DY 46 Poster

Time: Thursday 16:00–18:00 Room: P1

DY 46.1 Thu 16:00 P1

Level-Statistics of Disordered Systems: A Single Parametric Formulation — •Pragya Shukla — Department of Physics, IIT Kharagpur-721302, West Bengal, India

We present an analytical formulation for the statistics of energy levels of disordered systems, with/without e-e interactions, and, of arbitrary dimensions and boundary conditions. We find that the statistics behaves in a way similar to that of the single parametric Brownian ensembles. The latter appear during a Poisson → Wigner-Dyson transition, driven by a random perturbation. The analogy provides the analytical evidence for the single parameter scaling of the level-correlations in disordered systems at the metal-insulator transition as well as a tool to obtain them at the critical point for a wide range of disorders. The analogy also helps us to reveal many important features of the level-statistics in interacting systems e.g. a critical point behavior different from that of non-interacting systems, the possibility of extended states even in one dimension and a universal formulation of level correlations.

Reference:

(1) RANDOM MATRICES WITH CORRELATED ELEMENTS: A MODEL FOR DISORDER WITH INTERACTIONS PRAGYA SHUKLA, Phys. Rev. E, (71), (2005), 026266.

(2) LEVEL-STATISTICS IN DISORDERED SYSTEMS: A SINGLE PARAMETRIC SCALING AND CONNECTION TO BROWNIAN ENSEMBLES PRAGYA SHUKLA, J. Phys.: Condens. Matter 17, (2005) 1653-1677.

DY 46.2 Thu 16:00 P1

Some issues concerning oscillations in pedestrian crowds — •Tobias Kretz and Michael Schreckenberg — Universität Duisburg-Essen, 47057 Duisburg

"Oscillations" occur in pedestrian dynamics when two different groups of pedestrians with different directions of motion meet or intersect at a certain spot. We present a model of pedestrian motion that is able to reproduce the full range of oscillation as well as a method to quantify the strength of oscillations.

DY 46.3 Thu 16:00 P1

Real-Time-Traffic-Simulation and Prognosis in large scale Freeway-Networks — •Florian Mazur, Sigurdur F. Hafstein, Andreas Pottmeier, and Michael Schreckenberg — University Duisburg-Essen, Physics of Transport and Traffic, Lotharstr. 1, D-47057 Duisburg, Germany

Detailed and reliable information about the current traffic state is hardly obtainable by the road user. Therefore, we propose a web based visualization of the current and future traffic load of the autobahn network of North Rhine-Westphalia, Germany. This novel traffic information system named autobahn.NRW is based on an efficient and highly realistic traffic flow model, which is fed by traffic data from 4,500 detecting devices across the road network every minute. The approach of modelling entries and lane-blocks is completely new. The three-phases-approach which has a higher degree of realism then ordinary approaches, divides the road in front of the disturbance into three sections. Each section has a special function. The borders of the sections are based on a typing of different junctions and lane-blocks, which results from the different layouts. The results of the traffic simulation are published by a graphical user interface which can be accessed at http://www.autobahn.nrw.de/.

DY 46.4 Thu 16:00 P1

Self-assembly of pumps for microfluidic devices — •Stefan Bleil[1], David Marr[2], and Clemens Bechinger[1] — [1]2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [2]Chemical Engineering Department, Colorado School of Mines, Golden, Colorado 80401

The use of microfluidic devices requires active components (pumps or valves) which can direct and control liquids in such structures. We present a novel approach where pumps and valves are created by a self-assembly process which allows the realization of thousands of pumps at the same time. This is achieved by subjecting super paramagnetic colloidal particles to a circular polarized magnetic field, which results in a rotation of particles and thus leads to a fluid flow. Because the magnetic field induces additionally an attraction between adjacent particles, we can also create rotating particle clusters of different size. To control single pumps individually we use optical tweezers, which can stop or slow down the motion of particle clusters. In addition to the advantage of forming large arrays of individually addressable pumps, our approach allows also to scale the pumps down to the nanometer range by using smaller particles.

DY 46.5 Thu 16:00 P1

New Light on Like-Charge Attraction — •Jörg Baumgartl[1], Jose-Luis Arauz-Lara[2], and Clemens Bechinger[1] — [1]2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [2]Instituto de Física, Alvaro Obregón 64, 78000 San Luis Potosí, Mexico

A controversial debate in colloidal science has been launched in 1990 when Kepler and Fraden reported an unusual long-range attractive component in the pair potential of charged colloidal particles. This so-called like-charge attraction (LCA) was only observed in thin sample cells (typical plate separations < 10mm) while the pair-interaction in unconfined suspensions has been experimentally confirmed to be entirely repulsive which is in agreement with Poisson-Boltzmann theory. In the meantime it has been rigorously proven that the observed attraction can not be explained within the framework of mean field theories and several other approaches seem to fail to reproduce the experimental observations. We reinvestigate the pair-potential of charged colloidal particles in confined and unconfined geometries. We demonstrate that optical artifacts caused by the imaging process can lead to minute distortions in the particle distances as obtained by digital video microscopy. Those distortions result in an apparent minimum in U(r) which agrees with respect to its position and depth with the features observed in LCA. After correction of these distortions we obtain - independent of the confinement conditions - entirely repulsive pair interactions which show good agreement with linearized mean field theories. Thus, we can not support attractive components in the pair-interaction of confined colloidal suspensions.

