproduces their key features.

Yu Holovatch was supported by FWF (Austria), Projekt P16574, CvF by the European Community through MTKD-CT-2004-517186.

DY 30.19 Thu 16:00 Poster D

Topological self-organization and critical dynamics of input-driven threshold networks — •Thimo Rohlf — Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, NM 87501, USA

Based on a simple model of network self-organization by local rewiring rules [1], we study topological evolution of input-driven neural threshold networks. In addition to the original system, a subset of network nodes is driven by external input signals with a spiking rate ρ_{in}, that serves as a convenient new control parameter. Depending on $\rho_{in} > 0$, we find a much faster convergence towards topological and dynamical criticality [2] than in the original model (which has $\rho_{in} = 0$).

In particular, our extensive numerical simulations indicate that, at a critical driving rate $\rho_{in}^c(N)$, networks become self-organized critical even for finite numbers N of nodes. Several dynamical order parameters exhibit pronounced power-law scaling, long-range correlations and $1/f$ noise (including, e.g., the distribution of asymptotic Hamming distances of initially nearby system states).

Finally, we discuss possible applications of this model to problems in two fields: control of neural activity in the brain, and the evolution of signal processing by gene regulatory networks in biological cells.

[1] S. Bornholdt and T. Rohlf, *Phys. Rev. Lett.* **84**, 6114 (2000)
[2] T. Rohlf and S. Bornholdt, *Physica A* **310**, 245-259 (2002)

DY 30.20 Thu 16:00 Poster D

Microcanonical Analysis of Polymer Aggregation — •Christoph Junghans, Michael Bachmann, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig

We propose the use of microcanonical analyses for heteropolymer aggregation transitions [1,2]. Performing multicanonical Monte Carlo simulations of a simple hydrophobic-polar continuum model for interacting heteropolymers of finite length, we find a first-order-like behavior in the transition region between the phases of fragmented and aggregated configurations.

[1] C. Junghans, Diploma Thesis, Universität Leipzig (2006).
[2] C. Junghans, M. Bachmann, and W. Janke, Phys. Rev. Lett. **97**, 218103 (2006).

DY 30.21 Thu 16:00 Poster D

Self-driven particle and dynamic disorder — •Holger Grzeschik and Ludger Santen — Saarland University, Theoretical Physics, D-66041 Saarbrücken, Germany

We theoretically investigate self-driven particles, moving on an one dimensional lattice or track. The track is embedded in a cylinder, where the particles move diffusively. The self-driven particles can attach to and detach from the track such that the path length of the particles on the track is finite. At a given point in time the attach rates of the self-driven particles can be reduced due to the presence of a second type of particle, which is unable to perform a directed motion on the filament. This model is motivated by axonal transport, if one relates the self-driven particles to motor-proteins and the immobile particles to tau-proteins. For axons it is known that an excess of tau-proteins may cause a dysfunction of the neuron.

DY 30.22 Thu 16:00 Poster D

Vortex formation in Daphnia swarms — •Jürgen Vollmer, Bruno Eckhardt, and Christoph Lange — Fachbereich Physik, Philipps Universität, 35032 Marburg, Germany

We propose a self-propelled particle model for the swarming of Daphnia, which takes into account propulsion of the swimmers, mutual avoidance of close encounters and attraction to a centre. Various key parameters are identified in order to arrive at a phase diagram for qualitatively different steady-state motions. We find that a vertex is formed only in a finite range of propulsions, and analyse its transitions to other states. Hydrodynamic interaction between the swimmers can stabilise the vortex and change its velocity profile.

DY 30.23 Thu 16:00 Poster D

Collective motion of active brownian particles — •Jessica Strefler[1], Udo Erdmann[2], and Lutz Schimansky-Geier[1] — [1]Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin — [2]Helmholtz Gemeinschaft, Anna-Louisa-Karsch-Str. 2, 10178 Berlin

In nature complex collective dynamics within swarms of individual animals, e.g. fish can be observed. The swarming behavior originates from interactions between the indiviuals. The most common modes of motion are a coherent translation and a collective rotation. Motivated by this observations, we discuss a model of active Brownian particles in three dimensions interacting via a Morse-type potential. This model qualitativly reproduces the biological behavior. Numer-

ical simulations show either a coherent translatory or an incoherent rotating state. Depending on the number of particles and the noise intensity, phase transitions between the two states are observed.

DY 30.24 Thu 16:00 Poster D

Solvent dependence of protein secondary structures — •Hendrik Hansen-Goos[1,2], Roland Roth[1,2], Klaus Mecke[3], and Siegfried Dietrich[1,2] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — [2]ITAP, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart — [3]ITP, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Predicting the native state of a protein from a given sequence of amino acids is a task which has not been solved satisfactorily so far. An understanding of the mechanisms involved in protein folding is highly desirable as the 3D structure of a protein determines its function. Many approaches focus on energetic contributions from interaction between the amino acids and interaction with the solvent. There is, however, a contribution to the solvation free energy arising from the solvent entropy which varies for different protein configurations. We calculate solvent entropies for a protein represented in the simple tube model. Using the so-called morphometric approach, which makes calculations very efficient, we are able to scan over a large range of solvent configurations. For the particular case of a hard-sphere solvent, we discern regions where either a tightly packed helix, a sheetlike structure, or some unwinded helix minimizes the solvation free energy. Extensions to more realistic solvents and hydrophilic and hydrophobic interactions are presented.

DY 30.25 Thu 16:00 Poster D

Phase transitions in 2D colloidal crystals in presence of a 1D periodic potential — •Florian Bürzle and Peter Nielaba — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

2D melting transitions for model colloids in presence of a 1D external periodic potential are investigated using Monte Carlo simulation, thereby extending former studies [1]. We modelled the colloidal dispersions by hard disks in the canonical ensemble. In particular, we explore a hard disk system with commensurability ratio $p = \sqrt{3}a_s/2d = 2$, where a_s is the mean distance between the disks and d the period of the external potential. In this system one expects from theoretical considerations [2] a novel 'locked smectic' phase between the well known locked floating solid and the modulated liquid. This new phase, which was also observed in a recent experimental study [3], has been verified in our simulations. Furthermore, we used various statistical quantities like order parameters, their cumulants and response functions, to obtain a phase diagram for the transitions between the three phases.

