# DY 29: Poster II

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

DY 29.1 Thu 16:00 Poster C

**Constant Pressure Ensemble: Application to Small Systems and Relation to Einstein Fuctuation Theory.** — •Bernhard Joachim Mokross — Instituto de Fisica de Sao Carlos, Universidade de Sao Paulo, Sao Carlos, SP, Brasil, CEP 13560-970

The constant pressure ensemble is the most appropriate to deal with small systems (as clusters and nuclei) since experiments are usually performed under constant pressure conditions. The conjugate variable of the pressure is the volume wherefrom this ensemble partition function requires the sum over discrete unspecified volumes which may lead to errors, presented by the necessity of a correct volume scale, which increase with decreasing size of the system. In order to represent the partition function as a dimensionless integral Koper and Reiss placed the ensemble on a firm fundamental foundation with the derivation of a proper length scale applicable to isothermal fluctuations of any size in ideal fluids. In this paper, by a careful derivation, it is I shown that their result is not limited to isothermal fluctuations in ideal fluids. It applies as well to non-ideal fluids and describes fluctuations which may evolve under conditions not necessarily isothermal. It applies to small systems as well as to systems in the thermodynamic limit where it has a connection with Einstein fluctuation theory. It is also shown how it may be applied to nucleation processes.

DY 29.2 Thu 16:00 Poster C

**Efficiency at maximum work for quantum thermodynamic machines** — •Thomas Jahnke and Günter Mahler — Universität Stuttgart, 1. Institut für Theoretische Physik, Pfaffenwaldring 57, 70550 Stuttgart

Quantum thermodynamic processes can be described by means of a control model [1]: Introducing a statistical and a mechanical control parameter allows to define these processes as curves on the 2-dimensional control plane. Any process type known from macroscopic thermodynamics can thus be reformulated. Here we investigate the efficiency at maximum work for the Otto- and the Escher-Wyss-cycle acting between two baths of given temperatures. These efficiencies are found to lie between the Curzon-Ahlborn- and the Carnot-efficiency for all investigated spectra. We also discuss the limit, where the Curzon-Ahlborn-efficiency is reached.

[1] J. Birjukov, T. Jahnke and G. Mahler: Eur. Phys. J. B (submitted 2007)

DY 29.3 Thu 16:00 Poster C

**Chaotic and Stochastic Dynamics in Hysteretic Systems** — •Sven Schubert and Günter Radons — Chemnitz University of Technology, D-09107 Chemnitz

Many physical and technical systems such as shape memory alloys, magnetic nanoparticles, or certain friction models are characterized by a non-trivial hysteretic behavior, implying e.g. a complex dependence on previous input events (hysteretic memory).

On that score, we study properties of hysteretic output time series for different well understood input scenarios with similar characteristics using a discrete Preisach-hysteresis transducer.

For some aspects the chaotic trajectory of the logistic map and the corresponding stochastic process are treated differently under hysteresis. On the other hand, since hysteresis creates long-term memory we observe e.g. a slow decay of the autocorrelation function for both types of signals. For trajectories of higher iterations of the logistic map some of the observed properties converge to the results for the stochastic trajectory. The hysteretic memory, however, still distinguish between deterministic chaos and noise.

DY 29.4 Thu 16:00 Poster C

**Thermodynamic Casimir forces of $n$-component systems in slab geometries with free surfaces: Exact results for $n \to \infty$** — •Denis Comtesse, Alfred Hucht, Daniel Grüneberg, and Hans Werner Diehl — Fachbereich Physik, Universität Duisburg-Essen, D-47048 Duisburg

The $O(n)$ $\phi^4$-model on a three-dimensional slab of thickness $L$ and infinite lateral extension is investigated in the large-$n$ limit. The resulting self-consistent Schrödinger-type equation is solved numerically to determine the resulting Casimir force at and near the bulk critical temperature exactly. This enables us to study the physically relevant case of free boundary conditions, corresponding to a spherical model with separate constraints for each layer parallel to the confining surfaces. The resulting large-$n$ limit of the Casimir amplitude is obtained. To check the method, the Casimir amplitude for periodic boundary conditions is computed as well and found to be in excellent agreement with the analytically known exact result.

DY 29.5 Thu 16:00 Poster C

**Crossover from attractive to repulsive thermodynamic Casimir forces** — •Felix Schmidt and Hans Werner Diehl — Fachbereich Physik, Universität Duisburg-Essen, D-47048 Duisburg

Films whose long-length-scale behavior near the bulk critical point is described by $n$-vector $\phi^4$-models in slab geometries with free surfaces are considered. The confining surfaces are presumed to preserve the $O(n)$ invariance of the Hamiltonian. Local enhancements or weakenings of the pair interactions at the two boundary planes $\mathcal{B}_1$ at $z = 0$ and $\mathcal{B}_2$ at $z = L$ are allowed and taken into account through quadratic surface contributions with different interaction constants $c_1 \geq 0$ and $c_2 \geq 0$ on $\mathcal{B}_1$ and $\mathcal{B}_2$, respectively. When $c_1 \neq c_2$, the thermodynamic Casimir force that occurs near the bulk critical temperature can be repulsive or attractive. Using the field-theoretical renormalization group in $d = 4 - \epsilon$ dimensions, the thermodynamic Casimir force is determined at and near the bulk critical temperature for general positive values of $c_1$ and $c_2$. For appropriate choices of $c_1 - c_2$, crossovers from attractive to repulsive Casimir interactions (or vice versa) occur as the bulk critical temperature is approached.

DY 29.6 Thu 16:00 Poster C

**Techniques accelerating the dynamics of simulations of complex systems** — •Frank Beyer, Elmar Bittner, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, D-04009 Leipzig

Complex systems such as spin glasses simulated with local update schemes in the framework of Markov Chain Monte Carlo Simulations exhibit strong autocorrelations resulting in a slow dynamics especially pronounced in the temperature regime below the glass transition. Due to the rough energy landscape, trappings in local energy minima can be handled with (combinations of) different techniques such as parallel tempering and multicanonical simulations lowering relaxation times and autocorrelations. Our poster contains on the one hand a discussion of these methods with special attention to autocorrelation times giving a measure for assessing the goodness of a random walk. On the other hand it includes a survey on inherent structures and their highly degenerate configurations with minimal energy. Both issues concentrate on the 3d Edwards-Anderson spin glass model with bimodal interactions.

DY 29.7 Thu 16:00 Poster C

**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 $\chi$ and the planar surface tension $\tau$ (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 29.8 Thu 16:00 Poster C

**Thermodynamic Casimir effects at *m*-axial Lifshitz points** — •Matthias Burgsmüller, Daniel Grüneberg, and Hans Werner Diehl — Fachbereich Physik, Universität Duisburg-Essen, D-47048 Duisburg

Many-component spin systems with an $O(n)$-symmetrical Hamiltonian that have an $m$-axial bulk Lifshitz point in $d$ dimensions are considered in a slab geometry under periodic and free boundary conditions. The thermodynamic Casimir forces generated by thermal fluctuations at the Lifshitz point are found to depend on the slab's thickness $L$ in a distinct fashion, depending on whether the confining surfaces are perpendicular to one of the potential modulation axis or parallel to all of them. The small $\epsilon = d^*(m) - d$ expansion about the upper critical dimension $d^*(m) = 4 + m/2$ is utilized to study the Casimir effect via field-theoretic renormalization group methods and to determine the associated Casimir amplitudes for several boundary conditions.

DY 29.9 Thu 16:00 Poster C

**Scaling limit of groundstate dislocation lines in the solid-on-solid model** — •Karsten Schwarz and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, PF 151150, D-66041 Saarbrücken

In some cases, it has already been proven that Schramm-Loewner Evolution ($SLE_\kappa$) is the scaling limit of a discrete model, e. g. $SLE_2$ is the scaling limit of the planar loop-erased random walk.
We study dislocation-lines of the groundstate of the disordered two dimensional solid-on-solid model $H = \sum_{\langle i;j \rangle} (h_i - h_j)^2$ with $h_i = d_i + n_i$ ($d_i$ random offset $\in [0;1)$, $n_i \in \mathbb{Z}$). The main aim of our investigation is to answer the question whether the scaling limit of this discrete model can also be described by $SLE_\kappa$. So we simulate such lines on several different simply connected domains and control whether properties of $SLE_\kappa$ are satisfied. As our model is a frustrated system, it is hard to calculate the groundstate efficiently. So we also describe the used network algorithm.

DY 29.10 Thu 16:00 Poster C

**Equilibrium properties of the Wang-Landau algorithm** — •Mathias Aust, Elmar Bittner, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100920, 04009 Leipzig, Germany

The Wang-Landau method is generally considered to be an efficient Monte Carlo algorithm. It certainly is an easily implemented method to determine the density of states which is required for simulations on generalized ensembles such as multicanonical simulations. But since the Wang-Landau method uses strongly fluctuating, time-dependent weights instead of a fixed ensemble, there is no mathematical proof that the method yields reliable results.

This work provides a scheme to evaluate statistical data from time series lacking a fixed ensemble. The scheme is applied to Wang-Landau simulations of the two-dimensional Ising model measuring the energy and magnetization. The results are compared with data from exact enumerations on small lattices as well as with the exact Beale solution and magnetization data from multicanonical simulations for lattice sizes up to $64 \times 64$ to check for systematic errors of the algorithm.