DY 46.6 Thu 16:00 P1

Thermodynamics of Driven Brownian Particles — •Valentin Blickle[1], Thomas Speck[2], Laurent Helden[1], Udo Seifert[2], and Clemens Bechinger[1] — [1]2. Physikalisches Institut, Universität Stuttgart, Germany — [2]II. Institut für Theoretische Physik, Universität Stuttgart, Germany

A remarkable result in nonequilibrium statistical mechanics is the Jarzynski Relation (JR). It states that when a system is driven from state A to state B the free energy difference ΔF between A and B is connected to the work W done on the system: $< e^{-\beta W} >= e^{-\Delta F}$. In our experiment we study the motion of a Brownian particle in a non-harmonic potential, exposed to time dependent laser potentials. From its trajectory we can determine W and the heat exchange Q with the environment. Our well characterized system allows us to illustrate the first law of thermodynamics on a trajectorial level. In addition we study the JR and other related fluctuation theorems. In our experiments we observe a non-Gaussian distribution of W which has been predicted for non-harmonic potentials and is also supported by Focker-Planck calculations.

DY 46.7 Thu 16:00 P1

Experimental verification of a new scattering model for Total Internal Reflection Microscopy — •Christopher Hertlein[1], Laurent Helden[1], Elena Eremina[2], Thomas Wriedt[2], and Clemens Bechinger[1] — [1]2. Phys. Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart — [2]Institut für Werkstofftechnik, Universität Bremen, Badgasteiner Str. 3, 28359 Bremen

Total Internal Reflection Microscopy (TIRM) is a method for precise measurements of colloid - wall interaction potentials based on single particle evanescent wave light scattering. The technique is capable of resolving forces in the femtonewton range. In an evanescent field the scattering intensity strongly depends on the particle wall distance. The well established model used to interpret TIRM data is based on a simple exponential relation between intensity and distance. We developed a new model, that for the first time takes into account the exact experimental parameters. This model shows strong deviations from a purely exponen-

tial dependency of intensity and distance for certain parameters. These deviations can lead to severe artefacts in the measured interaction potentials. Using a TIRM-setup based on single-photon counting, we verified the dependency of the artefacts on experimental parameters such as average particle wall distance, penetration depth and polarisation of the evanescent wave.

DY 46.8 Thu 16:00 P1

Influence of external flows on dendritic growth: numerical investigation — •Dmitry Medvedev and Klaus Kassner — Otto-von-Guericke University Magdeburg, Universitaetsplatz 2, 39106 Madgeburg, Germany

We use a combined phase-field/lattice-Boltzmann scheme [1] to simulate dendritic growth from a supercooled melt in external flows. Several regions of the morphology diagram (in the supercooling – anisotropy – flow velocity coordinates) were explored.

At moderate to high undercooling and high anisotropy, data fall approximately onto unique curve in the Peclet number – tip radius plane. Hence, it could be argued that a parallel flow changes the selected tip radius and growth velocity solely by modifying (increasing) the Peclet number.

For smaller anisotropy, an interesting phenomenon is observed. The growth velocity for dendrites increases faster than for doublons with increase of the flow velocity (at the same undercooling and anisotropy). For some parameters, dendrites become faster, hence, external flow can appreciably change the morphology diagram.

For small anisotropy and Prandtl number, oscillations of the tip velocity are observed. Increase of the fluid viscosity damps these oscillations.
[1] D. Medvedev, K. Kassner, Phys. Rev. E 72, 056703 (2005)

DY 46.9 Thu 16:00 P1

Learning from examples in Neural Gas and Vector Quantization — •Michael Biehl, Anarta Ghosh, and Aree Witoelaar — Inst. of Mathematics and Computing Science, University Groningen, P.O. Box 800, 9700 AV Groningen, The Netherlands

The dynamics of training a neural gas for vector quantization in high dimensions is studied by means of methods from statistical physics. Prototype vectors for the repesentation of the data are updated either 'off-line' from an entire set of example data, or 'on-line' from a sequence of single data. In the first case, learning can be interpreted as to approach an equilibrium state and its typical outcome is studied in terms of macroscopic order parameters. For the on-line learning scenario, a description of the learning dynamics in terms of ordinary differential equations for the order parameters is possible. We explain the methods and present firstresults.

