

## DY 12: Poster I

Time: Tuesday 14:30–16:30

Location: P1A

DY 12.1 Tue 14:30 P1A

**Influence of broken rotational symmetry on granular segregation in horizontally vibrated systems** — ●AXEL FELTRUP<sup>1</sup>, INGO REHBERG<sup>1</sup>, and CHRISTOF KRÜLLE<sup>2</sup> — <sup>1</sup>Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth, Germany — <sup>2</sup>Maschinenbau und Mechatronik, Hochschule Karlsruhe - Technik und Wirtschaft, D-76133 Karlsruhe, Germany

A dish filled with glass beads is excited by a circular horizontal vibration. When inserting an intruder of different size or density, we can observe segregation of the intruder. Previous experiments were made in a circular dish[1,2]. By using non-circular dishes of different geometries we investigate the influence of broken rotational symmetry on the flow of the glass beads and the intruder.

[1]T. Schnautz, R. Brito, C. A. Kruelle, and I. Rehberg, A horizontal brazil-nut effect and its reverse, *Physical Review Letters* 95, 028001 (2005) [2]S. Aumaître, T. Schnautz, C.A. Kruelle, and I. Rehberg: Granular phase transition as a precondition for segregation, *Physical Review Letters* 90, 114302 (2003).

DY 12.2 Tue 14:30 P1A

**Microstructure and Pattern Formation during Zone Melting of Colloidal Crystals** — ●THOMAS PALBERG<sup>1</sup>, ENRIQUE VILANOVA VIDAL<sup>1</sup>, NINA LORENZ<sup>1</sup>, HANS-JOACHIM SCHÖPE<sup>1</sup>, and HARTMUT LÖWEN<sup>2</sup> — <sup>1</sup>Johannes Gutenberg Universität, Institut f. Physik, D-55128 Mainz, Germany — <sup>2</sup>Heinrich Heine Universität, Institut f. Theoretische Physik II, D-40225 Düsseldorf, Germany

We mimic the zone melting process of metals using colloidal model systems subjected to a gradient in particle interaction. We first study the continuous melting process of a confined one-component colloidal charged sphere crystal pushed up a gradient in salt concentration by a hydrostatic pressure difference along a slit cell. Here we study the dependence of interfacial morphology on system parameters and gradient strength. a polycrystalline to columnar transition is found, presumably caused by the applied shear. In addition we study the melting behavior if the salt is applied homogeneously and no drive is applied. Here we observe a swiss cheese morphology. Finally we study (again without drive) the morphology and the segregation behavior, when a second component is added, taking the role of an impurity. Contaminated crystals melt at low salt concentration, where purified crystals are still stable and in fact reform from the melt via heterogeneous nucleation. A zoo of interesting morphologies including dendrites and phase separation is observed.

DY 12.3 Tue 14:30 P1A

**Fluidization and segregation in a vertically vibrated quasi two-dimensional granulate** — ●JONATHAN KOLLMER<sup>1</sup>, CHRISTOF A. KRÜLLE<sup>1,2</sup>, and INGO REHBERG<sup>1</sup> — <sup>1</sup>Experimentalphysik V, Universität Bayreuth, 95447 Bayreuth, Germany — <sup>2</sup>Maschinenbau und Mechatronik, Hochschule Karlsruhe - Technik und Wirtschaft, 76133 Karlsruhe, Germany

An ensemble of hard spheres confined by two vertical glass plates forming a gap only slightly larger than the particle diameter - comparable to a Hele-Shaw cell - is vertically oscillated. To study segregation intruders are designed by gluing several spheres together. When a critical value of the forcing strength is reached, the granular bed begins to fluidize and - in the presence of intruders - segregation phenomena can be observed. By tracking of all granular particles, density and velocity fields of the system are measured. The question whether the intruders attract each other or are driven to a common location is addressed.

DY 12.4 Tue 14:30 P1A

**Two dimensional wet granular matter under shear** — ●KAI HUANG, MARTIN BRINKMANN, JAYATI SARKAR, and STEPHAN HERMINGHAUS — Max Planck Institute for Dynamics and Self-organization, Bunsenstr.10, 37073 Göttingen, Germany

The two dimensional clustering of wet particles under shear flow is studied experimentally and the results are compared with both molecular dynamic (MD) and Lattice Boltzmann (LB) simulations. Particles floating on a viscous liquid are wetted by an oil film, which gives rise to a hysteretic and short ranged capillary force between adjacent particles. This attractive force dominates other particle-particle interactions. Shear induced clustering of particles is captured by a high

speed camera and motions of individual particles are determined by an image processing procedure. The size distribution and fractal dimensions of clusters obtained by experiments show good agreement with MD simulation. Comparison to LB simulation indicates that hydrodynamic interaction does not play an important role. The average cluster size is shown to vary as  $\propto \dot{\gamma}^\alpha$  with  $\alpha \approx -2/3$ , where  $\dot{\gamma}$  is the applied shear rate. Our results can be well explained on the basis of a simple capillary model.

DY 12.5 Tue 14:30 P1A

**Phase field modeling: The interaction of interfaces** — ●ROBERT SPATSCHEK<sup>1,2</sup>, NAN WANG<sup>2</sup>, and ALAIN KARMA<sup>2</sup> — <sup>1</sup>ICAMS, Ruhr-Universität Bochum — <sup>2</sup>Northeastern University Boston

Nowadays, phase field models are an important tool for simulating the dynamics of e.g. solidification processes. Often, these models are used in the sharp or thin interface limit, where all relevant physical length scales are large in comparison to the intrinsic interface thickness, which is then used as a purely numerical parameter that does not influence the results.

In the recent time, pattern formation on the nanoscale has attracted much interest, and there the above scale separation breaks down. Interactions between interfaces are therefore an inevitable and essential new effect, raising the question to which extend they can be modeled by conventional multi-order parameter phase field models in a reliable and well-controlled way. I will demonstrate a theoretical procedure how to analyze these phase field interactions and show the limitations of the conventional models. Also, I will present a new model which overcomes these restrictions; furthermore, the influence of alloying and mechanical stress will be investigated.