Additionally, the Wang-Landau method is combined with the Transition Matrix evaluation scheme by Wang and Swendsen to find a good working estimate of the density of states even faster.

DY 29.11 Thu 16:00 Poster C

**Diffusion and dissipation in complex quantum systems** — •Dominik Samson and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, PF 151150, D-66041 Saarbrücken

The Hamiltonian of a quantum-mechanical system contains a time-dependent parameter $X$. The system is prepared in a highly excited eigenstate of the instantaneous Hamiltonian, and we compute the amplitudes $< n(t)|\phi(t) >$ to be in the eigenstates $|n >$ of the instantaeous Hamiltonian $H(X(t))$ at later times. It was already found for generic Systems that the occupation probability spreads diffusively away from the initial state [1]. The diffusion constant $D$ is now investigated numerically in random matrix models (GOE and GUE) as a function of $\dot{X}$. We are able to prove numerically the theoretical predictions in two limiting regimes of both matrix models: in the GOE case, we have two $D(\dot{X})$ behaviours, in the GUE case $D$ has an unitarity dependence, always corresponding to Ohmic dissipation predicted by the Kubo formula and Landau-Zener transitions. We also study the sample to sample fluctuation of energy, $\Delta E = \left\langle [E(t) - E(t=0)]^2 \right\rangle$ in both ensembles, which seems to have a sub-ohmic behaviour.

[1] Michael Wilkinson, Diffusion and dissipation in complex quantum systems, Phys. Rev. A **41**, 4645 (1990)

DY 29.12 Thu 16:00 Poster C

**Coulomb Gap Revisited** — •Arnulf Möbius[1], Peter Karmann[2], and Michael Schreiber[2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden — [2]Institut für Physik, Technische Universität Chemnitz

One of the most prominent features of the Coulomb glass is the Coulomb gap, a soft gap in the single-particle density of states around the chemical potential [1,2]. Previous numerical studies of the gap yielded densities considerably deviating from the analytical results.

Because of the long-range interaction, the energy region which could be considered in previous simulations was limited by severe difficulties arising from finite-size effects. To overcome this problem, we use a renormalization like iteration procedure: A cutoff length of the interaction is introduced which increases step by step during relaxation. In this way, simulations of samples of up to $2 \cdot 10^9$ sites were performed.

For one- to three-dimensional samples, we studied the influence of the disorder strength. The consideration of extremely large samples opens new insight: There is a tendency to universal behaviour in all three cases as predicted analytically in [1]. Asymptotic power laws with the predicted exponents seem to hold in the two- and three-dimensional cases, but the prefactors are smaller than predicted in [2] by factors of 2 to 3. However, this behaviour is observed only for very low energies so that the experimental relevance of the asymptotics has to be judged with reservation.

[1] A.L. Efros and B.I. Shklovskii, J. Phys. C 8, L49 (1975).
[2] A.L. Efros, J. Phys. C 9, 2021 (1976).

DY 29.13 Thu 16:00 Poster C

**Dynamic Analysis of Cup Anemometer Data** — •Mathias Hölzer[1,2], Michael Hölling[1,2], and Joachim Peinke[1,2] — [1]Universität Oldenburg — [2]ForWind, Oldenburg

The cup anemometer is one of the most used wind measuring instruments in wind energy related context. The asymmetric form, on which its movement is based on, is the source of a systematic overestimation of the mean windspeed, the so called "Overspeeding".

The instrument inherent error is the biggest drawback of the instrument, since an error up to 10% in windspeed means an error up to 30% in wind energy output due to the cubic dependency between windspeed and energy content. Error correction methods have been devolped since the mid 1950's by a couple of authors. All these approaches yield a certain correction, but are complicated as they require additional information about the exact cup anemometer geometry.

With our new approach we treat the cup anemometer as a stochastic system with Markov properties. The dynamics of such a system can be described by the Fokker-Planck equation. By calculating the drift coefficient from the measured data it is possible to determine the correct mean wind speed. In comparison with other algorithms the presented approach leads to better results. Furthermore it is not nesesary to have additional information of the geometry of the anemometer.

The presented approach can be a considerable advance for the correct forecast of wind energy output in the future as well as for previously measured data as long as it is possible to apply the method to timeseries to correct the mean wind speed of a site.

DY 29.14 Thu 16:00 Poster C

**Wetting on Geometrically Structured Surfaces** — •Monica Marinescu[1,2], Mykola Tasinkevych[1,2], and Siegfried Dietrich[1,2] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — [2]Universität Stuttgart, Institut für Theoretische und Angewandte Physik, Pfaffenwaldring 57, 70569 Stuttgart

Complete wetting on different geometrically structured substrates of a fluid close to its liquid-gas coexistence is studied. The system is described by an effective interface Hamiltonian which takes into account the long-range character of the substrate potential. Four structured geometries consisting of periodic arrays of rectangular and cylindrical pits and posts are considered. As a limiting case, wetting on a substrate with two rectangular, perpendicular "grooves" is also studied.

We describe wetting behaviour by the interfacial height function $l(\Delta\mu)$, where $l$ is the height of the liquid/gas interface at the cavity midpoint and $\Delta\mu$ the distance from bulk coexistence. Based on this function, we find a filling regime for all aforementioned geometries provided the system is driven close enough to bulk coexistence. In the

postfilling regime, universal scaling behaviour and covariance of the interfacial height function are analyzed.

DY 29.15 Thu 16:00 Poster C

**Replica-exchange cluster algorithm** — •Elmar Bittner and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

In typical finite-size scaling analyses of Monte Carlo simulations of a model exhibiting a second-order phase transition, one often needs an extended temperature/energy range around the critical point. By combining the replica-exchange algorithm with cluster updates and an adaptive routine to find the range of interest, we introduce a new flexible and powerful method for systematic investigations of second-order phase transitions. As a result, we gain two further orders of magnitude for 2D and 3D Ising models in comparison with the recently proposed Wang-Landau recursion for cluster algorithms based on the multibondic algorithm, which is already a great improvement over the standard multicanonical variant.

DY 29.16 Thu 16:00 Poster C

**Path Integrals Without Integrals** — •Antun Balaž[1], Aleksandar Bogojević[1], Ivana Vidanović[1], and Axel Pelster[2] — [1]Scientific Computing Laboratory, Institute of Physics Belgrade, Pregrevica 118, 11080 Belgrade, Serbia — [2]Fachbereich Physik, Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg, Germany

Studying the relationship between path integral discretizations of different coarseness, a hierarchy of discretized effective actions was recently derived, which yields an improved $(\beta/N)^p$ convergence of discretized transition amplitudes to the continuum limit up to $p = 12$ [1,2]. In this contribution we present a simpler procedure for obtaining these results through the derivation and solution of a set of recursive relations, and determine the effective actions even up to order $p = 25$. Higher values of $p$ make it possible to have higher precision results even for small values of $N$. Ultimately, for short propagation times $\beta < 1$ it is possible to set $N = 1$ and obtain closed analytic expressions for path integrals of a generic quantum-mechanical theory. We verify the obtained formula by comparison with perturbative expansion, loop expansion, and exact Monte Carlo simulations for the case of an anharmonic oscillator with quartic coupling. Finally, we discuss the numerical and analytical use of the obtained effective actions for long propagation times $\beta > 1$.

[1] A. Bogojevic, A. Balaz, and A. Belic, Phys. Rev. Lett. **94**, 180403 (2005)

[2] A. Bogojevic, A. Balaz, and A. Belic, Phys. Lett. A **344**, 84 (2005)

DY 29.17 Thu 16:00 Poster C

**Tackling Master Equations with a Loop Transform** — •Stephan Herminghaus, Klaus Roeller, Axel Fingerle, and Jürgen Vollmer — MPI für Dynamik und Selbstorganisation, Göttingen

A procedure is introduced which allows to represent the dynamics of a non-equilibrium system violating detailed balance by its steady state loop fluxes. It is shown that detailed balance is restored in this representation, such that the non-equilibrium steady state follows a simple Boltzmann distribution. It is thereby shown that the loop transform maps the complex behaviour of a large class of systems far from thermal equilibrium onto standard statistics of multilevel systems with degeneracies. A novel algorithm for the construction of the steady state densities naturally emerges. Furthermore, we find an expression for a free energy functional governing both the steady state and some aspects of the dynamic behavior of the system.

DY 29.18 Thu 16:00 Poster C

**Universal critical behaviour in wet granular matter** — Axel Fingerle, Klaus Roeller, Kai Huang, and •Stephan Herminghaus — MPI für Dynamik und Selbstorganisation, Göttingen

Wet granular matter is meanwhile established as a versatile model system for a large class of phenomena far from thermal equilibrium. We have studied phase transitions in vertically agitated piles of wet glass beads by experiment, simulation, and analytical theory. The full phase diagram is obtained, in mutual agreement of all three approaches. Quite remarkably, we find that details of the capillary force characteristics are irrelevant for most of the observed features. The only relevant parameters are the capillary force at contact and the total energy which is necessary to rupture a capillary bridge.