DY 46.10 Thu 16:00 P1

Experimental Observation of Stochastic Resonance in Coupled Systems — •Tobias Sawetzki, Carmen Schmitt, and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart

Since the introduction of the concept of Stochastic Resonance (SR) for the description of the periodic occurrence of ice ages, SR has been found in a great variety of examples in nature (e.g. the feeding behavior of paddlefish or human balance control) and experiments (Schmitt triggers, ring lasers). The essential feature of SR is that in nonlinear systems the presence of a certain level of noise can improve the detection of weak periodic signals.

We investigate SR by observing the motion of a colloidal particles in a modulated double well potential, which is generated by two neighboring optical traps. By adding further double well potentials in a square geometry, we study the effect of coupling between the different systems. If the modulation signals for the double wells are in phase, we observe two effects: (i) SR is enhanced compared to the isolated system and (ii) with increasing coupling the resonance is shifted towards smaller frequencies. When a phase shift is between the modulations in the square, coupling results in an asymmetry in the pobability distribution.

DY 46.11 Thu 16:00 P1

Relation between microscopic coevolutionary processes and macroscopic replicator equations: Meanfield dynamics in infinite populations and first-order corrections in finite populations — •Jens Christian Claussen[1], Arne Traulsen[2], and Christoph Hauert[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany — [2]Center for Evolutionary Dynamics, Harvard

Evolutionary game theory since Maynard Smith has served a powerful approach in biological systems as well as in agent-based models of social and economic systems. For infinite populations, a standard approach to analyze the dynamics are deterministic replicator equations, however lacking a systematic derivation. Additionally, in finite populations modelling finite-size stochasticity by Gaussian noise is not in general warranted [1]. We show that for the evolutionary Moran process and a Local update process, the explicit limit of infinite populations leads to the adjusted or the standard replicator dynamics, respectively. In addition, the first-order corrections in the population size are given by the finite-size update stochasticity and can be derived as a generalized diffusion term of a Fokker-Planck equation [2] thus giving a convenient framework of description. We explicitely discuss the differences for the Prisoner's Dilemma, where Moran evolution fixates faster [2], and Dawkin's Battle of the Sexes, where we show that the stochastic update fluctuations in the Moran process exhibit a finite-size dependent drift reversal [2].
[1] J.C. Claussen & A. Traulsen, Phys. Rev. E 71, 025101(R)
[2] A. Traulsen, J.C. Claussen, C. Hauert, Phys. Rev. Lett, 2005, in print

DY 46.12 Thu 16:00 P1

Thermal ratchet e ect in ferrofluids with mean-field interactions — •Volker Becker and Andreas Engel — Carl-von-Ossietzky-Universität, 26111 Oldenburg

Ferrofluids are suspensions of magnetic particles in an suitable carrier fluid.A thermal ratchet system for ferrofluids was introduced in [1]. Under the influence of a suitable time dependent magnetic field, rectification of orientation fluctuations of the magnetic grains become possible. The magnetic grains was modelled in [1] as non-interacting overdamped particles with frozen magnetic moments. To go beyond the the one particle approach we propose a simple model taking into account the interactions between the orientations of the magnetic grains. To keep things simple we consider a mean-field like attractive coupling between the orientations. It is possible to derive a mean-field Fokker-Planck equation for the orientation density. This equation has a similar form as one in the single particle approach, however with an self-consistently effective magnetic field. We study the influence of the particle interactions and in particular investigate whether the ratchet effect in many-particle systems may operate even with time choices of the time dependent fields which induce no ratchet effect in the single particle approach.
[1] A. Engel, H. W. Müller, P. Reimann, A. Jung, *Phys. Rev. Lett.* **91**, 060602(2003); A. Engel, P. Reimann, *Phys. Rev. E* **70**, 051107 (2004)

DY 46.13 Thu 16:00 P1

Calculation of the density of states in pseudointegrable quantum billiards — •Stefanie Russ — Institut für Theoretische Physik III, Universität Giessen, D-35392 Giessen

We calculate numerically the lengths and areas of the periodic orbit families for several pseudointegrable quantum billiards, as e.g. barrier billiards, L-shaped billiards and billiards with several steps until large orbit lengths. We use the periodic orbits to determine the integrated density of states for large energy intervals. Comparing the results to the known eigenvalues of the systems we find that the fluctuations of the density of states are reproduced in good accuracy by the periodic-orbit calculations. Finally, possible applications to experiments and a comparison to integrable systems is discussed.