[1] W. Strepp, S. Sengupta, P. Nielaba, Phys. Rev. E **63**, 046106 (2001)
[2] L. Radzihovsky, E. Frey, D. R. Nelson, Phys. Rev. E **63**, 031503 (2001)
[3] J. Baumgartl, M. Brunner, C. Bechinger, Phys. Rev. Lett. **93**, 168301 (2004)

DY 30.26 Thu 16:00 Poster D

Bubble dynamics on laser excited nanoparticles — •Anton Plech[1], Vassilios Kotaidis[1], Michael Wulff[2], Gero von Plessen[3], and Christian Dahmen[3] — [1]Fachbereich Physik, Uni Konstanz, Universitätsstr. 10, D-78457 Konstanz — [2]ESRF, BP 220, F-38043 Grenoble — [3]I. Physikalisches Institut der RWTH Aachen, Huyskensweg, D-52074 Aachen

Strong nonequilibrium exitation of gold nanoparticles can be achieved by femtosecond laser heating. The nanoscale provides cooling rates of 10^{13} K/sec in aqueous suspension. Consequently the phase transition in the adjacent water layer is of explosive nature with strong supersaturation. We have employed a pump-probe technique using femtosecond laser pulses as heat stimulus and pulsed x-rays as probe for the nanoscale structure relaxations. By a combination of x-ray techniques it was possible to measure the particle temperature, pressure transients in the water phase, vapor bubble morphology and particle shape. Bubbles forming around 9 nm particles expand to sizes in the 20 nm range before they recollapse within a subnanosecond interval. The bubble dynamics can be modelled by macroscopic fluid dynamics (Rayleigh Plesset equation) [1]. We found a supersaturation of the water phase to 85

[1] V. Kotaidis, A. Plech: Cavitation dynamics on the nanoscale, Appl. Phys. Lett., 84 (2005) 213102.
[2] V. Kotaidis, C. Dahmen, G. von Plessen, F. Springer, A. Plech: Excitation of nanoscale vapor bubbles at the surface of gold nanoparticles in water, J. Chem. Phys., 124, (2006) 184702.

DY 30.27 Thu 16:00 Poster D

Bubble dynamics on laser excited nanoparticles — •Anton Plech[1], Vassilios Kotaidis[1], Michael Wulff[2], Gero von Plessen[3], and Christian Dahmen[3] — [1]Fachbereich Physik, Uni Konstanz, Universitätsstr. 10, D-78457 Konstanz — [2]ESRF, BP 220, F-38043 Grenoble — [3]I. Physikalisches Institut der RWTH Aachen, Huyskensweg, D-52074 Aachen

Strong nonequilibrium exitation of gold nanoparticles can be achieved by femtosecond laser heating. The nanoscale provides cooling rates of 10^{13} K/sec in aqueous suspension. Consequently the phase transition in the adjacent water layer is of explosive nature with strong supersaturation. We have employed a pump-probe technique using femtosecond laser pulses as heat stimulus and pulsed x-rays as probe for the nanoscale structure relaxations. By a combination of x-ray techniques it was possible to measure the particle temperature, pressure transients in the water phase, vapor bubble morphology and particle shape. Bubbles expand to sizes in the nanometer range before they recollapse within a subnanosecond interval. The bubble dynamics can be modelled by macroscopic fluid dynamics (Rayleigh Plesset equation) [1]. We found a supersaturation of the water phase to 85 % of the critical temperature [2] as threshold process.

[1] V. Kotaidis, A. Plech: Cavitation dynamics on the nanoscale, Appl. Phys. Lett., 84 (2005) 213102.
[2] V. Kotaidis, C. Dahmen, G. von Plessen, F. Springer, A. Plech: Excitation of nanoscale vapor bubbles at the surface of gold nanoparticles in water, J. Chem. Phys., 124, (2006) 184702.

DY 30.28 Thu 16:00 Poster D

Excess free energy and Casimir forces in slabs with periodic boundary conditions at and above the bulk critical temperature — •Daniel Grüneberg and Hans Werner Diehl — Universität Duisburg-Essen (Campus Duisburg), Fachbereich Physik, D-47048 Duisburg, Germany

We consider systems that are describable by n-component short-range ϕ^4 models in a $\infty^{d-1} \times L$ slab geometry of finite thickness L with periodic boundary conditions along the finite dimension. Within these models the excess free energy and the thermodynamic Casimir force are evaluated at and above the bulk critical temperature $T_{c,\infty}$ using the renormalization-group improved perturbation theory in $d = 4 - \epsilon$ dimensions. This theory has recently been re-examined in Ref. [1], and is found to be ill-defined beyond two-loop order when the boundary conditions (bc) are such that the free propagator involves a zero-energy mode. This applies to periodic bc and special-special ones, and leads to a non-analyticity of the free energy for $L < \infty$ at the bulk critical point (bcp). The remedy is a reorganization of the field theory with regard to a proper treatment of the zero-energy mode [1]. This reorganized field theory is employed to derive the finite-size scaling functions of the excess free energy and the Casimir force. Their values at the bcp are related to the critical Casimir amplitude $\Delta_{\rm per}$, whose small-ϵ expansion is found to involve—besides integers powers of ϵ—fractional powers $\epsilon^{k/2}$ with $k \geq 3$, and powers of $\log \epsilon$. We present explicit results for $\Delta_{\rm per}$ to order $\epsilon^{3/2}$, which are used to estimate its value at $d = 3$.

[1] H. W. Diehl *et al.*, Europhys. Lett. **75**, 241 (2006)

DY 30.29 Thu 16:00 Poster D

Fractal dimension of domain walls in two-dimensional Ising spin glasses — •Oliver Melchert and Alexander K. Hartmann — Institut für Theoretische Physik, Georg-August-Universität Göttingen

We study the problem of finding domain-wall excitations on 2d Ising spin glasses in terms of a shortest-path problem. Purpose of this ground-state study is to shed light on the fractal dimension d_f of domain walls, where d_f describes the scaling of the mean domain wall length with the system size L, i.e. $\langle \ell \rangle \propto L^{d_f}$. Exploring systems up to $L = 300$ we yield $d_f = 1.271(1)$ for the case of gaussian disorder, in support of previous findings. The case of bimodal disorder exhibits a high degeneracy of ground states and thus allows for numerous domain walls with minimal energy. Here, we are able to give a true lower and an estimate for the upper bound of the fractal dimension: $d_f^{low} = 1.097(1)$ and $d_f^{up} = 1.396(10)$.