DY 12.6 Tue 14:30 P1A

**Quantitative tests of local porosity theory for single phase flow in porous media** — ●THOMAS ZAUNER<sup>1</sup>, JENS HARTING<sup>1</sup>, BIBHU BISWAL<sup>1</sup>, and RUDOLF HILFER<sup>1,2</sup> — <sup>1</sup>Institut für Computerphysik, Universität Stuttgart, 70569 Stuttgart — <sup>2</sup>Institut für Physik, Universität Mainz, 55099 Mainz

Understanding fluid transport in natural porous media such as sandstones is important for many industrial and ecological applications. Permeability is widely used for characterization because it is one of the measured transport parameters that is strongly correlated to the microstructure. We present quantitative comparison of permeabilities estimated from the geometrical characterization of the microstructure within the framework of local porosity theory [1] with those obtained from large scale lattice Boltzmann simulations via Darcy's law. With these two methods we analyze a laboratory scale continuum model of Fontainebleau sandstone [2] discretized at increasing resolutions ranging from 80 to 2.5  $\mu\text{m}$ . Furthermore, many cubic subsamples with sidelength from 0.0128 to 1.024 cm are investigated to gain information about the representative elementary volume for this kind of sandstone. The results provide information for estimating representative elementary volume and resolutions for reliable permeability calculations.

[1] R. Hilfer. *Adv. Chem Phys.*, XCII:299, 1996.

[2] B. Biswal et al. *Phys. Rev. E*, 75:061303, 2007.

DY 12.7 Tue 14:30 P1A

**Study of Droplet-Coalescence for Miscible Liquids** — ●STEFAN MENZEL and MICHAEL BESTEHORN — Lehrstuhl Statistische Physik/Nichtlineare Dynamik, Brandenburgische Technische Universität Cottbus, Deutschland

Two miscible droplets flowing together are studied numerically using an extension of the thin film equation. Recent experimental observations show that sessile droplets not only fuse instantaneously after peripheral contact but also coalesce delayed for many seconds [1]. This rather unusual behavior occurred for droplets with small contact angles consisting of different liquids. After initial contact a thin gap between the droplets was observed through which liquid is exchanged from the low to the high surface tension liquid.

[1] H. Riegler, P. Lazar, *Langmuir* Vol. 24 (2008) 6395-6398.

DY 12.8 Tue 14:30 P1A

**Dynamics of turbulent structures in a Rayleigh-Bénard-system** — ●MICHAEL PETERS and MICHAEL LANGNER — Uni Old-

enburg, Deutschland

Abstract: Langevin analysis of a time series essentially serves to work out the underlying deterministic law of the stochastic dynamical system considered. This method is applied to a measured time series of a Rayleigh-Bénard convection experiment in the turbulent region. The experimental setup consists of a water-filled cylindrical vessel heated from below. At the Rayleigh number  $Ra=6.8 \times 10^9$  a roll convection is observed with stochastic reorientations of the roll axis. The time series refers to the measurement of the vertical velocity component at a given point near the cylinder wall. The analysis of the corresponding one-dimensional Langevin equation reveals a deterministic double-well potential.

DY 12.9 Tue 14:30 P1A

**A D3Q19 lattice Boltzmann pore-list code with flow boundary conditions for permeability calculations** — ●ARIEL NARVÁEZ, MARTIN HECHT, and JENS HARTING — Institut für Computerphysik, Universität Stuttgart, 70569 Stuttgart

For a broad range of applications the most important transport property of porous media is its permeability, whose definition is related to the Darcy's law.

Here we present a new implementation of the well known D3Q19 lattice-Boltzmann method (single- and multi-relaxation time) using a pore-list instead of the matrix pore-space to characterize the pore structure. The input pore-list data is characterized for the position of the fluid nodes, the connectivity with each other, and also boundary conditions. The flow is driven by using a developed flow boundary conditions at the inlet and at the outlet [1]. This boundary condition acts locally on each lattice site and it is possible to specify the velocity exactly on the boundary nodes. In addition is independent on the details of the relaxation process during collision and contains no artificial slip.

This implementation reduces the computing time required to compute the flow field in steady-state for computational domain with a low porosity.

[1] General on-site velocity boundary conditions for lattice Boltzmann. preprint arXiv: 0811.4593.

DY 12.10 Tue 14:30 P1A

**Interaction of turbulent spots in pipe flow** — ●DEVANJAN SAMANTA, ALBERTO DELOZAR, and BJORN HOF — MPI for dynamics and self organisation Bunsenstrasse 10 gottingen 37073 lower saxony germany

The process of transition from laminar to turbulent regime in shear driven flows is still an unresolved issue. Localized turbulent regions or spots emerge in the laminar turbulent transition regime. A good understanding of these localized structures is crucial for the comprehension of the transition to turbulence. We investigate the interaction of such turbulent spots in pipe flow for Reynolds numbers from 1900 to 2500. Turbulence is created locally by injecting a jet of water through a small hole in the pipe wall. The spacing of the turbulent spots downstream is inversely proportional to the perturbation frequency. It is observed that for distances less than approximately 20 pipe diameters turbulent spots start to interact and annihilate each other. The interaction distance is measured as a function of Reynolds number. This investigation is closely related to spatially turbulent laminar periodic patterns which were earlier observed in other shear driven flows like Taylor-Couette or plane Couette.

DY 12.11 Tue 14:30 P1A

**Invariants of the velocity gradient tensor in turbulent flows** — ●ANTON DAITCHE, MICHAEL WILCZEK, and RUDOLF FRIEDRICH — Institut für Theoretische Physik, Wilhelm-Klemm-Str. 9, 48149 Münster

The velocity gradient tensor  $A_{ij} = \partial_j u_i$  can be used to characterize the fine scale motion of a turbulent flow. For example the local topology of the velocity field is determined by the rate of strain tensor and the rate of rotation tensor, which are the symmetric and asymmetric parts of  $A_{ij}$ . We study  $A_{ij}$  along Lagrangian trajectories in homogeneous, isotropic and stationary turbulence. Due to the isotropy the pdf of  $A_{ij}$  is a function of the invariants of this tensor. A detailed analysis of the statistics of these invariants will be presented. Furthermore we estimate the drift of these invariants and evaluate the statistical properties of its fluctuations.