DY 46.14 Thu 16:00 P1

Coherent exciton transport in dendrimers and continuous-time quantum walks — •Veronika Bierbaum, Oliver Mülken, and Alexander Blumen — Institute for Physics, University of Freiburg, Herrmann-Herder-Str. 3, 79104 Freiburg, Germany

We model coherent exciton transport in dendrimers by continuous-time quantum walks (CTQWs) [1]. Here only the topology of the dendrimer determines the dynamics. Depending on the initial excitation we find that the transport to certain nodes of the dendrimer is blocked and the long time average of the quantum mechanical transition probability between two nodes of the dendrimer shows characteristic patterns. Furthermore, for small dendrimers where the initial excitation is at the central node, the coherent transport shows perfect recurrence. For larger dendrimers, the recurrence is not perfect anymore. This resembles results for discrete quantum carpets [3]. When the initial excitation starts from the central node, the problem can be mapped onto a line which simplifies the computational effort. For the (space) average of the quantum mechanical probability to be still or again at the initial site, we obtain based on the Cauchy-Schwarz inequality a simple lower bound. \Zitat{1}{Oliver Mülken, Veronika Bierbaum, Alexander

Blumen; in preparation} \Zitat{2}{Oliver Mülken, Alexander Blumen; Phys. Rev. E 71, 016101 (2005)} \Zitat{3}{Oliver Mülken, Alexander Blumen; Phys. Rev. E 72, 036128 (2005)}

DY 46.15 Thu 16:00 P1

The free energy calculations of a system with soft mode. — •Małgorzata Sternik and Krzysztof Parlinski — Institute of Nuclear Physics Polish Academy of Sciences, ul.Radzikowskiego 152, Kraków

In regular crystals, where all phonon modes are harmonic, the free energy is a sum of the ground-state energy and vibrational configurations of noninteracting harmonic phonons. Using this approach, we performed the first-principle free-energy calculations of the tetragonal and monoclinic phases of zirconia. [1] The free energy for a cubic ZrO_2 crystal, which possesses a soft mode, was calculated using the double-well energy-displacement relation. The soft mode branch was considered as an ensemble of independent anharmonic oscillators of the parabola-plus-gaussian, or of the 2-4 polynomial forms.

The anharmonic contributions were included to reproduce the cubic-to-tetragonal phase transition. [2] The first results show that the cubic phase cannot be stabilized within the framework of the independent oscillators approach. The negative result could be a consequence of two reasons, that the thermal expansion of crystals and the phonon-phonon interaction are neglected.

This work was partially supported by the Polish State Commitee of Scientific Research (KBN), grant no 1 P03B 104 26.

[1] J.Chem.Phys. 122, 064707 (2005)
[2] J.Chem.Phys. 123, in print

DY 46.16 Thu 16:00 P1

Quantum echos at exceptional points — •Jonas Metz, Barbara Dietz, Thomas Friedrich, Maksim Miski-Oglu, and Florian Schäfer — Institut für Kernphysik, Schloßgartenstr.9, 64289 Darmstadt

We experimentally investigated quantum echos at exceptional points (EPs) with microwave billiards. First, two EPs were localized in the measured resonance spectrum. Then, the decay of these resonances with time was studied. The t^2-dependance predicted on the basis of a 2×2-matrix model for the two states degenerating at the EP could be verified, while for subcritical couplings of the two resonance states deviations from the theoretical model were found.

This work has been supported by DFG within SFB 634.

DY 46.17 Thu 16:00 P1

Gas diffusion in three-dimensional porous media in the Knudsen regime — •Stephan Zschiegner[1,2], Stefanie Russ[1], Armin Bunde[1], and Jörg Kärger[2] — [1]Institut für Theoretische Physik III, JLU Giessen — [2]Institut für Experimentelle Physik I, Universität Leipzig

In general, diffusion of gas particles depends on the collisions between the gas molecules as well as on the collisions of the gas with the pore walls. Of particular interest for many real gases is the range of the so-called Knudsen regime, where the interaction of the molecules with the pore walls plays the crucial role and intermolecular collisions can be neclected.

We implement pores with different roughness by considering the first four iterations of a generalized fractal Koch curve in three dimensions. For these model pores we have performed detailed investigations of self-diffusion and transport diffusion. We show that the diffusion can be mapped onto Levy walks and discuss the roughness dependence of the diffusion coefficients D_s and D_t of self- and transport diffusion, respectively. With further enhancement, by additionally calculating the statistical concentration within the pore, our results show equality of both diffusion coefficients D_s and D_t.

DY 46.18 Thu 16:00 P1

The Preisach model with stochastic input — •Falk Hesse and Günter Radons — University of Technology Chemnitz

Many materials in engineering and physics, such as piezoelectrics or shape memory alloys, show a strongly nonlinear input-output behaviour known as hysteresis. The Preisach formalism deals with the weigthed superposition of infinitely many independent elementary loops to model such hysteretic systems.

For the case of an Ornstein-Uhlenbeck process as input signal, we investigate the spectral density of the output generated by the Preisach operator. Since hysteresis deals with the history of the present input, the memory state of the system is taken into account. A correlation between the average memory length of the operator and the spectral density function of the generated output is shown. Furthermore the influence of the saturation for the average memory length is investigated. The importance of first-passage times of the underlying input process for the properties of the output as well of the memory is shown.