DY 29.19 Thu 16:00 Poster C

**Equation of state of wet granular matter** — Axel Fingerle, Klaus Roeller, and •Stephan Herminghaus — MPI für Dynamik und Selbstorganisation, Göttingen

Wet granular matter is meanwhile established as a versatile model system for a large class of phenomena far from thermal equilibrium. We present the equation of state of wet granular matter, consisting of spherical grains wetted by a certain amount of liquid, and externally agitated to some finite granular temperature (mean kinetic energy per degree of freedom). Following earlier studies which demonstrated the enhancement of the Kolmogorov-Sinai entropy due to the capillary forces [1,2], we find expressions for the pressure of a wet granular gas as a function of granular temperature. Excellent agreement with dynamical simulations is obtained in the full relevant range of packing fractions and liquid content.

[1] A. Fingerle, S. Herminghaus, and V. Zaburdaev, *Phys. Rev. Lett.* **95** (2005) 198001.

[2] A. Fingerle, S. Herminghaus, and V. Zaburdaev, *Phys. Rev. E* **75** (2007) 061301.

DY 29.20 Thu 16:00 Poster C

**The concept of correlated density and its application** — •Klaus Morawetz[1,2], Pavel Lipavsky[3,4], Jan Kolacek[4], Ernst Helmut Brandt[5], 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, Noethnitzer Str. 38, 01187 Dresden, Germany — [3]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic — [4]Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16253 Prague 6, Czech Republic — [5]Max Planck Institute for Metals Research, 70506 Stuttgart, Germany

The correlated density appears in many physical systems ranging from dense interacting gases up to Fermi liquids which develop a coherent state at low temperatures, the superconductivity. The underlying quantum statistical theory in nonequilibrium is the nonlocal kinetic theory developed earlier. One consequence of the correlated density is the Bernoulli potential in superconductors which compensates forces from dielectric currents which allows to access material parameters.

P. Lipavský, J. Kolacek, K. Morawetz, E. H. Brandt, T. Yang; *Bernoulli potential in superconductors - how electric fields help to understand superconductivity*, Lecture Notes in Physics , Vol. 733, Springer, Berlin, 2007

P. Lipavský, V. Spicka, K. Morawetz; *Kinetic equation for strongly interacting dense Fermi systems*, Ann. Phys. Fr., Vol. 26, N$^o$ 1, 2001, pp. 1-254, EDP Sciences

DY 29.21 Thu 16:00 Poster C

**From hyperbolic regularization to exact hydrodynamics via simple kinetic models** — •Matteo Colangeli[1], Martin Kröger[1], and Ilya Karlin[2] — [1]Polymer Physics, ETH Zürich, Switzerland — [2]Aerothermochemistry and Combustion Systems Lab, ETH Zürich, Switzerland

The derivation of hydrodynamics from a microscopic description is the classical problem of physical kinetics. The Chapman-Enskog method derives the solution from the Boltzmann Equation as a series in powers of Knudsen number. However, as demonstrated by Bobylev, even in the case of one-dimensional linear deviations from global equilibrium, the Burnett hydrodynamics violates the H-Theorem. We introduce a method to derive stable equations of linear hydrodynamics to any desired accuracy in Knudsen number. We first proceed with derivation from a thirteen Moments Grad System recovering and generalizing [1] the previous Bobylev result, including the proof of an H-theorem [2]. Further, we derive hydrodynamics from linearized Boltzmann Equation [3]. We demonstrate that stability of hydrodynamic equations arises as interplay between two basic features: dissipativity and hyperbolicity.

[1] M. Colangeli, I.V. Karlin, M. Kröger, From hyperbolic regularization to exact hydrodynamics for linearized Grad's equations, Phys. Rev. E 75 (2007) 051204. [2] M. Colangeli, I.V. Karlin, M. Kröger, Hyperbolicity of exact hydrodynamics for three-dimensional linearized Grad's equations, Phys. Rev. E 76 (2007) 022201. [3] M. Colangeli, M. Kröger, I.V. Karlin, "Eigen"-closure of linear Boltzmann equation from Invariant Manifold Theory (to be submitted).

DY 29.22 Thu 16:00 Poster C

**Features of Preferential Trapping on Energy Landscapes**

— •Andreas Fischer[1], Karl Heinz Hoffmann[1], and Christian Schön[2] — [1]TU Chemnitz, D-09107 Chemnitz, Germany — [2]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany

Understanding complex systems is a very important task as they occur in various situations. The wealth of different temporal phenomena which have been observed in such systems needs to be understood in detailed analysis of the connectivity and the respective time scales of the transitions in the state space.

The hierarchical tree model has proven to be highly suitable for the description of a complex system's state space. as its capabilities were tested in various scenarios. The dynamics in such a hierarchical system is governed by the flow of probability and the points where the tree structure branches out. This flow of probability is determined by different factors which need to be discussed in detail.

The research presented here deals with a split of a probability flow when it runs towards the more branched out parts of a tree structure. It is this special probability splitting which determines in the sequence of successive branches what the overall time behavior of a system will be. While such an analysis has already been made for systems with very special exponential densities of state we here expand our analysis to the more general case of polynomial densities of states and investigate what the differences in the behavior of the branching probability flows are. We observe new and unexpected behavior towards different phenomena which have not yet been reported before.

DY 29.23 Thu 16:00 Poster C

**Long-term correlations in human brain oscillations during sleep** — •Fabian Gans[1], Aicko Schumann[1], Thomas Penzel[2], and Jan Kantelhardt[1] — [1]Institut für Physik, MLU Halle, Germany — [2]Charité Center for Cardiology, Berlin, Germany

The human brain spontaneously generates complex oscillations in different frequency bands, which can be recorded by electroencephalography (EEG). Studying time series of the spontaneous amplitude of the oscillations in several frequency bands, we observe long-term correlated fluctuations as well as nearly uncorrelated fluctuations. The correlation behaviour is compared with similar long-term correlations observed in autonomously regulated functions, i.e., heartbeat, blood pressure and respiration during different sleep stages representing different physiological modes.

DY 29.24 Thu 16:00 Poster C

**Excitation of coherent oscillations in noisy medium** — •Jan Köhler, Jörg Mayer Mayer, and Heinz Georg Schuster — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts Universität, Olshausenstraße 40, 24098 Kiel, Germany

We study the influence of neuronal threshold modulation on the properties of cortical traveling waves. For that reason we simplify a Wilson-Cowan-type integro-differential equation model of propagating neocortical activity to a spatially discrete version. Further we introduce a noisy threshold. Depending on the noise level we find different states of the network activity, ranging from asynchronous oscillations, traveling waves, to synchronous oscillations. Finally we induce the transition between these different states by an external modulation.

DY 29.25 Thu 16:00 Poster C

**The thalamocortical system: An example for control of synchrony in a biological system** — Jörg Mayer[1], Heinz Georg Schuster[1], Jens Christian Claussen[1], •Hong-Viet Ngo[1], and Matthias Mölle[2] — [1]Institut für Theoretische Physik und Astrophysik, Christian-Albrecht-Universität Kiel — [2]Department of Neuroendocrinology, University of Lübeck

Thalamic circuits are able to induce state dependent oscillations with different frequencies and degrees of synchronization. Based on experimental results the simultaneous occurence of spindle oscillations over widespread territories of the thalamus are a consequence of corticothalamic projections, hence synchrony in a decorticated thalamus declines. Here we study the influence of corticothalamic projections on the degree of synchrony in a thalamic network. We uncover the underlying control mechanism, which yields a control method for a wide range of stochastically driven excitable units.

DY 29.26 Thu 16:00 Poster C

**Conformational mechanics of polymer adsorption transitions at attractive substrates** — •Monika Möddel, Michael Bachmann, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig

Conformational phases of a semiflexible off-lattice homopolymer model near an attractive substrate are investigated by means of multicanonical simulations. In our model, nonbonded pairs of monomers as well as monomers and the substrate interact via attractive van der Waals forces in addition to the chain's bending energy. We analyse thermal fluctuations of energetic and structural quantities and adequate docking parameters as a function of the temperature. Introducing a solvent parameter, that is related to the strength of the surface attraction, we discuss aspects of the solubility-temperature phase diagram. Apart from the main phases of adsorbed and desorbed conformations there is also a variety of other phase transitions such as the energetic transitions from filmlike surface-layer conformations to compact surface-attached globular structures.

DY 29.27 Thu 16:00 Poster C

**Effects of quenched randomness on predator-prey interactions in a stochastic Lotka-Volterra lattice model** — •Ulrich Dobramysl[1] and Uwe C. Täuber[2] — [1]Christian Doppler Labor für Oberflächenoptische Methoden, Johannes Kepler Universität Linz, Austria — [2]Virginia Polytechnic Institute and State University, Blacksburg, VA, USA

We study the influence of spatially varying reaction rates (i.e., quenched randomness) on a stochastic two-species Lotka-Volterra lattice model for predator-prey interactions using Monte Carlo simulations. The effects on the asymptotic population densities, transient oscillations, spatial distributions, and on traveling wave and invasion front speed velocities are investigated. We find that spatial variability in the predation rate yields an increase in the asymptotic population densities of *both* predators and prey.