DY 12.12 Tue 14:30 P1A

**Hysteresis in twophase flow in porous media - a numerical**

**experiment** — ●FLORIAN DOSTER<sup>1</sup>, PAUL ZEGELING<sup>2</sup>, and RUDOLF HILFER<sup>1,3</sup> — <sup>1</sup>Institute for Computational Physics, University of Stuttgart, 70569 Stuttgart, Germany — <sup>2</sup>Department of Mathematics, Utrecht University, 3584 CD Utrecht, Netherlands — <sup>3</sup>Institute for Physics, University of Mainz, 55099 Mainz, Germany

Existing theories for twophase flow in porous media at the scale of centimeters to hectometers show a number of deficiencies, particularly concerning hysteresis, upscaling and residual saturations. An alternative constitutive theory [1] has proposed to treat the percolating and the non-percolating fluid parts separately. We have now closed the set of nonlinear coupled partial differential equations of this theory selfconsistently. The set of equations is then solved for the initial/boundary value problem of raising a closed column by an adaptive moving grid algorithm [2]. Its solutions show that this new constitutive theory [1] is capable of predicting some hysteretic phenomena in twophase flow in porous media.

[1] R. Hilfer, Phys. Rev. E, 016307 (2006)

[2] J.G. Blom et al., ACM Trans. in Math. Software 20, 194, (1994)

DY 12.13 Tue 14:30 P1A

**New anemometers for atmospheric and laboratory turbulent flows** — ●JAROSLAW PUCZYLOWSKI, HENDRIK HEISSELMANN, MICHAEL HÖLLING, and JOACHIM PEINKE — ForWind - Center for Wind Energy Research, University of Oldenburg, Oldenburg, Germany

We present setups and measurement results of new anemometers, the 2D-Laser-Cantilever-Anemometer and the sphere anemometer.

Compared to cup-anemometers the sphere anemometer is a robust sensor for simultaneous detection of wind speed and direction with a high spatial and temporal resolution. The drag force raised by air flow acts upon a sphere resulting in a deflection of the supporting pipe. Using the technology of atomic force microscopes deflections in micrometer range can be detected. Via calibration the corresponding flow velocity in two dimensions can be obtained.

The 2D-Laser-Cantilever-Anemometer is equipped with a cantilever measuring the dimensions of few ten micrometers. Small deflections of the cantilever due to flow can be detected by means of the laser pointer principle. In view of the bending and twisting behavior of the cantilever, longitudinal and transversal velocity components can be measured at the same time. A two-dimensional PSD element is used to determine the position of the reflecting laser spot. The 2D-Laser-Cantilever-Anemometer allows measurements with a spatial and temporal resolution comparable to x-wire-anemometry.

The working principle of both anemometers is similar. The sphere anemometer is applicable for measuring atmospheric flows, the 2D-Laser-Cantilever-Anemometer can be used for flows on smaller scales.

DY 12.14 Tue 14:30 P1A

**Experimental and numerical studies of avalanche motion** — ●CHRISTIAN KRÖNER, BIRTE DOMNIK, and SHIVA P. PUDASAINI — Steinmann Institut, Universität Bonn

The motion of avalanches can be divided into three parts: starting zone, track and deposition area. Normally the flow along the track can be described by the Savage-Hutter model[1], a depth-integrated continuum model. Since in the beginning and the end of the motion the vertical velocity cannot be neglected, a non depth-integrated model is required. This also holds for the impact of an avalanche on obstacles, which are often mounted on avalanche paths for protection. The main challenge in modelling a real three dimensional flow, is to find an appropriate description of the stresses inside the material. Therefore, numerical simulations using different stress models[2] are compared to a model experiment.

[1] S.B. Savage, K. Hutter, J. Fluid Mech. 199,177-215 (1989)

[2] C. Fang, Y. Wang, K. Hutter, Continuum Mech. Thermodyn. 19,423-440 (2008)

DY 12.15 Tue 14:30 P1A

**Flight paths of vertically fluidized wet granulates** — ●ZEINA KHAN<sup>1</sup>, MARIO SCHEEL<sup>1</sup>, MARCO DI MICHIEL<sup>2</sup>, RALF SEEMANN<sup>1,3</sup>, and STEPHAN HERMINGHAUS<sup>1</sup> — <sup>1</sup>MPI for Dynamics and Self-Organization, Bunsenstr. 10, D-37073 Goettingen — <sup>2</sup>European Synchrotron Radiation Facility, BP 220 F-38043 Grenoble Cedex — <sup>3</sup>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 accel-

eration at which fluidization occurs increases acutely when compared with the dry case [1], however it is not yet known which flow patterns evolve in this three dimensional system. Using fast synchrotron X-ray imaging techniques we track the motion of tracer particles embedded in the bulk of the granulate flow. We report on the effects of varying the vibration amplitude and frequency on the resulting flow pattern and velocity statistics. 1. M. Scheel et al., J. Phys.: Cond Mat. 16, S4213 (2004).

DY 12.16 Tue 14:30 P1A

**Continuous and discontinuous jamming transitions** — ●CLAUS HEUSSINGER and JEAN-LOUIS BARRAT — Laboratoire de Physique de la Matière Condensée et Nanostructures Université Lyon 1

We discuss the jamming transition of frictionless elastic particles at zero temperature. A quasistatic shear simulation is implemented that probes the yield-stress of the system. By varying the volume-fraction across the jamming point we cannot only follow the yield-stress line but also discuss the flow properties of the fluid below jamming.

Previous studies have viewed jamming as a mixed continuous-discontinuous phase transition, as it has both a diverging correlation length and a discontinuous order parameter (number of particle contacts).

In contrast, our results suggest that the number of contacts is fully continuous across the transition and only shows a cusp singularity. Furthermore, we will discuss the mean-square displacement as well as four-point correlation functions to highlight the role of dynamical effects in the process of jamming.

DY 12.17 Tue 14:30 P1A

**Structure Factors of a Driven Granular Gas suffering Stokes' Drag** — ●ANDREA FIEGE<sup>1</sup>, TIMO ASPELMEIER<sup>1</sup>, and ANNETTE ZIPPELIUS<sup>1,2</sup> — <sup>1</sup>Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — <sup>2</sup>Institute of Theoretical Physics, University of Göttingen, Germany

We study a system of dissipative granular particles, i. e. spherical particles suffering energy loss due to inelastic collisions and Stokes' drag. An energy source (volume bulk driving) provides a stationary state, such that the Langevin equation for a tagged particle becomes

$$\frac{d}{dt} \mathbf{v}_i = -\gamma_S \mathbf{v}_i + \frac{\mathbf{F}_i}{m_i} + \boldsymbol{\xi}_i \quad (1)$$

where  $\mathbf{F}_i$  denotes the change in the velocities due to the systematic force representing the collisions. Adding a Stokes' drag force to a common driven granular fluid is expected to suppress the random walk of total momentum due to non-momentum-conserving driving.