DY 30.30 Thu 16:00 Poster D

Reduction of surface coverage of finite systems due to ge-

ometrical steps — •Klaus Morawetz[1,2], Carsten Olbrich[3], Sibylle Gemming[4], and Michael Schreiber[1] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [3]School of Engineering and Science, Jacobs University Bremen, 28725 Bremen, Germany — [4]Forschungszentrum Rossendorf, PF 51 01 19, 01314 Dresden, Germany

The coverage of vicinal, stepped surfaces with molecules is simulated with the help of a two-dimensional Ising model including local distortions and an Ehrlich-Schwoebel barrier term at the steps. An effective two-spin model is capable to describe the main properties of this distorted Ising model. It is employed to analyze the behavior of the system close to the critical points. Within a well-defined regime of bonding strengths and Ehrlich-Schwoebel barriers we find a reduction of coverage (magnetization) at low temperatures due to the presence of the surface step. This results in a second, low-temperature transition besides the standard Ising order-disorder transition. The additional transition is characterized by a divergence of the susceptibility as a finite-size effect. Due to the surface step the mean-field specific heat diverges with a power law. [cond-mat/0608013]

DY 30.31 Thu 16:00 Poster D

Boundary field induced first-order transition in the 2D Ising model: numerical study — •Elmar Bittner and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

In a recent paper, Clusel and Fortin [J. Phys. A.: Math. Gen. 39 (2006) 995] presented an analytical study of a first-order transition induced by an inhomogeneous boundary magnetic field in the 2D Ising model. They identified the transition that separates the regime where the interface is localized near the boundary from the one where it is propagating inside the bulk. To confirm the analytical results, we performed multimagnetic simulations and measured the probability density of the magnetisation and the spin-spin correlation function to determine the phase transition and the location of the interface. Our results are in very good agreement with the theoretical prediction.

DY 30.32 Thu 16:00 Poster D

Continuous time cluster Monte Carlo algorithm for the spin-boson model — •Andre Winter and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, PF 151150, D-66041 Saarbrücken

A Monte Carlo algorithm to explore the quantum phase transition between localized and delocalized phase of the sub-Ohmic spin-boson model is presented. Its partition function can be written as a path integral over spin-worldlines in imaginary time involving an effective action that contains long-range interaction between spin values at different times. This path integral is evaluated with a continuous (imaginary) time Monte-Carlo algorithm with cluster updates. In this way the usual Trotter-discretization is avoided and results of simulations using this algorithm are expected to be representative for the spin-boson model also in the sub-Ohmic regime. We compute the critical exponents of the phase transition and their dependence on the bath exponent characterizing the low frequency behavoir of the spectral function of the bosonic bath.

DY 30.33 Thu 16:00 Poster D

Effects of dissipation in random quantum magnets — •Heiko Rieger[1] and Gregory Schehr[2] — [1]Theoretische Physik, Universität des Saarlandes, PF 151150, D-66041 Saarbrücken — [2]Laboratoire de Physique Théorique, Université de Paris-Sud, F-91405 Orsay

Quantum phase transitions in a large class of one-dimensional and some higher-dimensional quantum magnets with quenched disorder are described by an infinite randomness fixed point. Unusual scaling laws and the occurence of Griffiths-McCoy singularities away from the critical point characterize theses universality classes, which have been studied with a strong disorder renormalization group (SDRG), exact diagonalization and quantum Mone-Carlo methods. A coupling of the spin degrees of freedom to a dissipative bosonic bath alters this scenario significantly: The sharp quantum phase transition is smeared and the Griffiths-McCoy singularities become dominated by a classical behavior of the susceptibility and specific heat below a crossover temperature T*. By combining the SDRG with a renormalization scheme for the spin-boson-system it became possible to describe this crossover quantitatively in random transverse field Ising systems and possibly also in other quantum spin systems.

DY 30.34 Thu 16:00 Poster D

Self-avoiding walks on fractals: scaling laws — •Viktoria Blavatska[1], Yurij Holovatch[2], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11, 04109 Leipzig, Germany — [2]Institute for Condensed Matter Physics, Svientsitski Str. 1, Lviv 79011, Ukraine

The scaling behaviour of linear polymers in disordered media, modelled by self-avoiding random walks (SAWs) on the backbone of three- and four-dimensional percolation clusters is studied by Monte Carlo simulations. We apply the pruned-enriched Rosenbluth chain-growth method (PERM). Our numerical results bring about the estimates of critical exponents, which characterise disorder averages of end-to-end distance and number of SAWs.

DY 30.35 Thu 16:00 Poster D

Beitrag abgesagt — •XXX XXX —

DY 30.36 Thu 16:00 Poster D

Structural Transitions of Three-dimensional Homopolymers on Regular Lattices — •Thomas Vogel[1], Michael Bachmann[1,2], and Wolfhard Janke[1] — [1]Institute for Theoretical Physics, University Leipzig, PF 100920, 04109 Leipzig, Germany — [2]Complex Systems Division, Lund University, Sweden

We employ recently developed flat histogram extensions [1,2] of the pruned-enriched Rosenbluth method (PERM) [3] to study the freezing collapse of flexible polymers on simple cubic (sc) and face-centered cubic (fcc) lattices at temperatures well below the Θ-transition. We find that the freezing collapse does not scale with the system size in this model, besides some fluctuations due to the underlying lattice. It dominates the thermodynamic behavior of small systems but becomes unimportant in the long-chain limit.

Our work was motivated by a recent study of another related system. The crystallization temperature there depends on the polymer length and coincides with the Θ-transition in the thermodynamic limit [4].

[1] M. Bachmann, W. Janke, Phys. Rev. Lett. **91** (2003) 208 105.
[2] T. Prellberg, J. Krawczyk, Phys. Rev. Lett. **92** (2004) 120 602.
[3] P. Grassberger, Phys. Rev. E **56** (1997) 3682.
[4] F. Rampf, W. Paul, K. Binder, Europhys. Lett. **70** (2005) 628.