DY 29.28 Thu 16:00 Poster C

**Spectra of Husimi cacti: Exact Results and Applications** — •mircea galiceanu and alexander blumen — Theoretische Polymerphysik, Universität Freiburg, Hermann-Herder-Straβe 3, D-79104 Freiburg, Germany

We determine analytically the complete spectra of the Husimi cacti, which are dual structures to the dendrimers, but, distinct from these, contain loops. Our solution makes use of a judicious analysis of the normal modes [1]. Although close to those of dendrimers, the spectra of Husimi cacti differ. From the wealth of applications for measurable quantities which depend only on the spectra, we display for Husimi cacti the behavior of the fluorescence depolarisation under quasi-resonant Förster energy transfer and the loss and storage moduli.

[1] Galiceanu M. and Blumen A., *J. Chem. Phys.,* **127, 134904 (2007)**

DY 29.29 Thu 16:00 Poster C

**Perturbation propagation in random and non-random Boolean Networks** — •Christoph Fretter[1,2], Agnes Szejka[1], and Barbara Drossel[1] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Deutschland — [2]Institut für Informatik, Martin-Luther-Universität Halle-Wittenberg, Deutschland

According to Derrida's definition of criticality, networks in which the perturbation of a single node propagates on an average to more (less) than one other node are chaotic (frozen). At the boundary between these two phases are critical networks. For Random Boolean Networks, the phase diagram can be derived analytically by considering the connectivity of the networks and the chosen update functions, and by using the annealed approximation. This consideration can be generalised to the Derrida plot, in which perturbations of all sizes are considered, and their value one time step later is evaluated.

By introducing a modification of this Derrida plot, we show that even Random Boolean Networks with a small size agree well with the results obtained by the annealed approximation, but non-random networks show a very different behaviour. We focus on networks that were evolved for high dynamical robustness. The most important conclusion is that the simple distinction between frozen, critical and chaotic networks is no longer useful, since such evolved networks can display properties of both frozen and chaotic networks.

DY 29.30 Thu 16:00 Poster C

**Damage Spreading and Criticality in Finite Random Dynamical Networks** — •Thimo Rohlf[1,2], Natali Gulbahce[3], and Christof Teuscher[4] — [1]Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, NM 87501, USA — [2]Max-Planck Institute for Mathematics in the Sciences, Inselstrasse 22, D-04103 Leipzig — [3]Los Alamos National Laboratory, T-Division and CNLS, MS B284, Los Alamos, NM

87545, USA — [4]Los Alamos National Laboratory, CCS-3, MS B287, Los Alamos, NM 87545, USA

We systematically study and compare damage spreading at the sparse percolation (SP) limit for random boolean and threshold networks with perturbations that are independent of the network size $N$. This limit is relevant to information and damage propagation in many technological and natural networks. Using finite size scaling, we identify a new characteristic connectivity $K_s$, at which the average number of damaged nodes $\bar{d}$, after a large number of dynamical updates, is independent of $N$. Based on marginal damage spreading, we determine the critical connectivity $K_c^{sparse}(N)$ for finite $N$ at the SP limit and show that it systematically deviates from $K_c$, established by the annealed approximation, even for large system sizes. Our findings can potentially explain the results recently obtained for gene regulatory networks and have important implications for the evolution of dynamical networks that solve specific computational or functional tasks.

DY 29.31 Thu 16:00 Poster C

**Self-organization of heterogeneous topology and symmetry breaking in networks with adapative thresholds and rewiring** — •Thimo Rohlf — Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, NM 87501, USA

We study an evolutionary algorithm that locally adapts thresholds and wiring in Random Threshold Networks, based on measurements of a dynamical order parameter. A control parameter $p$ determines the probability of threshold adaptations vs. link rewirings. For any $p < 1$, we find spontaneous symmetry breaking into a new class of self-organized networks, characterized by a much higher average connectivity $\bar{K}_{evo}$ than networks without threshold adaptation ($p = 1$). While $\bar{K}_{evo}$ and evolved out-degree distributions are independent from $p$ for $p < 1$, in-degree distributions become broader when $p \to 1$, approaching a power-law. In this limit, time scale separation between threshold adaptions and rewiring also leads to strong correlations between thresholds and in-degree. Finally, evidence is presented that networks converge to self-organized criticality for large $N$.

DY 29.32 Thu 16:00 Poster C

**Localization transitions in complex networks** — •Lukas Jahnke[1], Jan Kantelhardt[1], Richard Berkovitz[2], and Shlomo Havlin[2] — [1]Theoretische Physik, Martin-Luther-Universität, Halle / Saale, Germany — [2]The Minerva Center, Department of Physics, Bar-Ilan University, Ramat Gan, Israel

Transitions between localized and extended states have been studied in various disordered systems. The most well-known case is Anderson localization, where a disordered potential landscape on a regular lattice drives a metal-insulator transition of electrons described by the tight-binding equation. Similar transitions occur for vibrational modes and on non-regular structures, e.g., on percolation clusters. Using numerical techniques based on random matrix theory, we study such localization phenomena also with magnetic field and on more complex networks, i.e., on random graphs and scale free networks. We find that a localization-delocalization transition can be driven by several other parameters than standard on-site disorder strength. The results are compared with quantum percolation on standard lattices.

DY 29.33 Thu 16:00 Poster C

**Desiccation cracks on different substrates: simulation by a spring network model** — Supti Sadhukhan[2], Dibyendu Mal[2], Sujata Tarafdar[2], Tapati Dutta[3], Karl Heinz Hoffmann[1], and •Janett Prehl[1] — [1]Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz — [2]Condensed Matter Physics Research Center, Jadaypur University, Kolkata 700 032, India — [3]Physics Department, St Xavier's College, Kolkata 700016, India

Crack patterns formed due to desiccation of clay or similar materials show distinctive reprocucible patterns [1]. Plotting the cumulative area $A_{\rm cum}$ covered by the cracks versus their width $\geq W_{\rm min}$ a typical reproducible shape can be seen. In a log-log plot, this curve has two roughly linear regions with different slopes. For a ploypropylene substrate, there is a sharp change from a nearly horizontal line to a very steep line [2], whereas for a glass substrate, which is smoother, there is a gradual changeover between the two regions [3]. We propose a simple 1d and 2d spring chain model, in which reducing the natural length of the springs corresponds to the desiccation process. Springs may break, or slip over the substrate to accommodate strain beyond a specified threshold. The model successfully reproduces the successive stages of crack formation and behaviour of the cumulative area curve, as observed in experiments.

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[2] D. Mal, et al., *Fractals*, **14**, 283 (2006)
[3] D. Mal, et al., *J. Phys. Soc. Japan*, **76**, 014801 (2007)

DY 29.34 Thu 16:00 Poster C

**Evolution of Boolean networks under selection for a certain attractor** — •Christoph Jan Hamer and Barbara Drossel — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt

Gene regulation networks are shaped by their evolutionary history. In several cases, it has been shown that a Boolean model captures correctly the essential dynamics of a gene regulation network. The best known and most investigated example is the network regulating the cell cycle of budding yeast, which has been successfully modeled as a Boolean threshold network. This model network has a fixed point that can be reached from most starting points in state space, and the approach to this fixed point during the cell cycle follows a trajectory that is stable against perturbations. We address in this poster the question whether this trajectory can be obtained in other networks with the same number of nodes. We search for such networks by an evolutionary process. We first create random networks and successively select for mutant networks the dynamics of which reproduces correctly more and more steps of the desired trajectory.

DY 29.35 Thu 16:00 Poster C

**Detection of Modules in Boolean Networks** — •Matthias Rybarsch und Stefan Bornholdt — Institut für Theoretische Physik

We investigate methods for detecting modules in Boolean networks. In particular, we study a damage spreading perspective on modular organization in Boolean networks and relate this to criticality in these systems. We find that the modular organization of a network is sensitively dependent on the dynamical regime of the network. We characterize quantities as the number of resulting modules, as well as the distribution of module sizes in the different regimes of the network. Finally we discuss possible implications for biological systems where these networks are used as models.

DY 29.36 Thu 16:00 Poster C

**Gauge Dependence of the Critical Dynamics at the Superconducting Phase Transition** — Maxim Dudka[1], •Reinhard Folk[2], and Günter Moser[3] — [1]Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, UA–79011 Lviv, Ukraine — [2]Institut für Theoretische Physik, Johannes Kepler Universität Linz, A–4040 Linz, Austria — [3]Fachbereich Materialforschung und Physik, Universität Salzburg, A–5020 Salzburg, Austria

The critical dynamics of superconductors in the charged regime is reconsidered within field-theory. For the dynamics the Ginzburg-Landau model with complex order parameter coupled to the gauge field suggested earlier [Lannert et al. Phys. Rev. Lett. **92**, 097004 (2004)] is used. Assuming relaxational dynamics for both quantities the RG functions within one loop approximation are recalculated for different choices of the gauge. A gauge independent result for the divergence of the measurable electric conductivity is obtained only at the weak scaling fixed point - unstable in one loop order - where the time scales of the order parameter and the gauge field are different.

Supported by the Austrian Fonds zur Förderung der wissenschaftlichen Forschung, project No P19583.