DY 46.19 Thu 16:00 P1

Investigation of the self-diffusion processses in liquids — •Vitaliy Bardic — Kiev Taras Shevchenko University

The study of the temperature dependence of oneparticle contributions to the self-diffusion coefficient has been carried out. The theoretical values of the self-diffusion coefficient in liquid argon coincide with both experimental data and the results of a computer simulation obtained at the certain values of the intermolecular potential parameters, the autocorrelation function of the molecular velocity being approximated by a quadratic polynomial.

DY 46.20 Thu 16:00 P1

Stochastic Schrödinger equation and quantum-classical dynamics — •Wolfgang Wolff and Walter T Strunz — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3, 79104 Freiburg i.Br.

We develop a framework to derive non-Markovian stochastic Schrödinger equations for open quantum systems in any order of the coupling strength to the environment. The derivation is based on Heisenberg's equation of motion using the coherent state representation for the environmental degrees of freedom. It is further shown that this framework allows us to derive consistent time evolution equations for coupled quantum-classical dynamics. These may be applied to nonlinear baths and couplings.

DY 46.21 Thu 16:00 P1

Testing a cooperative shear model for bulk metallic glasses using ultrasonic measurement techniques — •Annelen Kahl[1], Mary Laura Lind[2], Stefan Buschhorn[1], Jörg Hachenberg[1], William L. Johnson[2], and Konrad Samwer[1] — [1]1. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]138-78 Keck Laboratory, California Institut of Technology, Pasadena, California 91125, USA

The mechanical and rheological properties of metallic glasses and super cooled liquids can be explained with a cooperative shear model [1]. These material properties can be deduced from inherent states in a potential energy landscape described for example by an extended Frenkel-like potential. The model explains a universal relation between the maximum resolved shear stress and the shear modulus. Furthermore a prediction for the temperature dependence of the shear modulus is given. By isothermally annealing a sample for different times, the as-prepared sample can be transferred to equilibrium states of various corresponding fictive temperatures. The shear modulus for samples in different annealing states is measured to interpolate the equilibrium line. Using ultrasonic sound waves we determine the acoustic velocities for different annealing times by measuring the sample length and the travel time of a high frequency pulse propagating through the sample. From the sound velocity and the density of the samples the shear modulus can be determined. We acknowledge SFB 602, TP B8 for financial support.

[1] W.L. Johnson, K.Samwer, PRL95, 195501(2005)

DY 46.22 Thu 16:00 P1

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

Recently we were able to identify Lyapunov modes in chaotic many-particle systems with softcore interactions (Lennard-Jones fluids). This was made possible by defining and investigating certain static and dynamic correlation funtions of the Lyapunov vectors associated with the spectrum of Lyapunov exponents. We present the methods of calculating and evaluating these correlation functions as well as some results for binary Lennard-Jones fluids.

DY 46.23 Thu 16:00 P1

Genetic attack on neural cryptography — •Andreas Ruttor and Wolfgang Kinzel — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, 97074 Würzburg

Different scaling properties for the complexity of bidirectional syn-

chronization and unidirectional learning are essential for the security of neural cryptography. Incrementing the synaptic depth of the networks increases the synchronization time only polynomially, but the success of the geometric attack is reduced exponentially. This attack is improved by adding a genetic algorithm, which selects the fittest neural networks. The probability of a successful genetic attack is calculated for different model parameters using numerical simulations. The results show that scaling laws observed in the case of other attacks hold for the improved algorithm, too. The number of networks needed for an effective attack grows exponentially with increasing synaptic depth. Therefore the neural key-exchange protocol is secure in the limit of infinite synaptic depth.

DY 46.24 Thu 16:00 P1

Spindle Oscillations in Thalamocortical Oscillators: From a conductance-based biophysical model to an extended Hindmarsh-Rose model — •Jörg Mayer, Jens Christian Claussen, and Heinz Georg Schuster — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts Universität, Olshausenstraße 40, 24098 Kiel, Germany

In the last ten years electrophysiological measurements in thalamic slices helped to gain more insight into the thalamocortical system. In particular sleep spindles have been investigated thoroughly by extracellular and intracellular patch-clamp recordings in thalamic cells. Based on these data the thalamocortical system is a structure for which computational models can be extremely useful in in order to understand the relationship between underlying dynamics and biophysics.
We use an extended Hinsmarsh-Rose model to reproduce a recent experiment by Le Masson *et al.* on the thalamocortical loop. In this framework we analyze the underlying dynamical mechanisms which lead to spindle oscillations. We find that ionic currents which work on different timescales lead to spindle oscillations and influence the information transfer in thalamocortical loops significantly. [1]
[1] Jörg Mayer, Heinz Georg Schuster, and Jens Christian Claussen, The role of inhibitory feedback for information processing in thalamocortical circuits, arxiv.org e-print q-bio/0510040

DY 46.25 Thu 16:00 P1

Rotational Diffusion under Spatial Restrictions — •Heidrun Gleissberg, Patrick Ilg, and Siegfried Hess — TU Berlin

In Order to study the influence of confining walls on the rotational dynamics of a molecule with emphasis on the rotational diffusion coefficient a simple model is proposed.