DY 30.37 Thu 16:00 Poster D

Ground-state structure and energy landscape of the number partitioning problem — •Alexander Mann and Alexander K. Hartmann — Institut für Theoretische Physik, Georg-August-Universität Göttingen

We study the number partitioning problem (NPP), a basic NP-hard optimization problem which presents a phase transition between a computationally easy phase with an exponential number of zero energy solutions and a computationally hard phase with unique non-zero energy ground states. We apply both exact optimization algorithms and parallel tempering Monte Carlo simulations. To get an impression of the structure of the energy landscape we study the clustering properties in the easy as well as in the hard phase. We also study the finite-size scaling behavior of a temperature driven phase transition and compare it to analytical work and to the results of the random-energy model.

DY 30.38 Thu 16:00 Poster D

Finite-size effects and universality in superfluid films — •Anna Maciolek[1,2,3] and Siegfried Dietrich[1,2] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart, Germany — [2]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, D-70569 Stuttgart, Germany — [3]Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, PL-01-224 Warsaw, Poland

Universal aspects and finite-size scaling of the critical Casimir force f_C and specific heat in wetting films of ^{3}He-^{4}He mixtures near their bulk tricritical point and of pure ^{4}He near λ transition are studied within models of corresponding universality class. For mixtures nonsymmetric boundary conditions impose nontrivial concentration profiles leading to the repulsive force which exhibit a rich crossover behavior between the tricritical point and the line of critical points. The theoretical results agree with published experimental data; for mixtures they emphasize the importance of logarithmic corrections to the scaling function. [1] A. Maciolek and S. Dietrich, Europhys. Lett. **74**, 22 (2006). [2] A. Maciolek and S. Dietrich, unpublished.

DY 30.39 Thu 16:00 Poster D

Theory of Low-Frequency Raman-Spectroscopy in Disordered Solids — •Bernhard Schmid and Walter Schirmacher — Phys.-Dept. E13, Technische Universität München, D-85747 Garching, Germany

Raman spectra of disordered solids in the regime near 50 wavenumbers show very often an intensity maximum ("boson peak"). According to a theory of Shuker and Gammon the intensity is proportional to the vibrational density of states (DOS), divided by the frequency squared. The existing data, however do not agree with DOS data measured e.g. by neutron inelastic scattering. We present a theory of vibrational excitations in disordered solids [1] and their observation by Raman spectroscopy, based on the assumption that the elastic moduli and the opto-elastic coupling constants (Pockels constants) fluctuate in space. Comparing our theory with experimental data gives not only good agreement, but enables us to compare with other related anomalous vibrational properties such as neutron and synchrotron radiation spectra, as well as specific heat and thermal conductivity data.

[1] W. Schirmacher, Europhys. Lett. 73, 892 (2006)

DY 30.40 Thu 16:00 Poster D

Description of redox reaction and nanoparticle formation in glass with a reaction-diffusion system — •Knud Zabrocki[1], Steffen Trimper[1], Manfred Dubiel[1], and Klaus-Dieter Schicke[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Deutschland — [2]Experimental Department II, Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle (Saale), Deutschland

Nanoparticle formation of precious metals like silver and gold in glass is a current field of investigation because of its technically interesting applications. The size, shape and concentration of the particles and especially the control of these parameters during the formation process of the nanoparticles are of great importance for various applications. Detailed experiments on ion-exchanged glasses (EDX, TEM) build up the basis for our description of the formation process starting with a redox reaction of silver ions and glass containing ferrous ions. We use a system of reaction-diffusion equations to analyze the different concentration profiles of the reactants. Furthermore, the reaction-diffusion fronts are calculated where the particle formation as a clustering process sets in. The influence of the different parameters like reaction rate, diffusion coefficients and boundaries are studied in detail.

DY 30.41 Thu 16:00 Poster D

Lattice Gas Simulation of Liesegang Pattern Formation in Glass — •Lukas Jahnke and Jan Werner Kantelhardt — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

Liesegang patterns are a self-organized quasi-periodic structuring that occurs in diffusion-limited chemical reactions with two components. A wide range of mean-field theories based on differential equations exists, and they describe the basic properties of the pattern formation. In recent experiments (Mohr et. al., 2000), where silver nanoparticles in glass are generated behind a moving hydrogen front, Liesegang patterns also emerge. Due to the mesoscopic character of these experiments the mean field approaches do not seem to be fully adequate. Alternatively, the microscopic reaction-diffusion process can be modelled by Monte-Carlo simulations in a lattice gas approach (Chopard et. al., 1994). We present simulation results going beyond the mean field approch for parameters inside and outside the pattern formation regime. We also discuss the stability of the patterns and possible modifications of the process that might help to obtain photonic crystals.

DY 30.42 Thu 16:00 Poster D

The description of ion dynamics in silicate glasses in terms of energy landscapes — •Heiko Lammert and Andreas Heuer — Westfälische Wilhelms-Universität, Institut für Physikalische Chemie, Corrensstr. 30, D-48149 Münster

A hopping picture is widely accepted for the description of ion dynamics in amorphous solids. The underlying energy landscape for ionic motion is highly complex due to the disordered structure of the materials, and also because of the changing Coulomb interactions between the mobile ions.

Computer simulations have shown that the Coulomb interaction is required for a completely correct reproduction of e. g. the Mixed Alkali Effect. Meanwhile many qualitative theories of the ion dynamics neglect the Coulomb interactions and work with independent particles and perfectly random distributions of energies and barriers.

We test these common assumptions using realistic molecular dynamics simulations of alkali silicates. Our method for the identification of individual ionic sites from the trajectories enables a treatment in terms of ion hopping. A new analysis of different contributions to the site energies allows a direct comparison to models using simplified energy landscapes.

The results demonstrate the important role of the Coulomb interaction for the fundamental behavior of the system. However the simple picture of independent particles on a random landscape can be recovered, when vacancies are treated instead of ions.

DY 30.43 Thu 16:00 Poster D

Distribution of cavity fields of a m-component spin glass on a Bethe lattice — •Axel Braun and Timo Aspelmeier — Institut für theoretische Physik, Universität Göttingen

Using an extension of the cavity method to m-component vector spins on a Bethe lattice, we write down a self-consistent equation for the distribution of cavity fields, with m going to infinity. With it, we show that there is a replica-symmetric low-temperature phase. We extend these findings by calculating corrections for a finite number of spin components. The results of a numerical analysis confirm replica symmetry and the finite-size-exponent for the sample-to-sample-fluctuations of the free energy is obtained.