DY 29.37 Thu 16:00 Poster C

**Liquid interfaces in Ising fluids** — •Wolfgang Fenz[1], Igor Omelyan[1,2], Reinhard Folk[1], and Igor Mryglod[1,2] — [1]Institute for Theoretical Physics, Linz University, A-4040 Linz, Austria — [2]Institute for Condensed Matter Physics, 1 Svientsitskii Street, UA-79011 Lviv, Ukraine

We study the thermodynamic properties and microscopic structure of liquid-liquid and liquid-vapor interfaces in Ising spin fluids by an integral equation approach. The coupled set of the Lovett-Mou-Buff-Wertheim equations for the inhomogeneous one-particle distribution functions and the Ornstein-Zernike equations for the bulk two-particle correlation functions complimented by the closure relation are solved using a modified soft mean spherical approximation. The two-particle inhomogeneous direct correlation functions are consistently constructed by nonlinear interpolation of the bulk ones corresponding to the coexisting phases. The density and magnetization profiles at the

liquid-liquid and liquid-vapor interfaces are calculated in a wide range of temperatures including subcritical regions. The liquid-liquid adsorption coefficient and the liquid-vapor surface tension are evaluated as well. The influence of the external magnetic field on the structure of the liquid-vapor interfaces is also analyzed.

Supported by the Austrian Fonds zur Förderung der wissenschaftlichen Forschung, project No. P18592.

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DY 29.38 Thu 16:00 Poster C

**Melting transitions in 2D model colloids in presence of a 1D periodic potential** — •Florian Bürzle and Peter Nielaba — Physics Department, University of Konstanz, 78464 Konstanz, Germany

In our work, we investigate phase transitions in 2D model colloids in presence of a 1D external periodic potential using Monte Carlo simulation techniques in the NVT ensemble. Thereby we extend former computational studies [1]. In particular, we explore a hard disk system with commensurability ratio $p = \sqrt{3}a/(2d) = 2$, where $d$ is the period of the external potential and $a$ is the mean distance between the disks. In this case, theoretical considerations [2] suggest a novel "locked smectic" phase between the well known locked floating solid and the modulated liquid. In our simulations this new phase, which has already been observed in an experimental study [3], was verified. Furthermore, by definition of appropriate order parameters, we were able to obtain a phase diagram [4] based on the cumulant intersection method.

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[3] J. Baumgartl, et al., Phys. Rev. Lett. 93, 168301 (2004)
[4] F. Bürzle and P. Nielaba, Phys. Rev. E 76, 051112 (2007)

DY 29.39 Thu 16:00 Poster C

**Scaling behavior of domain walls at the T=0 ferromagnet to spin-glass transition** — •Oliver Melchert and Alexander K. Hartmann — Institut für Physik, Universität Oldenburg, 26111 Oldenburg

We study domain walls in two-dimensional Ising spin systems in terms of a minimum-weight path problem. The disorder has a fraction $\rho$ of ferromagnetic bonds and $(1-\rho)$ of gaussian bonds with zero mean and unit width. We first study the magnetization to locate the critical point $\rho_c$, where the ferromagnet to spin-glass transition occurs. Further, for distinguished values of $\rho$ close to the critical point, we investigate the stiffness exponent $\theta$, which describes the scaling of the domain-wall energy with the system size $L\times L$ according to $\Delta E \sim L^{\theta}$ and we obtain the fractal dimension $d_f$, describing the scaling of the average domain-wall length, i.e. $\langle \ell \rangle \sim L^{d_f}$. We perform a finite-size scaling analysis for systems up to $L = 512$. We find that both exponents remain constant in the spin-glass phase, i.e. $\theta = -0.28(1)$ and $d_f = 1.274(1)$. This is consistent with conformal field theory, where it seems possible to relate the expontents via $d_f - 1 = 3/[4(3+\theta)]$. Moreover we find that the scaling of the average domain-wall length near the critical point can be described by $\langle \ell \rangle \sim L^{d_f^c} f[(\rho-\rho_c)L^{1/\nu}]$, with the critical fractal dimension $d_f^c = 1.221(1)$, the critical exponent of the correlation length $\nu = 1.49(7)$ and a scaling function $f[\ldots]$.

DY 29.40 Thu 16:00 Poster C

**Melting of trapped few particle systems** — •Jens Böning[1], Alexei Filinov[1], Patrick Ludwig[1], Henning Baumgartner[1], Michael Bonitz[1], and Yurii Lozovik[2] — [1]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Institute for Optics and Spectroscopy of the RAS, Troitsk, Russia

Solid or liquid behavior are collective properties of macroscopic systems. Nevertheless, collective behavior emerges already in small systems. But, how many particles are required and how to reliably detect liquid or solid behavior and the melting point in a small system? While in large systems there exist many equivalent quantities, in small systems the predicted melting point strongly depends on the choice of quantity and on the way it is computed yielding ambiguous and even divergent results [1]. We present a very simple quantity which allows to overcome these problems – the variance of the block averaged interparticle distance fluctuations [2].

[1] D.D. Frantz, J. Chem. Phys. **115**, 6136 (2001)

[2] J. Böning, A. Filinov, P. Ludwig, H. Baumgartner, M. Bonitz, and Yu.E. Lozovik, arXiv:0711.1124.

DY 29.41 Thu 16:00 Poster C

**Interfaces in Three-Dimensional Ising-like Systems** — •Michael Köpf and Gernot Münster — Institut für Theoretische Physik, Universität Münster, Wilhelm-Klemm-Str. 9, 48149 Münster

We consider interfaces in systems belonging to the universality class of the three-dimensional Ising model. They can be described in the framework of the broken-symmetry phase of three-dimensional $\phi^4$-theory. A proper choice of boundary conditions enforces the existence of an interface, which in mean-field theory resembles the well-known Cahn-Hilliard profile. To include thermal fluctuations to first order in the semiclassical approximation, an equation of motion for the interfacial profile is derived via the effective action formalism. The renormalized solution to this equation yields an interface which is shown to exhibit the behaviour predicted by capillary wave theory, i.e. the interfacial thickness diverges logarithmically with increasing system size. Ensuing a detailed investigation of interfacial features we estimate the region of validity of the approximation.

DY 29.42 Thu 16:00 Poster C

**Colloids in External Fields and in Micro-Channels** — Kerstin Franzrahe, Peter Henseler, and •Peter Nielaba — Physics Department, University of Konstanz, 78457 Konstanz

By Monte Carlo simulations we investigate the effect of an external periodic field on the structural properties and the phase diagram of a two-dimensional binary model colloid [1]. Interesting melting scenarios for the subsystems are analyzed. The layering formation in colloidal systems in micro-channels in external gravitational fields is explored by Brownian Dynamics simulations [2]. Interesting layer-reduction effects are found in the flow direction.

References:
[1] K. Franzrahe, P. Nielaba, Phys. Rev. **E**, in press.
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DY 29.43 Thu 16:00 Poster C

**Anisotropic three-dimensional Heisenberg antiferromagnets in a field** — •Georg Bannasch and Walter Selke — Institut für Theoretische Physik, RWTH Aachen

Three-dimensional anisotropic Heisenberg antiferromagnets, the xxz-model as well as variants, in a field are investigated. Based on ground state considerations and Monte Carlo techniques, the role of biconical fluctuations and structures is studied. Results are compared to findings on two-dimensional anisotropic Heisenberg antiferromagnets [1,2,3,4].

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DY 29.44 Thu 16:00 Poster C

**Quantum Monte Carlo study of the 2D quantum compass model** — •Sandro Wenzel and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04109 Leipzig

The so-called two-dimensional compass models have recently attracted interest in both the classical and quantum case due to its relevance for describing orbital interactions, arrays of superconducting Josephson junctions and as a model for protecting qubits in quantum computation [1]. Recently it was shown [2] that the classical version has a directional-ordering transition in the Ising universality class and it was proposed that this also holds for the quantum version [3–4]. Here we contribute to this question with a dedicated Quantum Monte Carlo study of the directional-ordering transition in the quantum compass model at finite temperatures. We obtain the critical temperature and the critical exponents and compare with reference [5].

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[3] J. Dorier, F. Becca, and F. Mila, Phys. Rev. B **72**, 024448 (2005).
[4] H.-D. Chen, C. Fang, J. Hu, and H. Yao, Phys. Rev. B **75**, 144401 (2007).

[5] T. Tanaka and S. Ishihara, Phys. Rev. Lett. **98**, 256402 (2007).

DY 29.45 Thu 16:00 Poster C

**Segregation Dynamics and Local Order Parameters at Binary Alloy Surfaces** — •Sebastian Kapfer[1], Harald Reichert[2], and Klaus Mecke[1] — [1]Institut für Theoretische Physik I, Erlangen, Germany — [2]Max-Planck-Institut für Metallforschung, Stuttgart, Germany

Ordering phenomena in alloys are known to be heavily modified by the presence of surfaces. Recent X-ray scattering experiments reveal surprising effects in the ordering dynamics of $Cu_3Au$ [Europhys. Lett. **53**, 570 (2001)]. A T-CVM (tetrahedron cluster variation method) free energy expression is used which reproduces correctly the topology of the experimental phase diagram. The CVM is extended for systems with a surface to study in a kinetic model the effect of surface segregation on the dynamics of the ordering process following a rapid quench.

In a complementary effort, we study time-resolved transmission electron microscopy of $Cu_3Au$ surfaces with atomic resolution. The monitored fluctuations of the local order parameter can be analyzed by morphological measures and compared with a Gaussian field theory in real space.