In particular, two approaches are considered. The first one employs a recently introduced time reversible thermostat for rotational motion [1]. The other utilizes the irreversible Langevin equation.

Priority is given to the comparision of numerical results obtained via these strategies for a molecule in a channel.
[1] S.Hess, Z. Naturforsch. **58a**, 377 (2003)

DY 46.26 Thu 16:00 P1

Anomalous transport in disordered iterated maps — •Andreas Fichtner and Günter Radons — Chemnitz University of Technology, 09107 Chemnitz

Anomalous diffusion is not only restricted to systems with many degrees of freedom. It is also observable in low dimensional systems such as random walks in random environments. Sinai diffusion characterizes a class of random walks for which the so called Golosov phenomenon was proven rigorously. We extend the Sinai model to random walks whose transitions are not restricted to nearest-neighbours. Thereby a vanishing global bias is guaranteed by a generalization of binary disorder.

For Sinai disorder exact results exist for the disorder averaged mean square displacement, the density of states of the propagator, and the size-dependence of the escape rate, or, the mean first passage time, respectively. For each of them one can define a characteristic exponent. We show that in our extension of the Sinai model these exponents depend in a non-trivial way on the system parameters. This is a consequence of the generic absence of detailed balance.

DY 46.27 Thu 16:00 P1

Stochastic Resonance and Resonant Activation in Colloidal Suspensions — •Carmen Schmitt and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart, Germany

Stochastic Resonance and Resonant Activation are two prominent examples for noise-induced phenomena in nonlinear systems. Studying the dynamics of colloidal particles fluctuating in double well potentials created by optical tweezers, we have the experimental tools to investigate both effects in the same system. We present systematic measurements on *bona fide* Stochastic Resonance and compare the behavior of three different measures used in this context: the area under the first peak of the residence time distribution, the hysteresis loop area and phase synchonization. In addition to Stochastic Resonance we also observe Resonant Activation in our system. We demonstrate that the 'resonances' are located at different modulation frequencies.

DY 46.28 Thu 16:00 P1

Statistical analysis of noise-driven coupled nonlinear oscillators with Kerr-type nonlinearity — •Stanislav Derevyanko[1] and Jaroslaw Prilepskiy[2] — [1]Photonics Research Group, Aston University, Aston Triangle, Birmingham, UK — [2]B.I. Verkin Institute for Low Temperature Physics and Technology, Kharkov, Ukraine

We present exact analytical results for the statistics of nonlinear coupled oscillators under the influence of additive white noise. We suggest a perturbative approach for analysing the statistics of such systems under the action of a determanistic perturbation, based on the exact expressions for probability density functions for noise-driven oscillators. Using our perturbation technique we show that our results can be applied to studying the optical signal propagation in noisy fibres at (nearly) zero dispersion as well as to weakly nonlinear lattice models with additive noise. The approach proposed can account for a wide spectrum of physically meaningful perturbations and is applicable to the case of large noise strength.

DY 46.29 Thu 16:00 P1

Coupling induced dynamics in a ring of discrete bistable systems — •Johannes Werner, Thomas Stemler, and Hartmut Benner — Institut für Festkörperphysik, TU Darmstadt

Unidirectionally coupled bistable systems can show oscillations even in the absence of external forcing. These oscillations occur when an odd number of elements are negatively coupled to form a ring and the coupling strength λ is increased above a critical value λ_c. The frustration induced by the coupling leads to enhanced sensitivity to external signals. Recently, this was utilised in the construction of a highly sensitive magnetometer [1].

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 reproduces most results from [1], it also shows several experimental constraints resulting from the finite frequency response and a small asymmetry of the elements.
[1] Bulsara et al. PRE 70, 036103 (2004)

DY 46.30 Thu 16:00 P1

Noisefree Stochastic Resonance at an Interior Crisis — •Thomas Jüngling, Thomas Stemler, and Hartmut Benner — Institut für Festkörperphysik, TU Darmstadt

We report on the oberservation of noisefree stochastic resonance in an externally driven diode oscillator close to an interior crisis. At sufficiently high excitation amplitudes the diode resonator shows a strange attrator which after the collision with a unstable period 3 orbit exhibits a crisis induced intermittency. In the intermittency regime the system jumps between the previously stable chaotic attractor and the new phase space regions obtainend by the crisis. This random jumping between the two states of the dynamical system can be used to amplify a weak periodic signal via the mechanism of stochastic resonance. In contrast to conventional stochastic resonance no external noise is needed, but its role is taken over by the fast intrinsic chaotic dynamics. We compare our data obtained from the diode resonator with numerical simulations of the logistic map, where a similar crisis induced intermittency is observed.