We investigate the influence of momentum conservation on static structure factors using fluctuating hydrodynamics. A method to incorporate Stokes' drag into standard event driven molecular dynamic simulations is introduced allowing us to carry out extensive numerical work and compare results to our theoretical predictions.

DY 12.18 Tue 14:30 P1A

**Elasticity of wet fiber networks** — ●OHLE CLAUSSEN, MARTIN BRINKMANN, and STEPHAN HERMINGHAUS — MPI for Dynamics and Self-Organization, Bunsenstrasse 10, D-37073 Göttingen

Networks of elastic fibers change their mechanical properties when they become wetted by a liquid. Capillary forces induce an aligning torque between overlapping fibers which causes the formation of fiber bundles. We present a 2D model of randomly distributed straight elastic rods with periodic boundary conditions representing a 3D network of entangled fibers that exhibit both stretching and bending modes. Besides permanent crosslinks we introduce sliding bonds exerting a hysteretic torque on the network in order to model the effects of capillarity. The fibers are coupled to an oscillating external field inducing a time dependent strain in the network. Depending on the amplitude of the strain different dynamic regimes can be observed. We investigate the dissipated energy and the effective shear loss modulus of the fiber network for varying excitations numerically.

DY 12.19 Tue 14:30 P1A

**Pattern formation of granulates in a flat rotating container** — ●FRANK RIETZ and RALF STANNARIUS — Universität Magdeburg, FNW, IEP, Abteilung Nichtlineare Phänomene

What happens inside a rotating Hele-Shaw cell that is filled with a granular mixture you'll see at this poster. Depending on the fill level we find either stripe patterns, traveling waves or convection rolls. Relations to other pattern forming systems are apparent however an explanation is still missing.

DY 12.20 Tue 14:30 P1A

**The entropy of the Hard-Core Model mimicking disordered systems** — ●ANDREA WINKLER<sup>1</sup>, GEROLD ALSMEYER<sup>1</sup>, and ANDREAS HEUER<sup>2</sup> — <sup>1</sup>Institut für mathematische Statistik WWU, 48149 Münster — <sup>2</sup>Institut für physikalische Chemie WWU, 48149 Münster

A very simple model of particle interaction is the Hard-Core Model. Here one considers  $n$  particles on a two-dimensional square-cell lattice with  $N$  sites subject to the condition that the particles can not overlap. It can be regarded as a discrete version of the hard disc system. We calculate the entropy of this model, firstly, with the analytical method according to [1] and, secondly, with numerical methods via Monte-Carlo-simulations. We find a scaling relation  $S(\rho) = a(\rho) + b(\rho) \frac{\ln c(\rho)N}{N}$  for large  $N$  and the density  $\rho = \frac{n}{N}$ . Furthermore the deviations for small system sizes are discussed.

[1] R.B.McQuistan, J.L.Hock, Composite nearest-neighbor degeneracies for several kinds of simple particles distributed on two-dimensional, square-cell lattices (J.Math.Phys 33, August 1992)

DY 12.21 Tue 14:30 P1A

**Pseudo-knots in helical structures** — FERNAO VISTULO DE ABREU<sup>1</sup>, RICARDO DIAS<sup>1</sup>, and ●CHRISTIAN VON FERBER<sup>2,3</sup> — <sup>1</sup>Department of Physics, Aveiro University, Portugal — <sup>2</sup>Applied Mathematics Research Centre, Coventry University, UK — <sup>3</sup>Physikalisches Institut, Universität Freiburg

It is generally accepted that physical entanglements are essential to explain some mechanical properties of polymers, like viscoelasticity. The current view is that entanglements behave as dynamic links that are destroyed and created in time. It is less clear whether entanglements could alternatively produce local and stable links, with similar effects to chemical bonds. Here we show that local and stable entanglements, that we call physical pseudo-knots, exist and are formed with high probability in helical structures. The energies required to create and destroy physical pseudo-knots can differ by at least one order of magnitude. Together with their localized nature this makes them controllable, opening the possibility for a wide range of applications in material science, nano- and biotechnology. Physical pseudo-knots may also have implications for living systems, that may use them, or try to avoid them and hence be related to disease. [Soft Matter 4:731 (2008)]

DY 12.22 Tue 14:30 P1A

**Molecular dynamics simulation of Ostwald ripening** — ●THOMAS KRASKA — Institut für Physikalische Chemie, Universität zu Köln

Ostwald ripening is a process taking place in the late stages of a phase transition after the system has already a low or vanishing supersaturation. Small particles dissolve or evaporate due to their high solubility or high vapour pressure while the large particles grow. The particle size distribution caused by ripening has been modelled by various theories while there are few atomistic or molecular simulations of single ripening processes. Here molecular dynamics simulations of liquid argon droplets in the saturated vapour phase are performed [1] because evaporation and condensation of droplets as well as the diffusion in the vapour phase are fast processes. It allows monitoring ripening in a time frame of 100 nanoseconds simulation time. Although the examined system models a gas-liquid transition one finds many analogies with experimental results of solid-liquid ripening processes such as for the water system being important for the stability of ice cream.

[1] T. Kraska, J. Phys. Chem. B. 112, 12408 (2008)

DY 12.23 Tue 14:30 P1A

**Relaxation into stationary nonequilibrium** — ●JAKOB MEHL, VALENTIN BLICKLE, and CLEMENS BECHINGER — 2. Physikalisches Institut, Universität Stuttgart, Germany

By now, the physics of equilibrium states is well understood. One remarkable feature is that equilibrium states are characterized by a relaxation time, which is independent of initial conditions. In contrast, the relaxation of a nonequilibrium stationary state (NESS) is *a priori* unknown. By combining colloidal particles, rotating laser tweezers, and video microscopy, we study experimentally the transitions between two well-defined NESS. Our experiments prove, that likewise to an equilibrium state, a NESS is characterized by an intrinsic relaxation time. Furthermore, this time constant crucially depends on how far the system is driven out of thermal equilibrium. In accordance with theoretical predictions, the relaxation time monotonically increases with

driving strength.