DY 30.44 Thu 16:00 Poster D

Hydrodynamic Lyapunov modes in binary Lennard-Jones fluids — •Christian Drobniewski, Günter Radons, and Hong-Liu Yang — Chemnitz University of Technology, 09107 Chemnitz

In analogy to the microscopic definition of structure factors of molecular hydrodynamics we introduced static and dynamic correlation functions for Lyapunov vectors ([1],[2]). By this it was made possible to identify Lyapunov modes in chaotic many particle systems with soft-core interactions (Lennard-Jones fluids). Binary Lennard-Jones fluids are a well known class of systems, which were thoroughly investigated in the context of the glass transition. For binary systems we generalize these Lyapunov vector correlation functions in analogy to the so-called partial structure factors. With these correlation functions we provide a new tool for the investigation of the Lyapunov instability in binary extended systems. We present results obtained by calculating and investigating these correlation functions and find, for instance, signatures indicating the glass transition taking place in the system.

[1] H.L. Yang and G. Radons, Phys. Rev. E 73, 016202 (2006)
[2] G. Radons and H. L. Yang, arXiv nlin. CD/0404028

DY 30.45 Thu 16:00 Poster D

Quantum mechanical model of the conductivity of alkali glasses — •Joachim Sohns and Michael Schulz — Institut für Theoretische Physik, Universität Ulm, 89069 Ulm, Germany

Our aim is to reproduce the mixed alkali effect and other important properties of the conductivity of alkali glasses in the framework of qunatum mechanics. Our model includes direct interaction between the particles, static interaction between the glass and the ions and the interaction between the ions and phonons in the glass. Because the system is assumed to be out of thermal equilibrium, we use the Keldysh technique and calculate two particles Green's functions. The conductivity of the system follows from the Kubo formula.

DY 30.46 Thu 16:00 Poster D

Mean field theory for relaxation in random dipolar systems — •Hartmut Grille[1], Wolfgang Dieterich[2], Philipp Maass[1], and Michael Schulz[3] — [1]Technische Universität Ilmenau, 98684 Ilmenau, Germany — [2]Universität Konstanz, 78457 Konstanz, Germany — [3]Universität Ulm, 89069 Ulm, Germany

Disordered materials often exhibit nearly frequency-independent dielectric loss spectra. This unique feature is far from being understood. By kinetic Monte Carlo simulations it has recently been shown that a dipolar system with positional randomness can provide a mechanism for that "nearly constant loss"(NCL) response [1]. With respect to analytical theories, the long-range and tensorial character of dipole-dipole interactions clearly are complicating factors. In this work we propose a mean field theory for a disordered, dilute system of dipoles, capable of dealing with these problems [2]. The magnitude of dipole moments and their positions are frozen. We derive an approximate expression for the dielectric loss spectra and evaluate it numerically. Influences of different forms of positional randomness and of the sys-

tem size on the dielectric susceptibility are investigated and compared with the simulations.

[1] For a review, see W. Dieterich, P. Maass, Chem. Phys. **284**, 439 (2002).

[2] M. Schulz, W. Dieterich, P. Maass, Z. Phys. Chem. **218**, 1375 (2004).

DY 30.47 Thu 16:00 Poster D

Non-linear conductivity effects in disordered systems: a theoretical approach — •Lars Lühning and Andreas Heuer — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Germany

The nonlinear conductivity effects of thin ionic conductors under the influence of ac- and dc electric fields are studied numerically and analytically using a regular hopping model with a characteristic hopping distance representing the typical distance between adjacent ionic sites.

Here we analyze a single-particle hopping model. The transition rates are deduced from a sequence of randomly distributed trapping sites using periodic boundary conditions. An analytical expression for the stationary current under a constant and periodic force in one dimension is given and verified by numerical calculations. Numerical results for the stationary current in two and three dimensions are also presented. It turns out that the stationary current depends on the sample thickness. Interestingly, the first corrections to the linear response display a non-trivial behavior in the thermodynamic limit.

DY 30.48 Thu 16:00 Poster D

How to model surface diffusion using the phase-field approach — •Klaus Kassner — Institut für Theoretische Physik, Otto-von-Guericke-Universität Magdeburg, Postfach 4120, D-39016 Magdeburg

It is demonstrated that the description of surface diffusion controlled dynamics via the phase-field method is less trivial than appears at first sight. A seemingly straightforward approach previously used in the literature is shown to fail to produce the correct asymptotics, albeit in a subtle manner. An apparently obvious alternative fails for a complementary reason. Finally, a model is constructed that asymptotically approaches known sharp-interface equations without adding undesired constraints. For all the models, linear stability of a planar front is investigated both analytically and numerically, in order to assess their utility in numerical simulations.

DY 30.49 Thu 16:00 Poster D

The Evolution of Stressed Coherent Interfaces — •Michael Fleck and Robert Spatschek — Institut fuer Festkoerperforschung, Forschungszentrum 52425 Juelich

Understanding the influence of elasticity on the evolution of surfaces or interfaces is of great scientific and technological importance, because it is directly related to fracture. Nonequilibrium interface kinetics are driven by a chemical potential which sensitively depends on the elastic state of the system. We present a method how to derive the chemical potential of two coherently connected linear elastic media from fundamental variational principles. It turns out that the coherency conditions, which is the absence of slips and detachments at the interface, has important implications.

We analyze the onset of the Asaro-Tiller-Grinfeld (ATG) instability - i.e. the elastically induced morphological surface instability of a solid body subjected to a uniaxial stress - including effects from dynamic elasticity, surface tension and effects from the modification due to coherency.

The results of the linear stability analysis are compared to numerical results from phase field modelling. In the late stage of the instability this process can lead to fracture.

DY 30.50 Thu 16:00 Poster D

Dendritic melting along a grain boundary — •Claas Hueter, Efim Brener, and Dmitri Temkin — Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

Dendritic growth is a process which is very important in materials science. It can occur not only in solidification, but also in melting processes. Specifically, we discuss the melting of an overheated crystal along a grain boundary, in the framework of the symmetric model of diffusion-limited growth.

In contrast to the conventional dendritic growth, which requires the consideration of the anisotropy of the surface tension to provide a selection of the characteristic length scale of the appearing pattern and the growth velocity, the situation is here rather different: The presence of the triple junction at the tip allows a steady growth even for isotropic surface tension. This pattern formation problem is solved entirely analytically for specific parameter ranges. To our best knowledge, this is the first case of an entirely analytical solution in dendritic growth. In other cases, the corresponding nonlinear eigenvalue problem is solved numerically.