DY 29.46 Thu 16:00 Poster C

**Comparison of phase-field models for surface diffusion** — •Clemens Müller-Gugenberger[1], Robert Spatschek[1,2], and Klaus Kassner[3] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich — [2]Center for Interdisziplinary Research on Complex Systems, Northeastern University, Boston, MA 02115, USA — [3]Otto-von-Guericke-Universität Magdeburg, Postfach 4120, 39016 Magdeburg

Many pattern-forming systems require the understanding of the dynamics of the moving boundary between different phases. While phase-field approaches have proven to be versatile tools for tackling such problems, they mostly dealt with nonconservative interface dynamics. But in many cases, like for elastically induced morphological instabilities, the description of surface-diffusion controlled dynamics, which leads to conserved dynamics, is desirable.

We show that a seemingly straightforward approach from the literature to model surface diffusion via the phase-field method fails to produce the correct asymptotics. Two models that approximate known sharp interface equations without adding undesired constraints are constructed. The numerical implications that come with the use of a given model are compared.

DY 29.47 Thu 16:00 Poster C

**Velocity Selection Problem in the Presence of the Triple Junction** — efim brener, •claas hueter, denis pilipenko, and dmitri temkin — Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich

The melting processes along a grain boundary and the growth of an eutectoid dendrite are considered. In our previous work we have shown that under some assumptions it is possible to solve the corresponding integro-differential equation analytically. Here we consider also the growth of a eutectoid dendrite. In both cases the presence of a triple junction serves as selection mechanism. This theory is applicable to the practical important system: Dendritic growth of ferrite on an austenite grain boundary.

DY 29.48 Thu 16:00 Poster C

**Thin film growth of binary alloys** — •Mario Einax[1], Wolfgang Dieterich[2], and Philipp Maass[1] — [1]Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau, Germany — [2]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

We investigate several growth stages of binary alloys, formed by co-deposition of A and B atoms on a flat substrate. We show that several so far unknown features emerge under co-deposition of two kinds of atoms: (i) Novel scaling relations for the density of stable islands in terms of the incoming fluxes, adatom diffusion coefficients and binding energies [1]. (ii) Perpendicular magnetic anisotropy (PMA) in a certain temperature window as a result of a competition of shape and segregation effects [2]. (iii) Increase of structural anisotropy and PMA upon application of a strong magnetic field during growth. This latter feature is suggested by calculations based on Landau theory and can be confirmed by kinetic Monte Carlo simulations [3].

[1] M. Einax et al., Phys. Rev. Lett. **99**, 016106 (2007).

[2] S. Heinrichs et al., Phys. Rev. B **75**, 085437 (2007).

[3] M. Einax et al., J. Phys. Condens. Matter **19**, 086227 (2007); M. Einax et al., Mat. Sci. Eng. C **27**, 1325 (2007).

DY 29.49 Thu 16:00 Poster C

**Controlling surface morphologies by time-delayed feedback** — •Michael Block[1], Michael Wünscher[1,2], Eckehard Schöll[1], and Beate Schmittmann[3] — [1]Institut f. Theo. Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Institut für Kristallzüchtung, Max-Born Str. 2, 12489 Berlin — [3]Department of Physics, Virginia Tech, Blacksburg, VA 24061, USA

We investigate methods to control the roughness of a growing surface, via a time-delayed feedback scheme. The method can be applied to a wide range of non-equilibrium growth phenomena, from solid-state epitaxy to tumor growth. As an illustration, we consider (i) stochastic growth equations and (ii) a Kinetic Monte Carlo (KMC) model, and show that the effective growth exponent of the surface width can be stabilized at different values. By comparison of the two models we establish a correspondence between parameters of the stochastic differential equations and the tuning of the temperature in the KMC simulation. Possible experimental realizations are suggested and the relation to experiments without feedback is shown in detail.

References:

[1] M. Block, B. Schmittmann, and E. Schöll, Phys. Rev. B 75, 233414 (2007).

DY 29.50 Thu 16:00 Poster C

**Dynamic behaviour of granular matter in a circular vibrated conveyor** — •Michael Heckel, Christof A. Kruelle, and Ingo Rehberg — Universität Bayreuth, 95447 Bayreuth, Germany

Understanding the behaviour of vibrated granular matter is important because many industrial processes rely on mixed multicomponent substances. The system has to be driven with energy to stay in motion due to dissipative particle interactions. In studies this is mostly achieved by horizontal or vertical stimulation.

A horizontal and vertical oscillation with the same amplitude was superposed at a phase shift of $\pi/2$. In this way a circular oscillation for each point of the annular container is achieved. As granulate a binary mixture of black glass beads with a diameter of 1 mm and white glass beads with a diameter of 4 mm are used.

Above a threshold frequency of the excitation the bigger particles move to the top of the granulate which is known as the Brazilnut effect (BNE). If a second threshold frequency is exceeded, another separation begins to dominate which can be seen as well-separated monodisperse domains in the vibrated bed. By increasing the shaker frequency even further, a final state can be achieved where both particle species are completely separated in two distinct domains.

DY 29.51 Thu 16:00 Poster C

**Granular Dynamics Of Nonspherical Particles** — •Wilhelm August, Ingo Rehberg, and Christof Krülle — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuht

In our experiment we shake a monolayer of rice with an industrial conveyor which has been slightly altered. The vibration form possesses besides the vertical a horizontal azimuthal component which leads to a collective transport of the monolayer. We are able to focus on some tracers. Their velocity and orientation has been monitored for a long time interval. This method is an important tool for observing interesting dynamic phenomena [1]. We also measured the decay of the rotational diffusion constant over some decades [2]. Moreover, this setup allows to observe some other phenomena typical for granular matter, like e.g. segregation or heaping.

[1] Igor S. Aranson, Dmitri Volfson, and Lev Tsimring, Phys. Rev. E 75, 051301 (2007)

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DY 29.52 Thu 16:00 Poster C

**Mini-Ripples in fine granular matter** — •Simon Fischer, Ingo Rehberg, and Christof Krülle — Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth

In 1940 R.A. Bagnold, one of the pioneers in the field of wind blown grains, discovered a small scale ripple structure in very fine sand in wind tunnel experiments. He described these ripples to have an - in

comparison to known structures in coarse sand - extremely small wavelength, of about one centimetre near the threshold for grain motion. Moreover, he noticed an "interesting change in the ripple formation" towards "new ripples on a much larger scale" when the wind reached a certain critical strength [1]. Although many theories, simulations and experiments have been performed on wind driven ripple formation in coarse granular matter [2], science has not taken a closer look to structures in fine granular matter. In our setup we are able to investigate the formation, growth and long time behaviour of these mini-ripples to gain a better understanding of this phenomenon and its relation to other ripple structures observed in nature.

[1] R.A. Bagnold, The physics of blown sand and desert dunes (Chapman & Hall, London 1941)

[2] B. Andreotti, P. Claudin, O. Poliquen, Phys.Rev.Lett.. 96,028001 (2006)

DY 29.53 Thu 16:00 Poster C

**Sequential random packings of spheres and ellipsoids** — •Pedro Lind[1], Reza Baram[2], and Hans Herrmann[2] — [1]Institute for Computational Physics, Universität Stuttgart, Pfaffenwaldring 27, D-70569 Stuttgart, Germany — [2]Computational Physics, IfB, HIF E12, ETH Hönggerberg, CH-8093 Zürich, Switzerland

This study has two parts. First, we generalize the recent study of random space-filling bearings to a more realistic situation, where the spacing offset varies randomly during the space-filling procedure, and show that it reproduces well the size-distributions observed in recent studies of real fault gouges. In particular, we show that the fractal dimensions of random polydisperse bearings sweep predominantly the low range of values in the spectrum of fractal dimensions observed along real faults, which strengthen the evidence that polydisperse bearings may explain the occurrence of seismic gaps in nature. Second, we present some new remarks on sequential algorithms for packing ellipsoids.

DY 29.54 Thu 16:00 Poster C

**Granular Robots** — •Z. S. Khan[1], A. Steinberger[1], M. Scheel[1], R. Seemann[1,2], and S. Herminghaus[1] — [1]MPI for Dynamics and Self-Organization, Bunsenstr. 10, D-37073 Goettingen — [2]Experimental Physics, Saarland University, D-66041 Saarbruecken

We have recently observed that when a bidisperse mixture of glass beads is moistened by a fluid and shaken sinusoidally in a vertical container, small agglomerates of beads held together against the wall by liquid capillary bridges take off from the surface of the pile and rapidly climb up the container walls against gravity. These self-organized agglomerates have one large grain at the head of the structure with one or more small grains trailing behind. When similar agglomerates are placed on a horizontally vibrating substrate they travel horizontally along the axis of vibration. We report our investigations of this novel system, including the agglomerate speed as a function of the applied acceleration, viscosity of the wetting fluid and agglomerate structure.