DY 12.24 Tue 14:30 P1A

**Nonequilibrium phase transitions in finite arrays of globally coupled Stratonovich models: Strong coupling limit** — FABIAN SENF, •PHILIPP M. ALTROCK, and ULRICH BEHN — Institut für Theoretische Physik, Universität Leipzig, Deutschland

A finite array of  $N$  globally coupled Stratonovich models exhibits a continuous nonequilibrium phase transition. In the limit of strong coupling there is a clear separation of time scales of center of mass and relative coordinates. The latter relax very fast to zero and the array behaves as a single entity described by the center of mass coordinate. We compute analytically the stationary probability and the moments of the center of mass coordinate. The scaling behavior of the moments near the critical value of the control parameter  $a_c(N)$  is determined. We identify a crossover from linear to square root scaling with increasing distance from  $a_c$ . The crossover point approaches  $a_c$  in the limit  $N \rightarrow \infty$  which reproduces previous results for infinite arrays. The results are obtained in both the Fokker-Planck and the Langevin approach and are corroborated by numerical simulations. For a general class of models we show that the transition manifold in the parameter space depends on  $N$  and is determined by the scaling behavior near a fixed point of the stochastic flow.

DY 12.25 Tue 14:30 P1A

**Separation of variables in MD simulation: A criterion to estimate the quality of the approximation** — •ADOLFO POMA and LUIGI DELLE SITE — Max-Planck-Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz, Germany

We propose a simple method to evaluate the approximation of separation of variables (ASV) in Molecular Dynamics (MD) and related fields. It is based on a point-by-point evaluation of the difference between the true potential and the corresponding potential where the separation of variables is applied. The major advantage of such an approach is the fact that it requires only the analytical form of the potential as provided in most of the MD codes. We provide an application of this criterion for the alkane (aliphatic) chain and compare the efficiency for two different Mapping Schemes (MS).

DY 12.26 Tue 14:30 P1A

**Size Distribution of Hanging Dew Droplets** — •TOBIAS LAPP, JOHANNES BLASCHKE, JÜRGEN VOLLMER, and BJÖRN HOF — MPI for Dynamics and Self-Organization, 37073 Göttingen, Germany

The formation, growth and coarsening of dew droplets on flat surfaces has widely been studied in the physics literature under the keyword "Breath Figures". Surprisingly, little attention has been devoted however to hanging dew droplets. In this case coarsening comes to rest due to dripping off of droplets from the surface, and gravity changes the relation of droplet volume and surface release in coalescence events. We present experimental data for the droplet distribution, and discuss how these gravity induced effects influence Family and Meakin's classical expressions for the size distribution of droplets.

DY 12.27 Tue 14:30 P1A

**Statistical mechanical description of polarizable liquid systems in electric field** — •SEMION STEPANOW and THOMAS THURN-ALBRECHT — Institut für Physik, Universität Halle, D-06099 Halle

We formulate the statistical mechanical description of liquid systems without permanent dipoles in an electric field in the  $\mathbf{E}$ -ensemble, which is the pendant to the thermodynamic description in terms of the free energy at constant potential. The contribution of the electric field to the configurational integral  $\tilde{Q}_N(\mathbf{E})$  in the  $\mathbf{E}$ -ensemble is given in an exact form as a factor in the integrand of  $\tilde{Q}_N(\mathbf{E})$ . We also calculate the contribution of the electric field to the Ornstein-Zernike formula for the scattering function in the  $\mathbf{E}$ -ensemble. As an application we calculate the shift of the critical temperature for the van der Waals gas in the electric field, and show that the shift is downward in  $\mathbf{E}_0$ -ensemble (constant charges) and upward in  $\mathbf{E}$ -ensemble.

DY 12.28 Tue 14:30 P1A

**Shape Dependence of Free Energies** — •ANATOLY DANILEVICH, THORSTEN HIESTER, and KLAUS MECKE — Institut für Theoretische Physik Universität Erlangen-Nürnberg, Staudtstrasse 7, 91058 Erlangen, Germany.

Thermodynamic potentials of a fluid bounded by a finite, arbitrarily shaped convex container  $K \subset \mathbb{R}^d$  are expected to be dependent only

on  $d + 1$  morphometric measures, the so-called Minkowski functionals  $M_i(K)$ , and additional terms which decrease exponentially with the size of  $K$  [1]. This conjecture has been tested analytically for lattice models and - by reducing the problem to integral geometric calculations - also for a cluster expansion of a continuous fluid model. The results can be used in combination with density functional theory to derive an explicit expression for the Tolman length, i.e., the curvature correction to the surface tension of a spherical drop.

[1] P. König, R. Roth and K. Mecke, Phys. Rev. Lett. **93**, 160601 (2004).

DY 12.29 Tue 14:30 P1A

**Noise driven hysteresis** — •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 non-trivial hysteretic behavior. The fact that either deterministic external fields are superimposed by thermal noise or input seems to be entirely erratic itself leads to questions concerning stochastic processes under hysteresis. We mainly investigate spectral properties and autocorrelation of Preisach hysteresis models driven by stochastic input scenarios.

Since hysteresis is able to create long-term memory, it is possible to observe an algebraic decay of the output autocorrelation function and  $1/f$ -noise even for  $\delta$ -correlated input trajectories [1]. We always observe an emphasized low frequency regime, respectively an increase in correlation times, for  $\delta$ -correlated noise driven hysteresis.

Furthermore, we investigate how correlated input processes, including fractional Gaussian noise (fGN), are transformed by hysteretic operators. In contrast to uncorrelated input processes, a further increase in output correlation times is not enforced for fGN driven hysteresis. Additionally, first results are presented on how similarly correlated processes from different sources are treated under the influence of hysteresis.

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

DY 12.30 Tue 14:30 P1A

**Phase transition as a mechanism of fullerene formation** — •ADILAH HUSSEIN, ALEXANDER YAKUBOVICH, ANDREY SOLOV'YOV, and WALTER GREINER — Frankfurt Institute for Advanced Studies, Goethe University, Ruth-Moufang-Str. 1, Frankfurt am Main 60438, Germany

Phase transition in fullerenes  $C_{60}$  and  $C_{240}$  are investigated by means of constant-temperature molecular dynamics simulations. In the phase transition region, the assembly (and fragmentation) of the  $C_{60}$  cage from (and to) the gaseous state is demonstrated via the dynamical coexistence of two phases. In this critical region, the fullerene system is seen to continuously oscillate between the carbon cage (the solid phase) and the state of carbon dimers and short chains (the gas phase). These oscillations correspond to consecutive disintegration and formation of the fullerene. Furthermore, the temperature-dependent heat capacity of the fullerene features a prominent peak, signifying the finite system analogue of a first-order phase transition. The simulations were conducted for 500 ns using a topologically-constrained pairwise force-field which was developed for this work. Results of the simulations were supplemented by a statistical mechanics analysis to account for entropy and pressure corrections, corresponding to experimental conditions. These corrections lead to a phase transition temperature of 3800-4200 K for pressure 10-100 kPa, in good agreement with available experimental values.