DY 30.51 Thu 16:00 Poster D

2d barchan dunes made in the lab — •Christopher Groh[1], Christof Krülle[1], Andreas Wierschem[2], Nuri Aksel[2], and Ingo Rehberg[1] — [1]Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth — [2]Technische Mechanik und Strömungsmechanik, Universität Bayreuth, D-95440 Bayreuth

For a long time people are fascinated by the dynamics of sand dunes. And so it is not surprising that there are a lot of studies outdoors, which give an overview about the facts of the formation of dunes in the desert or at the beach. In recent years scientists looked for theoretical models to give answers to the basic questions of the physical mechanisms of dune formation and migration [1,2]. In our setup we are able to investigate the dynamics of a well defined two-dimensional single barchan dune under the force of a shearing water flow. This allows easily the validation of the existing two-dimensional theoretical models with our experimental data. Beyond that, several unexpected new features have been observed.

[1] B. Andreotti, P. Claudin, and S. Douady, Eur. Phys. J. B 28, 341-352 (2002)

[2] K. Kroy, G. Sauermann and H. J. Herrmann Phys. Rev. E 66, 031302 (2002)

DY 30.52 Thu 16:00 Poster D

Coefficient of restitution: The effect of finite duration of collisions — Thomas Schwager and •Thorsten Poeschel — Charité, Augustenburger Platz 1, 13353 Berlin

The dynamics of a granular systems may be computed by Molecular Dynamics based on the interaction forces or by event-driven Molecular Dynamics using the coefficient of restitution. Knowing the forces the coefficient of restitution can be derived by integrating Newton's equation of motion. The end of a particle collision should be characterized by the time when the repulsive force between the particles conceals. So far, however, for simplicity it was assumed that the collision ends when the distance of the particle exceeds the sum of the radii. We show that the latter assumption leads erroneously to effective attractive forces and, thus, to an overestimation of the coefficient of restitution. Applying the improved condition for the duration of collisions, we derive the coefficient of restitution for the most frequently used particle interaction models. For the case of viscoelastic particles we find a novel dependence of the coefficient of restitution on the impact rate.

DY 30.53 Thu 16:00 Poster D

Granular gas cooling and relaxation to the steady state in regard to the overpopulated tail of the velocity distribution — •Thorsten Poeschel[1], Nikolai Brilliantov[2], and Arno Formella[3] — [1]Charité, Augustenburger Platz, 10439 Berlin — [2]Institut für Physik, Universität Potsdam, Am Neuen Palais 10, 14469 Potsdam — [3]Universidad de Vigo, Department of Computer Science, Edificio Politécnico, 32004 Ourense, Spain

We present a universal description of the velocity distribution function of granular gases, $f(v)$, valid for both, small and intermediate velocities where v is close to the thermal velocity and also for large v where the distribution function reveals an exponentially decaying tail. By means of large-scale Monte Carlo simulations and by kinetic theory we show that the deviation from the Maxwell distribution in the high-energy tail leads to small but detectable variation of the cooling coefficient and to extraordinary large relaxation time.

Reference: T. Pöschel, N. Brilliantov, and A. Formella, Phys. Rev.E 74, 041302 (2006)

DY 30.54 Thu 16:00 Poster D

Bottom-to-Top-Restructuring for the simulation of nanopowders — •Thomas Schwager[1], Thorsten Pöschel[1], and Dietrich E. Wolf[2] — [1]Charite, Augustenburger Platz 1, 13353 Berlin — [2]Fachbereich Physik, Universität Duisburg-Essen, D-47048 Duisburg

When repeatedly redepositing chunks cut out of a two-dimensional packing of adhesive rigid particles one converges to a losely packed assembly whose fractal dimension is close to one. On a system of a few

million particles we studied the structural properties of these packings. We found that the system adopts a universal structure which is determined by the chunk size. Moreover, the short-range structure of these assemblies is independent even of the chunk size. To obtain statistically significant results one has to consider systems of particle numbers far higher than one million particles. Granular systems of such sizes are beyond the capabilities of methods like force-based or event-driven Molecular Dynamics. Instead we applied a generalization of the Bottom-to-Top-Restructuring (Visscher and Bolsterli, Nature 239:504, 1972) which allows the simulation of hundred million particles. The results from this study can be applied to packings of nano-powders.

DY 30.55 Thu 16:00 Poster D

Experimental Study towards Granulates on Planetary — Antje Brucks[1] and •Jürgen Blum[2] — [1]Zentrum für angewandte Raumfahrttechnologie und Mikrogravitation, Am Fallturm, 28359 Bremen — [2]Institut für Geophysik und extraterrestische Physik, Technische Universität zu Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig

We present a study on low-gravity surface flows of granular materials. Planetary surfaces of small solar-system bodies are usually covered by granulates called regolith. We are interested in the static and dynamic characteristics of such granulates under low-gravity conditions prevailing on the surfaces of small bodies in the solar system. We are particularly interested at which lower boundary in g-level particles become dominated by cohesive forces.

We investigated the effect of the reduction of the gravitational acceleration on the granular flow behaviour. The experiments were performed under microgravity conditions in the Bremen Drop Tower and were using a slowly rotating centrifuge for simulating low-gravity environments. Surface flow effects were simulated in two flat (quasi-2D) sand glass experiments, in a rotating tumbler and in an avalanche box. We will present results from 15 microgravity experiments in an acceleration range between 1 g_0 and 0.01 g_0.

DY 30.56 Thu 16:00 Poster D

Horizontal Brazil-nut effect in a binary mixture — •Christian Kröner, Christof Krülle, and Ingo Rehberg — Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth, Germany

The segregation of one big sphere in a monolayer of spheres rolling on a circularly vibrating table in a circular container is observed. The granular system consists of a binary mixture with size ratio 3 to 2. Depending on the ratio of the particles' material density and size, migration of the large intruder particle occurs either towards center or to the boundary. This is called the horizontal (reverse) Brazil-nut effect (H(R)BNE)[1]. The crossing point between HBNE and HRBNE is determined by varying the intruder's size and maintaining its material density. By varying the proportion of small particles in the binary mixture it was observed that the average particle size is a crucial parameter. For a better understanding of the mechanisms the interaction between the intruder and the binary mixture are studied in detail.