DY 29.55 Thu 16:00 Poster C

**Flight paths of vertically fluidized wet granulates** — •Z. S. Khan[1], M. Scheel[1], M. Di Michiel[2], R. Seemann[1,3], and S. Herminghaus[1] — [1]MPI for Dynamics and Self-Organization, Bunsenstr. 10, D-37073 Goettingen — [2]European Synchrotron Radiation Facility, BP 220 F-38043 Grenoble Cedex — [3]Experimental Physics, Saarland University, D-66041 Saarbruecken

When dry granulates are shaken vertically and the peak acceleration exceeds the force of gravity, the grains move irregularly like the molecular motion of a fluid while they remain densely packed. It has been shown that when a fluid is added to the granulate, the critical acceleration at which fluidization occurs increased strongly when compared to the dry case [1], however it is not yet known which flow patterns evolve in this three dimensional system. Using fast synchrotron X-ray tomography techniques we track the motion of tracer particles embedded in the bulk of the granulate flow. We report on the effects of varying the frequency and amplitude of vibration as well as the liquid content on the granulate motion.

1. M. Scheel et al., J. Phys.: Cond Mat. 16, S4213 (2004).

DY 29.56 Thu 16:00 Poster C

**Mimetic intruders in a two dimensional system of vertically excited granulate** — •Jonathan Kollmer, Christof A. Kruelle, and Ingo Rehberg — Universität Bayreuth, 95440 Bayreuth, Germany

An initially close packed granular bed of hard spheres is confined by two glass plates with a separation only slightly larger than the particle diameter. In this experiment one or more intruders are inserted and the container is exposed to sinusoidal oscillations. When a critical value of the forcing strength is reached, the granular bed begins to fluidize[1] and segregation as well as intruder-intruder interaction can be observed. While common experiments[2] to study these effects use large disks as intruders this approach utilizes intruders composed of the same beads as the granulate.

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[2] D.A. Sanders, M.R. Swift, R.M. Bowley and P.J. King - Europhys. Lett., **73**(3), pp. 349-355 (2006)

DY 29.57 Thu 16:00 Poster C

**Fluidization of granulates wetting by liquid Helium** — •Kai Huang, Masoud Sohaili, and Stephan Herminghaus — Max Planck Institute for Dynamics and Self-Organization, Goettingen

To fluidize wet granulates by vertical vibration, extra force is necessary to overcome the capillary force. We explore experimentally the fluidization of a granulate wetted by liquid Helium, because of its special liquid properties. By varying temperature around the $\lambda$ point, we study how liquid Helium changes the dynamic properties of granulates. For superfluid wetting, the critical acceleration for fluidization increases almost linearly with film thickness. This indicates that superfluid starts to flow and forms liquid bridges. For wetting by normal fluid Helium, the critical acceleration shows a relatively steep increase close to saturation. Above saturation, both superfluid and normal fluid give rise to a plateau of the critical acceleration, because the capillary force depends only weakly on the volume of the bridge. The plateau value is found to vary with temperature and shows a peak around the $\lambda$ point, which indicates the influence of the specific heat of liquid Helium.

DY 29.58 Thu 16:00 Poster C

**Dynamics of gas bubble in vibrofluidized wet granulates** — •Kai Huang, Axel Hager-Fingerle, Klaus Roeller, and Stephan Herminghaus — Max Planck Institute for Dynamics and Self-Organization, D-37073, Goettingen

Recent studies on phase transitions of wet granulates show that the liquid-gas transition of wet granulates is dominated by the injected energy, because the hysteretic interaction of capillary bridges formed between particles introduces a characteristic energy scale. Between the liquid and the gas phase, there exists a co-existence regime where we always observe at least one stable gas bubble wandering around in the granular fluid. The gas bubble tends to reduce its surface and keep a circular shape, suggesting the existence of surface tension. Here we present an experimental study on the dynamic behavior of granular gas bubbles, including the nucleation, merging and vanishing processes. We use different methods to measure the velocity profile across the gas bubble. Inside the gas bubble, the velocity distribution is obtained by statistics on the track lengths of particles. In the fluid phase, the mean velocity is obtained by tracing Ruby particles illuminated with a green light source.

DY 29.59 Thu 16:00 Poster C

**Synthetic microcomputertomography of a laboratory scale sandstone core with authigenic clay** — •Bibudhananda Biswal[1] and Rudolf Hilfer[1,2] — [1]ICP, Universität Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany — [2]Institut für Physik, Universität Mainz, 55099 Mainz, Germany

A continuum geometrical modeling technique for reconstructing three dimensional pore scale microstructure of multiscale porous media [1] is extended to generate the first laboratory scale computer model of a sandstone with chlorite cementation, quartz overgrowth and kaolinite pore fillings. The core plug, 2.5 cm in diameter and 2.5 cm long, contains roughly $10^{11}$ crystallites with sizes varying from roughly 1 mm down to 100 nm. The continuum representation of the pore scale geometry allows discretization at arbitrary resolutions and makes available, for the first time, truly multiscale synthetic $\mu$-CT images for flow simulation. The method can be used to reconstruct pore scale microstructure of a large variety of clay textured sandstone morphologies.

[1] B. Biswal et al., Phys. Rev. E, **75**, 61303 (2007)

DY 29.60 Thu 16:00 Poster C

**Transport of ferrofluid due to traveling-stripe forcing** — •Thomas Friedrich, Christian Gollwitzer, Reinhard Richter,

and Ingo Rehberg — Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth

Transport of ferrofluid can be achieved by rotating [1] or by traveling magnetic fields [2,3]. We apply a traveling-stripe forcing of the magnetic induction [4] to a shallow layer of magnetic liquid. The volume transport in the subcritical and overcritical regime of the Rosensweig instability [5,6] is studied by means of radioscopy.


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- [3] K. Zimmermann, I. Zeidis, V.A. Naletova, V.A. Turkov, J. Magn. Magn. Mater. **268** 227 (2004)
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- [5] M. D. Cowley and R. E. Rosensweig, J. Fluid Mech. **30** 671 (1967)
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DY 29.61 Thu 16:00 Poster C

**Hexagon–Square Transition of the Rosensweig Instability in the presence of a magnetic ramp** — •Leonhard Wiesen, Christian Gollwitzer, Reinhard Richter, and Ingo Rehberg — Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth

The Rosensweig instability has been predicted [1] and found experimentally [2] to show a hexagon-square transition. In a recent experiment we unveiled by means of radioscopy [3] that this transition does show an inverse hysteretic behaviour (proteresis) [4]. In our contribution we reinvestigate this transition in a container with larger aspect ratio and under the influence of a magnetic ramp.


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[2] B. Abou, J.-E. Wesfreid, S. Roux, J. Fluid Mech. **416**, 217 (2001).
[3] R. Richter and J. Bläsing, Rev. Sci. Instrum. **72**, 1729 (2001).
[4] C. Gollwitzer, I. Rehberg, and Richter, J. Phys. Condens. Matter **18**, 2643 (2006).


DY 29.62 Thu 16:00 Poster C

**Interactions of colloidal particles with periodically deformed director fields in liquid crystalline free standing films** — •Kirsten Harth, Christian Bohley, and Ralf Stannarius — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, D-39106 Magdeburg, Universitätsplatz 2

We investigate textures of ferroelectric and paraelectric free standing liquid crystal films in the smectic C and C* phases by means of polarizing microscopy, with focus on colloidal liquid or solid inclusions. Periodic patterns have been observed around such inclusions and at film thickness steps. The inclusions interact with the director field, forming regular patterns, chains and lattices. An experimental investigation of the interactions between periodic patterns and inclusions is performed and the director field is analysed within an elastic continuum model.

DY 29.63 Thu 16:00 Poster C

**Structure formation in bidisperse ferrofluid monolayers: Theory and Simulations.** — •Sofia Kantorovich[1,2], Juan Cerda[3], and Christian Holm[1,3] — [1]MPI-P, Ackermannweg 10, D-55128, Mainz, Germany — [2]USU, Lenin av. 51, 620083, Ekaterinburg, Russia — [3]FIAS, Ruth-Moufang-Str. 1, D-60438, Frankfurt am Main, Germany

Molecular dynamics (MD) and Density functional theory are used to study thoroughly the mircrostructure formation in bidisperse ferrofluid monolayers. The simulation technique is close to the one used for monodisperse monolayers [Cerda et al., JP:CM, in print]. We show, that depending on the particle size ratio $d_L/d_S$ (where $d_{L(S)}$ stands for the diameter of the Large (Small) particles), the presence of small particles can lead to the poisoning effect observed in 3D [Kantorovich, Ivanov, PRE, 70, 021401,(2004)] and 2D [Klokkenburg et al., private communication] ferrofluid samples with the size ratio $d_L/d_S \sim 1.5$, but also to the cluster growth, when $d_L/d_S > 2$ due to the depletion forces. An extensive comparison of theory to the simulation results is provided.

DY 29.64 Thu 16:00 Poster C

**Non-periodic locked phase of a 2D colloidal system in a 1D quasicrystalline potential** — •Michael Schmiedeberg and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany

We study a two-dimensional charge-stabilized colloidal system under the influence of a one-dimensional quasicrystalline optical lattice. The resulting quasicrystalline potential consists of two modulations with wave vectors whose magnitudes differ by a factor of $\tau^2$, where $\tau$ is the number of the golden mean. For high values of the potential strength, periodically ordered structures do not exist [1].