DY 12.31 Tue 14:30 P1A

**Thermodynamic effects of an endohedral atom on the phase transition of fullerenes** — •ADILAH HUSSEIN<sup>1</sup>, ANDREY LYALIN<sup>2</sup>, and ANDREY SOLOV'YOV<sup>1</sup> — <sup>1</sup>Frankfurt Institute for Advanced Studies, Goethe University, Ruth-Moufang-Str. 1, Frankfurt am Main 60438, Germany — <sup>2</sup>Division of Chemistry, Graduate School of Science, Hokkaido University, Sapporo 060-0810, Japan

Encapsulation of a species within a fullerene can be regarded as an impurity which modifies the thermodynamic properties of the fullerene cage. The magnitude of the induced change is dependent upon the interaction of the carbon atoms in the fullerene and the type of endohedral species. In this work, we demonstrate that an Argon encapsulated within  $C_{60}$  can be regarded as intrinsic pressure on the fullerene cage. This intrinsic pressure leads to a shift in the temperature required to

fragment the fullerene cage, therefore affecting the phase transition behaviour of the fullerene from the cage structure to a gaseous state of carbon dimers. In this work, we construct a statistical mechanics model to explain this behaviour, as well as molecular dynamics simulations using the Tersoff potential. We demonstrate that the intrinsic pressure from the encapsulated species causes the fullerene system to be in one of its many isomer states. When the species is ejected out of the cage at high temperatures, the fullerene cage remains in the higher energy isomer state, therefore requiring less energy for a phase transition to its final gaseous phase of carbon dimers.

DY 12.32 Tue 14:30 P1A

**Stochastic Resonance in a ring of bistable elements** — ●JOHANNES WERNER and HARTMUT BENNER — Institut für Festkörperphysik, Technische Universität Darmstadt

A plethora of effects can be observed in unidirectionally coupled bistable systems. They include auto oscillations and enhanced sensitivity to external signals (e.g. [1]) as well as pattern formation [2]. These effects require an odd number of elements as well as an inverting, sufficiently strong coupling.

We show experimental results obtained from a ring of three negatively coupled Schmitt triggers, which are bistable electronic systems easy to realize. This ring was driven by different types of input signals. While our setup could reproduce most results from [1], it also showed several experimental constraints resulting from the finite frequency response and a small asymmetry of the elements.

In contrast to results from similar systems, e.g. [2], we were able to observe stochastic resonance like phenomena, specifically, an increased cross correlation between periodic input and response of the system. The results are supported by numerical experiments.

[1] Bulsara et al. PRE 70, 036103 (2004)

[2] Palacios et al. PRE 74, 021122 (2006)

DY 12.33 Tue 14:30 P1A

**Computer simulations of 2D colloidal crystals: elastic constants and effects of periodic, external fields** — ●KERSTIN FRANZRAHE and PETER NIELABA — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Minimization trends in physics and technology have caused a lot of interest in monolayers and their interactions with a substrate lately. Colloidal suspensions have proven to be ideal model systems for studies on such systems. The question of how the addition of another length scale into such a system will influence the intricate competition between adsorbate-adsorbate interaction and adsorbate-substrate interaction is addressed by studying a binary 50% hard disk mixture under the influence of a 1D spatially periodic substrate potential. The phase diagram is investigated by Monte Carlo simulations[1,3]. Furthermore we analyze the elastic properties of two dimensional colloidal crystals. The nonlocal elastic response function is crucial for understanding many properties of soft solids. It may be obtained by measuring strain-strain autocorrelation functions. We use computer simulations as well as video microscopy data of superparamagnetic colloids to obtain these correlations for two-dimensional triangular solids. Elastic constants and elastic correlation lengths are extracted by analyzing the correlation functions[2,3].

[1] K. Franzrahe, P. Nielaba, Phys. Rev. E 76, 061503 (2007); [2] K. Franzrahe, P. Keim, G. Maret, P. Nielaba and S. Sengupta, Phys. Rev. E 78, 026106 (2008); [3] K. Franzrahe et al., J. Phys.: Condens. Matter 20, 404218 (2008)

DY 12.34 Tue 14:30 P1A

**A Sinai-Billiard Model for Wet Granular Matter** — ●FRANZISKA GLASSMEIER, JÜRGEN VOLLMER, and MARTIN BRINKMANN — Dept. Dynamics of Complex Fluids, MPI for Dynamics & Self-Organization, 37073 Göttingen, Germany

We generalize the collision rules of the Sinai billiard to mimic collisions of two wet disks in a system with periodic boundary conditions. Within this framework we discuss the phase-space structure of invariant measures, and the entropy production involved in free cooling. Our results are compared to numerical data for the free cooling of large assemblies of wet disks.

DY 12.35 Tue 14:30 P1A

**Scaling in a One-Dimensional Model of Cyclic Interactions** — ●ANTON WINKLER<sup>1</sup>, TOBIAS REICHENBACH<sup>2</sup>, and ERWIN FREY<sup>1</sup> — <sup>1</sup>Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität

München, Theresienstraße 37, 80333 München — <sup>2</sup>Laboratory of Sensory Neuroscience, The Rockefeller University, 1230 York Avenue, New York, NY 10065, U.S.A.

Cyclic (rock-paper-scissors-type) population models serve to mimic complex species interactions. We have studied the effect of mutations on such a paradigmatic three-species model in one dimension, utilizing simple renormalization arguments complemented with exact calculations for certain limiting cases. We have thus achieved to build up a comprehensive picture of the system's dynamics. As the final arbiter of the validity of our results, we have employed stochastic simulations, which corroborate our predictions. Our methods and findings are potentially relevant for the spatio-temporal evolution of other non-equilibrium processes.