[1] T. Schnautz, R. Brito, C. A. Kruelle, and I. Rehberg, Phys. Rev. Lett. 95, 028001 (2005)

DY 30.57 Thu 16:00 Poster D

Coarsening of segregation patterns in a continuously rotating drum — •Tilo Finger and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg

The radial and axial segregation of granular mixtures in a long horizontal rotating drum has become one of the standard problems in the investigation of the physics of granular matter. Nevertheless the phenomena are incompletely understood so far. We investigate experimentally the structural properties and long term dynamics of the axial stripe pattern in a cylindrical drum which is initially half filled with a mixture of glass beads of different sizes and filled up with a liquid. The standard system is embedded in water. Rotation rates are chosen at low Froude numbers ($Fr \ll 1$). After starting a constant rotation rate a regular stripe pattern along the cylinder axis appears on the time scale of a few minutes. On a time scale of hours or days, the pattern coarsens by spontaneous dissolving of individual stripes. This was studied by optical and NMR methods [1]. We investigate the influence of viscosity and density of the interstitial fluid on the coarsening process. The relation between the level of segregation and the energy dissipation in the driving process is recorded and analyzed.

[1] T. Finger *et al.*, Phys. Rev. E **74**, 031312 (2006)

DY 30.58 Thu 16:00 Poster D

Rheological properties and the disturbance of the pair correlation function in clusters of oriented dipolar particles — •Stefan Fruhner and Siegfried Hess — Institut für Theoretische Physik, Technische Universität Berlin, D-10623, Germany

Clusters of colloidal dipolar particles are studied with the help of Non Equilibrium Molecular Dynamics (NEMD). This allows to study the local structure and rheological properties in magneto-rheological fluids [1] and in (inverted) ferro-fluids. A surrounding wall potential keeps the particles together. It can be regarded either as effective interactions with the surrounding fluid or as "walls" of a particle trap. The paricles are exposed to a homogeneous shear flow and they are subjected to a Gaussian thermostat. The dipole-dipole interaction and the shear flow render a distortion of the pair correlation function. A more complex anisotropic description for the directional dependence is needed [2]. The pair correlation function can also be approximated by the Maxwell-Stokes relation [3] for small shear rates. With the knowledge of the pair correalation function other quantities can be computed, i.e. the pressure and viscosity. The pressure tensor can also be obtained directly from the simulation, so a comparision of both methods is possible.

[1] M.Kröger, P.Ilg and S. Hess, J. Phys.: Condens. Matter 15(2003) S1403-S1423
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DY 30.59 Thu 16:00 Poster D

Magnetic fields generated in dipolar nematic liquid crystals under shear — •S. Grandner[1], S. Heidenreich[1], P. Ilg[1,2], S.H.L. Klapp[1,3], and S. Hess[1] — [1]Institute for Theoretical Physics, TU Berlin, 10623 Berlin, Germany — [2]Institute for Polymers, ETH Zürich, 8093 Zürich, Switzerland — [3]Stranski-Laboratorium for Physical and Theoretical Chemistry, TU Berlin, 10623 Berlin, Germany

The orientation of a tumbling nematic liquid crystal shows a time dependent response in a stationary Couette flow. This behavior can be described by a nonlinear transport equation for the alignment tensor [1]. Here, we generalize this approach to investigate a liquid crystal consisting of particles with an electric dipole moment [2]. The coupling between the alignment tensor and the electric polarisation is taken into account via an extended Landau-de Gennes potential. For certain ranges of the coupling parameter one can find a macroscopic electric polarisation in the nematic state without shear. The dynamic equations in the presence of shear are solved revealing complex dynamic behavior characterized by different states such as *tumbling*, *wagging* or *chaotic* [3]. According to the inhomogeneous Maxwell equation the time dependence of the electric polarisation yields a magnetic field, which is of measurable strength.

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DY 30.60 Thu 16:00 Poster D

Viscous behaviour of the nonlinear Maxwell model with a generalization for magnetorheological fluids. — •Bastian Arlt and Siegfried Hess — Institut für Theoretische Physik, Technische Universität Berlin, D-10623, Germany

A generalization of the Maxwell model where the relaxation is associated with a modification of the rheological model introduced by O. Hess, Ch. Goddard and S. Hess [1] is considered. The nonlinear Maxwell model equation involves the derivative of a potential function with respect to the stress tensor. In dependence on [1] where terms up to the 4^{th} order were used, here an alternative potential with terms up to 6^{th} order is studied. Furthermore, in order to treat the behaviour of dense magnetorheological fluids [2] additional terms associated with an applied magnetic field are taken into account [3]. Consequences of the model, in particular the shear stress, the first and second normal stress difference are presented for a plane Couette flow.

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DY 30.61 Thu 16:00 Poster D

Quantitative measurement of directed fluctuations in a fer-

rofluid ratchet — •Christian Müller, Thomas John, and Ralf Stannarius — Universität Magdeburg, ANP, Universitätsplatz 2, 39106 Magdeburg

Ferrofluids as many particle systems stabilized by thermal fluctuations are well suited to compare theoretical model predictions for a nanoscale thermal ratchet [1] with experimental results. We study the influence of the field frequency and wave form on the time-averaged macroscopic torque generated in a ferrofluid volume. Two pairs of Helmholtz coils are used to generate an oscillating (non-rotation) magnetic field. This field induces a ratchet potential for the ferrofluid particles. In combination with thermal fluctuations, this symmetry breaking potential leads to a net rotation of the particles, which is transferred to the sample liquid by viscous forces. The total macroscopic torque is measured and compared with predictions based on a microscopic model [2].

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DY 30.62 Thu 16:00 Poster D

Switching Behavior of Thermoreversible Nematic Gels — •Matthias Müller[1], Andreas Timme[2], Wolfgang Schöpf[1], Günter Lattermann[2], and Ingo Rehberg[1] — [1]Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth — [2]Makromolekulare Chemie I, Universität Bayreuth, D-95440 Bayreuth

We investigated the physical properties of a thermoreversible (physical) gel consisting of a nematic liquid crystal mixed with an organogelator in the planar configuration. In our sample materials the temperature of the gel-sol transition lies above the clearing point of the liquid crystal. Therefore the director stays aligned, after the gel network has formed. The main interest of this study is the change in the switching behavior between the gel and the pure liquid crystalline material, when applying an electric field. As expected, we found an increase of the threshold voltage for the Fréedericksz transition due to the gel network. Beyond that we experienced hysteresis effects, the are induced by the gelator.