DY 46.31 Thu 16:00 P1

How to describe a traffic breakdown physically? — •Julia Hinkel[1], Reinhard Mahnke[1], and Reinhart Kuehne[2] — [1]Institute of Physics, Rostock University, D–18051, Rostock — [2]German Aerospace Center, Institute of Transportation Research, D–12489, Berlin

We would like to calculate the traffic breakdown probability distribution which is related to a first-order phase transition from free flow to congested flow. Intuitively we introduce the notion of breakdown probability density as a function of time to reach some significant large car cluster size (first passage time problem). The calculations are based on initial–boundary–value Fokker–Planck equation including balance condition of probability flux.

[1] R. Kühne, R. Mahnke, International Symposium on Transportation and Traffic Theory, Washington, 2005
[2] J. Hinkel, How to calculate traffic breakdown probability? TGF2005, Berlin, 2005 (preprint)

DY 46.32 Thu 16:00 P1

Control of noise-induced patterns in a semiconductor nanostructure — •Grischa Stegemann[1], Alexander Balanov[1,2], and Eckehard Schöll[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin — [2]School of Physics and Astronomy, University of Nottingham, University Park, Nottingham NG7 2RD

We study the constructive influence of noise upon the nonlinear dynamics of current density patterns in a semiconductor nanostructure, and its control by time delayed feedback methods. In particular, we investigate noise-induced pattern formation in a double barrier resonant tunnelling diode described by a nonlinear reaction-diffusion model.

The parameters of the system are fixed at values below a Hopf bifurcation where the only stable state of the *deterministic* system is a spatially inhomogeneous "filamentary"steady state, and oscillating space-time patterns do not occur. We show that the addition of weak Gaussian white noise to the system gives rise to spatially inhomogeneous oscillations. As the noise intensity grows, the oscillations tend to become more and more spatially homogeneous, while simultaneously the temporal coherence of the oscillations decreases. We demonstrate that the application of a time delayed feedback loop, similar to that used in deterministic chaos control, allows one to either increase or decrease the regularity of the noise induced dynamics in this spatially extended system. Using linear stability analysis we can explain these effects, depending on the length of the delay interval.

DY 46.33 Thu 16:00 P1

Data analysis of periodically forced stochastic systems with time delay — •Andreas Wilmer, Dr. Till D. Frank, and Prof. Dr. Rudolf Friedrich — Institute for Theoretical Physics, WWU Münster, Wilhelm-Klemm-Str. 9, D-48149 Münster, Germany

A wide class of stochastic processes can be described by a system of Langevin equations. We shall consider stochastic systems, which include periodic forces and a time delayed feedback. These are relevant for various systems like seasonal systems in biology, engineering or movement control.
If we consider a univariate process with the stochastic variable $X(t)$, a time delay τ and a periodic force $f(t) = f(t+T)$, the Langevin equation reads as follows:

$$\frac{d}{dt}X(t) = h\left(X(t), X(t-\tau), f(t)\right) + g\left(X(t), X(t-\tau)\right)\Gamma(t)$$

where $\Gamma(t)$ is the fluctuating uncorrelated Langevin force with $\langle\Gamma_i(t)\Gamma_j(t')\rangle = 2\delta_{ij}\delta(t-t')$, the deterministic part $D^{(1)} = h$ called drift and the stochastic part g corresponding to the diffusion coefficient $D^{(2)} = g^2$.
We shall present a method, which enables the discrimination of a stochastic and deterministic force of time series and allows the estimation of the drift and diffusion coefficients from data.

DY 46.34 Thu 16:00 P1

Rotational Diffusion under Spatial Restrictions — •Heidrun Gleissberg and Siegfried Hess — Institut für Theoretische Physik, Technische Universität Berlin, D-10623, Germany

In Order to study the influence of confining walls on the rotational dynamics of a molecule with emphasis on the rotational diffusion coefficient a simple model is proposed.

In particular, two approaches are considered. The first one employs a recently introduced time reversible thermostat for rot ational motion [1]. The other utilizes the irreversible Langevin equation.

Priority is given to the comparision of numerical results yielded by these strategies for a molecule in a channel.

[1] S.Hess, Z. Naturforsch. **58a**, 377 (2003)

DY 46.35 Thu 16:00 P1

Control of noisy oscillations with extended time-delayed autosynchronization in the Van der Pol system — •Jan Pomplun[1], Eckehard Schöll[1], and Alexander Balanov[1,2] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, 10623 Berlin — [2]School of Physics and Astronomy, University of Nottingham, University Park, Nottingham NG7 2RD

We consider the Van der Pol system as a generic model of a nonlinear oscillator. Below the Hopf bifurcation the introduction of Gaussian white noise provokes noise-induced oscillations. It is shown that essential oscillation properties such as coherence and timescales can be controlled effectively by a feedback control loop with multiple time delays. This control scheme turns out to be much superior to single-time delay control. The occurrence of two different timescales in the system is observed, which can be modified by choosing appropriate values for the control parameters. An analytical treatment of the system explains these effects and shows excellent agreement with results from numerical simulations.