DY 12.36 Tue 14:30 P1A

**Flow equation analysis of the strong interaction Hubbard model** — ●ALEXANDER HOFFMANN and STEFAN KEHREIN — Physics Department, ASC, and CeNS, Ludwig-Maximilians-Universität, Theresienstraße 37, 80333 Munich, Germany

We employ unitary transformations to diagonalize the Hubbard model with strong Coulomb repulsion. The diagonal form permits us to investigate the equilibrium dynamics in the Mott insulating regime in a  $t/U$ -expansion. As an outlook, it can also serve as the basis for studying the non-equilibrium dynamics after a sudden interaction quench.

DY 12.37 Tue 14:30 P1A

**Preferential Trapping in State Space Dynamics** — ●ANDREAS FISCHER<sup>1</sup>, KARL HEINZ HOFFMANN<sup>1</sup>, and CHRISTIAN SCHÖN<sup>2</sup> — <sup>1</sup>TU Chemnitz, D-09107 Chemnitz, Germany — <sup>2</sup>Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany

The understanding of complex systems' dynamics is the basis for a successful modeling of a large variety of experimental results. This requires a in detailed analysis of the connectivity and the respective time scales of the transitions in the state space.

The hierarchical tree has proven to be a very useful model for a complex system's state space, as its capabilities have been frequently tested. The dynamics in such a hierarchical system is governed by the flow of probability and the tree's branching points, which is determined by different factors which need to be discussed in detail.

The research presented here analyzes the distribution of the probability when it flows towards the tree structures leafs. It is the way of this probability splitting which determines the over all time behavior. In this work the analysis is being expanded to more general approaches for the density of states.

DY 12.38 Tue 14:30 P1A

**Effect of disorder on equilibrium conformations of semiflexible polymers** — ●SEBASTIAN SCHÖBL, KLAUS KROY, and WOLFHARD JANKE — Institut für Theoretische Physik, Universität Leipzig

The structure and behaviour of biological cells is essentially affected by the biomechanical properties of semiflexible polymers. In the form of networks, such as the cytoskeleton, they build up the basic scaffold of eukaryotic cells. In order to study the mechanical properties of these highly complex systems, both interactions of the polymer with the surrounding network and further perturbing influences have to be taken into account.

We investigate the equilibrium structure of semiflexible polymers in different potential landscapes by Monte Carlo simulations. In our simulations we use two approaches, a lattice and an off-lattice model. In the first, the polymer is represented by a self-avoiding walk on a lattice with defects that represent the disorder. In the second, the semiflexible polymer is described by a Heisenberg chain, a discretized wormlike chain model. Relevant observables such as the end-to-end distribution function and the tangent-tangent correlation function are discussed. The disorder potential is modeled according to the underlying experimental biological system.

DY 12.39 Tue 14:30 P1A

**Transport on inhomogeneous filament networks** — ●PHILIP GREULICH and LUDGER SANTEN — Fachrichtung Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany

We present a model for intracellular vesicle transport on submembranal actin networks. These networks are created by stochastic growth dynamics of actin filaments leading to an inhomogeneous structure. The dynamics of vesicles are implemented by an interplay of active transport on filaments and diffusion in the cytosol, while steric interactions

of vesicles are taken into account. One observes the formation of vesicle clusters in a wide range of parameter space. We investigate the distribution of cluster sizes and compare these results to a system without filaments but attractive interactions between vesicles.

DY 12.40 Tue 14:30 P1A

**Analysing the reflectance spectra of human skin** — ●LIOUDMILA BELENKAIA<sup>1</sup>, PHILIPPE-A. BOURDIN<sup>1</sup>, VERA STERZIK<sup>2</sup>, MICHAEL BOHNERT<sup>2</sup>, and ANDREAS W. LIEHR<sup>1</sup> — <sup>1</sup>Freiburger Materialforschungszentrum, Stefan-Meier-Str. 21, 79104 Freiburg — <sup>2</sup>Institut für Rechtsmedizin, Albertstr. 9, 79104 Freiburg

Analysing the measurement data of a complex system always means interpreting the data with respect to a certain model. For the interpretation of the reflectance spectra of human skin, we use a twofold model. Part one of the model relates mesoscopic quantities like concentrations of skin dyes and the scatterer size distribution to characteristic optical parameters. The second part is a simulation of the experiment, which relates the reflectance to the optical parameters and therefore enables the estimation of the mesoscopic parameters on the basis of the measured reflectance [1]. In order to apply this model to topics of legal medicine a scientific information repository has been developed, which enables the physicist to store the measured reflectance spectra and to browse the analysis performed by the physician [2]. This contribution discusses the twofold model, the scientific information repository, and the experimental verification that the discolouration of livor mortis due to cooling is caused by re-oxygenation [3].

[1] Bohnert et al.: Int J Legal Med, 2005, 119, 355-362

[2] Belenkaia et al: arXiv:cs.DB/0612123

[3] Bohnert et al: Int J Legal Med, 2008, 122, 91-96

DY 12.41 Tue 14:30 P1A

**Wave localization in complex networks with high clustering** — ●LUKAS JAHNKE<sup>1</sup>, JAN W. KANTELHARDT<sup>1</sup>, RICHARD BERKOVITZ<sup>2</sup>, and SHLOMO HAVLIN<sup>2</sup> — <sup>1</sup>Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany — <sup>2</sup>Minerva Center and Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel

We study localization phenomena in complex optical networks. We find that strong clustering of links, i.e., a high probability of triadic closure, can induce a localization-delocalization quantum phase transition (Anderson-like transition) of coherent excitations. For example, the propagation of light wave-packets between two distant nodes of an optical network (composed of fibers and beam splitters) will be absent if the fraction of closed triangles exceeds a certain threshold. We suggest that such an experiment is feasible with current optics technology. We determine the corresponding phase diagram as a function of clustering coefficient and disorder for scale-free networks with different degree distributions characterized by an exponent  $\lambda$ . Without disorder, we observe no phase transition for  $\lambda < 4$ , a quantum transition for  $\lambda > 4$  and an additional distinct classical transition for  $\lambda > 4.5$ . Disorder reduces the critical clustering coefficient such that phase transitions occur for smaller  $\lambda$ . Ref.: Jahnke, Kantelhardt, Berkovits, and Havlin, Phys. Rev. Lett. 101, 175702 (2008)