DY 30.63 Thu 16:00 Poster D

Experimental realisation of the Rosensweig instability with ferrogels — •Christian Gollwitzer[1], Marina Krekhova[2], Ingo Rehberg[1], Günter Lattermann[2], and Reinhard Richter[1] — [1]Experimentalphysik V, Universität Bayreuth — [2]Makromolekulare Chemie I, Universität Bayreuth

Ferrogels are an interesting new class of materials that enhance the properties of magnetic fluids by elastic components [1]. The most striking phenomenon in ferrofluids, namely the Rosensweig instability, shows also up in ferrogels under certain conditions. Bohlius et al. [2] predict, that compared to the pure ferrofluid, the critical magnetic field is shifted to higher values due to elastic forces, and the critical wavenumber to remain the same.

We use a thermoreversible ferrogel [3] and expose it to a homogeneous magnetic field. By controlling the temperature we can easily change the elastic modulus over several orders of magnitude. The surface profile of the ferrogel is then recorded using an X-ray technique.

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DY 30.64 Thu 16:00 Poster D

Response of a ferrofluid to travelling stripe forcing — •Achim Beetz, Reinhard Richter, and Ingo Rehberg — Universität Bayreuth

A travelling stripe forcing excitation is applied for the first time to the surface of magnetic liquids in the advent of the Rosensweig instability. We investigate the response of the ferrofluid, in particular the amplitude of travelling waves, under variation of the magnetic field strength and the driving velocity. If the native propagation velocity v of the ferrofluid corresponds to the driving speed, the amplitude of the travelling waves shows a maximum. By fitting the data with an amplitude equation of a damped forced oscillation, one can obtain the critical Rosensweig field (at $v = 0$) and a part of the dispersion relation at a fixed wavenumber.

DY 30.65 Thu 16:00 Poster D

Transport Behavior of Colloids in Micro-Channels — •Peter Henseler and Peter Nielaba — Fachbereich Physik, Universität Konstanz, D-78457 Konstanz

The transport behavior of a system of gravitationally driven colloidal particles is investigated. The particle interactions are determined by the superparamagnetic behavior of the particles. They can thus be arranged in a hexagonal order by application of an external magnetic field. Therefore the motion of the particles through a narrow channel is governed by this positioning and a layered structure forms parallel to the walls. The arrangement of the particles is perturbed by diffusion and the motion induced by gravity. Due to these combined influences a density gradient forms along the direction of motion of the particles. A reconfiguration of the ordered structure is observed leading to a reduction of the number of layers. Experiments and Brownian dynamics (BD) simulations show that this is due to the density gradient along the channel. Furthermore we present simulation results for various channel geometries and the effect of obstacles within the channel.

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DY 30.66 Thu 16:00 Poster D

Dynamics in Thin Films of Blockcopolymer — •Peter Fey, Sabine Scherdel, Marcus Böhme, Nicolaus Rehse, and Robert Magerle — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

Thin films of blockopolymer are of scientific interest because their structure can easily be adjusted. Their dynamics can be controlled by solvent vapors. We observe the surfaces of thin films of blockopolymer with tapping mode scanning probe microscopy (TM-SPM). TM-SPM allows in-situ observations of the polymer film under solvent vapor atmosphere and gives information about the topology as well as mechanical properties of the surface. At the given volume ratio of the two blocks typical surface structures include lamellae, perforated lamellae, and cylinders oriented perpendicular or parallel to the surface, depending on film thickness and the solvent vapor pressure.

In our work we mainly focus on cylinders parallel to the surface. These cylinders show characteristic fluctuations close to the phase transition in width and orientation. We examine these fluctuations for typical periodicies using image processing algorithms.

DY 30.67 Thu 16:00 Poster D

Phase diagram of a colloidal adsorbate on a quasicrystalline substrate — •Michael Schmiedeberg and Holger Stark — Max-Planck-Institute for Dynamics and Self-Organization, D-37073 Göttingen, Germany

Using Monte-Carlo simulations, we study the phase behavior of a 2D charged-stabilized colloidal suspension in a potential with decagonal symmetry that can be realized by five interfering laser beams. As one may expect, we find a triangular to liquid phase transition for small potential values and a ten-fold symmetric quasicrystalline phase for high laser intensities. However, in an intermediate regime a quasicrystalline phase exist that only exhibits a 20-fold bond orientational order. It occurs due to the delicate interplay between the interacting colloids and the substrate potential.

DY 30.68 Thu 16:00 Poster D

On the behaviour of short Kratky-Porod chain — •Semjon Stepanow — Universität Halle, Institut für Physik, 06099 Halle

Using the exact computation of a large number of moments of the distribution function of the end-to-end distance G(r,N) of the wormlike chain, we have established the analytical form of the coefficients in Taylor expansions of the moments for short chain lengths N. The knowledge of these coefficients enabled us to resummate the moment expansion of G(r,N) by taking into account consecutively the deviations of the moments from their stiff rod limit. Within this procedure we have derived the short-chain expansion for G(r,N), the scattering function, and the extension-force relation, which take into account the deviations of the moments from their stiff rod limit to the seventh order in N.

DY 30.69 Thu 16:00 Poster D

Collapse and Freezing Transitions of Polymers on Regular Lattices — •Thomas Vogel[1], Michael Bachmann[1,2], and Wolfhard Janke[1] — [1]Institute for Theoretical Physics, University Leipzig, PF 100920, 04109 Leipzig, Germany — [2]Complex Systems Division, Lund University, Sweden

We present simulation results for the thermodynamical behavior of flexible polymers (interacting self-avoiding walks) on simple cubic (sc) and face-centered cubic (fcc) lattices. Beside the well-known collapse

transition, we concentrate ourselves on the freezing transition ocurring at lower temperatures.

We show how this transition, also called crystallization, liquid-solid [1] or globule-groundstate transition [2], is influenced by the lattice and how the transition depends on the system size.

We employ the pruned-enriched Rosenbluth method (PERM) [3] and generalized extensions of it [4,5].

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