By using Brownian dynamics symulations, we studied the dynamics of the non-periodic phases in the regime of high potential values and determined a phase transition between the well-known modulated liquid phase for small values of the Debye screening length and a non-periodic locked phase for large screening lengths. Details of our study will be presented.

[1] M. Schmiedeberg, J. Roth, and H. Stark, Phys. Rev. Lett. **97**, 158304 (2006)

DY 29.65 Thu 16:00 Poster C

**A novel off-lattice cluster Monte Carlo algorithm for fluid simulation** — •Markus Bellion[1], Ludger Santen[1], Heiko Rieger[1], and Werner Krauth[2] — [1]Saarland University, Theoretical Physics, D-66041 Saarbrücken, Germany — [2]CNRS-Laboratoire de Physique Statistique, Ecole Normale Supérieure 24, rue Lhomond, F-75231 Paris Cedex 05, France

The invention of Cluster Monte Carlo algorithms allowed for a much larger computational efficiency compared to local update schemes. By using cluster algorithms it was possible to reduce critical slowing down or even to avoid this problem. However, up to now most such cluster algorithms have been designed for classical and quantum mechanical models that are defined on a lattice. In fact, currently there are very few cluster algorithms that work for off-lattice models, because the identification of appropriate clusters while satisfying the detailed balance condition is even more challenging for continuous systems. Existing algorithms rely essentially on a geometric symmetry operation. Although these algorithms have been successfully applied to several model systems of complex fluids, their efficiency breaks down for higher densities. Here we report on an alternative algorithm: Particle clusters are identified by iterating a translational elementary move. The main advantage is the possibility to tune the size of generated clusters by varying the step size of the translation. As the trial step is not self-inverse, establishing detailed balance is a highly non-trivial task related to a well-known graph-theoretical problem. We show how this problem can be tackled or possibly circumvented for systems of hard particles.

DY 29.66 Thu 16:00 Poster C

**Vibrational excitations in systems with correlated disorder** — •Walter Schirmacher[1], Bernhard Schmid[2], Constantin Tomaras[1], Gabriele Viliani[3], Giacomo Baldi[4], Giancarlo Ruocco[5], and Tullio Scopigno[5] — [1]Phys.-Dept. E13, TU München — [2]FB Physik. Uni Mainz — [3]Dipt. di Fisica, Univ. di Trento, Italy — [4]INFM-CNR CRS-SOFT OGG c/o ESRF, Grenoble, France — [5]Dipt. di Fisica, Univ. di Roma; CRS SOFT-INFM-CNR c/o Univ. di Roma, Italy

We investigate a $d$-dimensional model ($d$ = 2,3) for sound waves in a disordered environment, in which the local fluctuations of the elastic modulus are spatially correlated with a certain correlation length. The model is solved analytically by means of a field-theoretical effective-medium theory (self-consistent Born approximation[1]) and numerically on a square lattice. As in the uncorrelated case [1,2] the theory predicts an enhancement of the density of states over Debye's $\omega^{d-1}$ law ("boson peak") as a result of disorder. This anomaly becomes reinforced for increasing correlation length $\xi$. The theory predicts that $\xi$ times the width of the Brillouin line should be a universal function of $\xi$ times the wavenumber. Such a scaling is found in the $2d$ simulation data, so that they can be represented in a universal plot. In the low-wavenumber regime, where the lattice structure is irrelevant, there is excellent agreement between theory and the simulation [3].


[1] W. Schirmacher, Europhys. Lett. **73**, 892 (2006)
[2] W. Schirmacher *et al.* Phys. Rev. Lett. **98**, 025501 (2007)
[3] W. Schirmacher *et al.* cond-mat 0711.1329


DY 29.67 Thu 16:00 Poster C

**Brillouin spectroscopy of disordered systems** — •Andreas Meier-Koll, Johannes Wiedersich, Peter Müller-Buschbaum, and Walter Schirmacher — Physik-Department E13, TU München

We have measured the longitudinal and transverse sound velocities in sodium silicate melts and polymeric materials by means of Brillouin spectroscopy using a tandem Fabry-Perot interferometer. In both material classes the relaxation processes can be observed from the smooth steps in the sound velocities and the maxima in the line widths. We interpret our data in terms of pertinent relaxation models.

DY 29.68 Thu 16:00 Poster C

**Coupling effects to describe macroscopic glass-forming systems** — •Christian Rehwald and Andreas Heuer — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität, 48149 Münster

Studying the potential energy landscape of different small glass-forming systems with periodic boundary conditions common features can be identified, giving rise to the notion of ideal Gaussian glass formers [1]. In agreement with the experiment this model system displays deviations from the Stokes-Einstein relation which are, however, too large. We introduce a model of interacting elementary subsystems of ideal Gaussian glass formers to reproduce macroscopic glass-formers. The interaction reduce the long tails of the waiting time distribution and renders the relaxation function $S_0(t)$ less non-exponential. In particular, now the violation of the Stokes-Einstein relation is close to experimental observations. Furthermore we check the model with respect to finite size effects, extract some information about four point correlation functions and discuss the relation to facilitated spin models [2].

[1] A. Heuer, submitted to J. Phys.: Cond. Mat. (2007)
[2] Y. Jung, J. Garrahan, D. Chandler, Phys. Rev. E **69** (2004)

DY 29.69 Thu 16:00 Poster C

**Modelling of susceptibility spectra of glass forming propylen carbonate with a schematic model of mode-coupling theory above and below $T_c$** — •Markus Domschke[1], Thomas Blochowicz[1], Thomas Voigtmann[2], and Bernd Stühn[1] — [1]TU Darmstadt, Germany — [2]Deutsches Zentrum für Luft- und Raumfahrt, Germany

Recently the glass former propylen carbonate was investigated by a two-component schematic model of the extended mode-coupling theory (MCT). It was possible to describe the dynamic susceptibilities from microscopic frequencies down to the GHz range, but it was not successful to find a realistic model of the $\alpha$ peak and excess wing at the low-temperature regime [1,2]. Therefore we introduced a phenomenological frequency-dependent hopping parameter $\Delta(\omega)$ to model the $\alpha$ process even below $T_c$. This leads to a proper description of measured data by dielectric spectroscopy and depolarized-light scattering in the whole frequency and temperature range, derived from a common density correlator.

[1] H Z Cummins, J. Phys.: Condens. Matter **17**, 1457 (2005)
[2] W. Götze and Th. Voigtmann, Phys. Rev. E **61**, 4133 (2000)

DY 29.70 Thu 16:00 Poster C

**Lattice Gas Simulation of Liesegang Pattern Formation** — •Lukas Jahnke — Theoretische Physik, Martin-Luther-Universität, Halle / Saale, Germany

Liesegang patterns are a self-organized, quasi-periodic structuring that occur in diffusion-limited chemical reactions with two components. In recent experiments, where silver nano particles in glass are being generated behind a moving hydrogen front, Liesegang patterns emerge also. Due to the mesoscopic character of these experiments it is not clear whether the mean field approaches are adequate. Alternatively, the microscopic reaction-diffusion process can be modeled by Monte-Carlo simulations in a lattice gas approach. We present simulation results going beyond the mean field approach by studying the role of fluctuations. We show that the fluctuation have a major impact on the results for small concentrations of the reacting particles.

DY 29.71 Thu 16:00 Poster C

**Nonlinear ion transport and resulting jump pathways in disordered systems** — •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 single particle hopping model which contains a characteristic hopping distance between adjacent sites. The transition rates are deduced from different kinds of distributions of the trapping sites using periodic boundary conditions.

An analytical expression for the stationary current densities under a constant field in one dimension is presented and verified by numerical simulations. It turns out that the stationary current densities depend on the sample thickness and, interestingly, the first correction to the linear response display a non-analytical behaviour in the thermodynamic limit.

Numerical calculations of the current densities are expanded both to the ac regime and to two dimensional systems and compared with experimental results. In two dimensions possibly resulting jump pathways due to a percolation approach are also presented.

Furthermore, transition rates are extracted from three dimensional hopping dynamics analyzed by molecular dynamics simulations.

DY 29.72 Thu 16:00 Poster C

**Role of ion-ion interaction for diffusion paths and residence sites in glassy electrolytes** — •Egbert Zienicke, Christian Müller, and Philipp Maass — Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau, Germany

Properties of diffusion paths and residence sites for mobile ions in glassy elctrolytes are essential to understand ionic tranport in these complex materials. An important question is, whether the diffusion paths and residence sites can be determined from knowledge of the network structure, as e.g. provided by reverse Monte Carlo modelling of neutron or X-ray diffraction data. To study this question we analyze structures of a lithium silicate glasses obtained from molecular dynamics simulations [1]. We first check how far the mere network potential of the immobile ions determines the diffusion paths. Then we investigate the influence of the Coulomb interaction betweeen the mobile Li ions with the help of Monte Carlo simulations. Our results suggest that path properties are largely determined by the network, but that the location of residence sites is strongly influenced by Li-Li interactions.

In relation to this work it is necessary also to critically examine the reliability of the potential models for modified network glasses commonly used in molecular dynamics simulations. A new approach is presented to develop such models by means of electronic structure calculations based on disordered partial structures.

[1] C. Müller, E. Zienicke, S. Adams, J. Habasaki, and P. Maass, Phys. Rev. B **75**, 014203 (2007).