DY 12.42 Tue 14:30 P1A

**Rule 150 cellular automata on 2D and Bethe lattices** — ●JENS CHRISTIAN CLAUSSEN — Neuro- und Bioinformatik, U zu Lübeck — Theoret. Phys. & Astrophys., CAU Kiel

The rule 150 cellular automaton is a remarkable discrete dynamical system, as it shows  $1/f^\alpha$  spectra if started from a single seed [1]. Despite its simplicity, a feasible solution for its time behavior is not obvious. Its self-similarity does not follow a one-step iteration like other elementary cellular automata. In this contribution [2] it is shown how its time behavior can be solved as a two-step vectorial, or string, iteration, which can be viewed as a generalization of Fibonacci iteration generating the time series from a sequence of vectors of increasing length. This allows us to compute the total activity time series more efficiently than by simulating the whole spatiotemporal process or even by using the closed expression. The results are further extended to the generalization of rule 150 to the two-dimensional case and to Bethe lattices, where two new corresponding integer sequences [3, 4] arise.

[1] J Nagler and J. C. Clausen, Phys. Rev. E 71, 067103 (2005)

[2] Jens Christian Clausen, Rule 150 cellular automata on 2D and Bethe lattices, Journal of Mathematical Physics 49, 062701 (2008)

[3] Jens Christian Clausen, Total activity of the Rule 150 cellular automaton on a Bethe lattice with coordination number 3, Online En-

cyclopedia of Integer sequences A138276

[4] Jens Christian Clausen, Total activity of the Rule 150 cellular automaton on a Bethe lattice with coordination number 4, Online Encyclopedia of Integer sequences A138277

DY 12.43 Tue 14:30 P1A

**Monte Carlo generation of complex random graphs with given functional weights** — ●HANNES NAGEL, BARTLOMIEJ WACLAW, and WOLFHARD JANKE — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig

We propose a C++ library for generating and handling random graphs with given statistical weights. The modular and extendable set of functions allows the user to easily create a program that generates complex networks with prescribed node-degree distribution, node-node correlations and assumed global structure (trees, simple graphs or degenerated graphs), with no a-priori limitation on the size of graph. The library also contains functions to perform statistical estimations on graphs or to export the graphs for further external processing.

DY 12.44 Tue 14:30 P1A

**Evolution of Boolean networks with different selection criteria and different update rules** — ●AGNES SZEJKA and BARBARA DROSSEL — Institut für Festkörperphysik, TU Darmstadt, Hochschulstrasse 6, 64289 Darmstadt, Germany

We study the evolution of Boolean networks under various selection criteria. Inspired by biological networks, we select simultaneously for robust attractors and for the ability to respond to external inputs by changing the attractor. Mutations change the connections between the nodes and the update functions. In order to investigate the influence of the type of update functions, we perform our simulations with canalizing as well as with threshold functions. We compare the properties of the fitness landscape that results for different versions of the selection criterion and the update functions, and the properties of the “solutions” found by the evolutionary process.

DY 12.45 Tue 14:30 P1A

**Anisotropy of the interface tensions of the three-dimensional Ising model** — ●ELMAR BITTNER, ANDREAS NUSSBAUMER, and WOLFHARD JANKE — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, D-04009 Leipzig, Germany

We determine the interface tension for the 100, 110 and 111 interface of the simple cubic Ising model with nearest-neighbour interaction using novel simulation methods. To overcome the droplet/strip transition and the droplet nucleation barrier we use a newly developed combination of the multimagnetic algorithm with the parallel tempering method. We investigate a large range of temperatures to study the anisotropy of the interface tension in detail.

DY 12.46 Tue 14:30 P1A

**Plateau formation in the twist parameter of the bond alternating AF  $S=1/2$  Heisenberg spin chain** — ●RAINER BISCHOF and JANKE WOLFHARD — Institut für Theoretische Physik, Universität Leipzig, Germany

The twist (order) parameter was introduced in [1] to signal a quantum phase transition between different valence bond configurations in various 1D quantum spin systems. We present quantum Monte Carlo simulations combined with quantum reweighting methods. At non-zero temperature we find the formation of a plateau in the twist (order) parameter around the (zero temperature) quantum critical point. We investigate the possibility that this plateau is related to the quantum critical region that fans out from the quantum critical point.

[1] M. Nakamura, S. Todo: Phys. Rev. Lett. 89, 077204 (2002).

DY 12.47 Tue 14:30 P1A

**Bose condensation for attractive interaction?** — ●MICHAEL MÄNNEL<sup>1</sup>, PAVEL LIPAVSKÝ<sup>2,3</sup>, KLAUS MORAWETZ<sup>4,5</sup>, and MICHAEL SCHREIBER<sup>1</sup> — <sup>1</sup>Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — <sup>2</sup>Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16253 Prague 6, Czech Republic — <sup>3</sup>Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic — <sup>4</sup>Research-Center Dresden-Rossendorf, Bautzner Landstr. 128, 01328 Dresden, Germany — <sup>5</sup>International Center of Condensed Matter Physics, University of Brasilia, 70904-970, Brasilia-DF, Brazil

We investigate a Bose gas with finite range interaction using a scheme to eliminate successive collisions as well as a single-channel T-matrix

approximation. For attractive interaction we find a Evans-Rashid transition from a quasi-ideal Bose gas to a BCS like phase with a gaped dispersion. The gap decreases with increasing density. At another critical point the gap vanishes, the dispersion becomes linear for small momenta and a Bose condensate appears. It is well known, that a Bose gas with contact interaction and a negative scattering length becomes instable and undergoes a gas-liquid or gas-solid transition. Looking for this instability we also calculate the pressure for the three phases.

DY 12.48 Tue 14:30 P1A

**Efficient free-energy calculation based on a generalized work fluctuation theorem** — •ALJOSCHA MARIA HAHN and HOLGER THEN

— Institut für Physik, Carl-von-Ossietzky-Universität Oldenburg

Traditional methods for the calculation of free-energies often converge extremely slow making it difficult to obtain accurate results. An example is the numerical computation of chemical potentials of fluids in the high density regime. The problem is that after inserting a test particle, the underlying phase space distribution does no longer coincide with its previous form.

A generalized work fluctuation theorem which includes bijective mappings of the underlying phase spaces allows the derivation of a maximum-likelihood estimator for the free-energy. By use of an appropriate map this estimator can, in principle, be made arbitrarily fast convergent.