DY 46.36 Thu 16:00 P1

Light-induced oscillations of a cavity mirror — •Max Ludwig, Clemens Neuenhahn, and Florian Marquardt — Sektion Physik, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 München

A Fabry-Perot cavity with a moving mirror represents one of the simplest examples where the radiation pressure interacts with micromechanical degrees of freedom. This can give rise to an instability leading to self-induced oscillations, as demonstrated in two recent experiments [1,2]. Our theory [3] predicted and explained multiple stable dynamical attractors of the resulting mechanical motion. Here, we extend this work to cover situations involving several light modes inside the cavity, as well as the chaotical regime of motion, displaying a rich variety of behaviour.

We present both analytical and numerical results and comment on the direct relevance for experiments [1,2].
[1] C. Höhberger-Metzger and K. Karrai, Nature 432, 1002 (2004); Proceedings of the 4th IEEE conference on nanotechnology, p. 419 (2004).
[2] T. Carmon, H. Rokhsari, L. Yang, T. J. Kippenberg, and K. J. Vahala, Phys. Rev. Lett. 94, 223902 (2005).
[3] F. Marquardt, J. Harris, and S. Girvin, cond-mat/0502561 (2005).

DY 46.37 Thu 16:00 P1

High-order resonance in spiral wave dynamics under traveling wave modulation — •Sergey Zykov[1,2], Vladimir Zykov[1], Vasilij Davydov[2], and Harald Engel[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Moscow Institute of Radioengineering, Electronics and Automation, Russia

Resonance effects are well-known for different oscillating systems subjected to external periodic forcing. Here we consider the resonant drift of spiral waves rotating in a two-dimensional excitable medium under a spatio-temporal forcing in the form of a traveling wave modulation. We analyze the dependence of the direction and the velocity of the drift on the frequency, the wavelength and the amplitude of the external modulation. In contrary to a spatially uniform, pure time-periodic external forcing, high-order synchronization bands (2:1 and 3:1) are obtained, where the phase of the spiral wave is synchronized by the external force. Results of the direct integration of the reaction-diffusion equations agree well with those of the kinematical description of spiral tip motion.

DY 46.38 Thu 16:00 P1

Classes of integrable spin systems — •Robin Steinigeweg and Heinz-Jürgen Schmidt — Physics Department, University of Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

We investigate certain classes of integrable classical (and quantum) spin systems of Heisenberg type. The first class is characterised by the recursively defined property P saying that the spin system consists of a single spin or can be decomposed into two uniformly coupled or uncoupled subsystems with property P. For these systems the time evolution can be explicitly calculated. The second class consists of spin systems where all non-zero coupling constants have the same strength possessing $N-1$ independent, commuting constants of motion of Heisenberg type. These systems have the above property P and can be characterised as spin graphs not containing chains of length four. Applications to the construction of symplectic numerical integrators for non-integrable spin

systems, e.g., a recently synthesised magnetic molecule, are briefly discussed.

DY 46.39 Thu 16:00 P1

Possible destabilizations of stationary dissipative solitons in three-component reaction-diffusion system — •S. V. Gurevich, Sh. Amiranashvili, and H.-G. Purwins — Institute of Applied Physics, WWU Münster, Corrensstr. 2-4, 48149 Münster, Germany

We investigate stability of the localized stationary solutions in a three-component reaction-diffusion system with one activator and two inhibitors. The change of the time constants of inhibitors can lead to various destabilization scenarios, e.g., to drift- or breathing bifurcation. A more complicated case, where both unstable modes are excited together also is considered. These situations are analyzed performing a two-time-scale expansion and the corresponding amplitude equations are obtained. Also numerical simulations are carried out showing good agreement with our analytical predictions.

DY 46.40 Thu 16:00 P1

Relation between drift-diffusion and reaction diffusion systems — •Sh. Amiranashvili, S. V. Gurevich, and H.-G. Purwins — Institute of Applied Physics, WWU Münster, Corrensstr. 2-4, 48149, Münster, Germany

We deal with a three-component transport equation that currently is used in gas-discharge and other electrical transport systems. We discuss the behavior of this system on the long time scale. Instead of directly solving the equation we introduce an asymptotical multi-scale expansion to reduce the system to a simpler one. The latter belongs to the class reaction-diffusion systems and is much more simpler to analyze and implement numerically. Direct comparison of the available numerical solutions for the two systems shows that the approximation works perfectly good. Thereafter we apply the simpler system to describe physical phenomena in gas discharge. Nowadays these phenomena hardly can be directly calculated in the framework of the original equations. The presented work lays the foundation for the universal behavior of patterns observed in electrical transport systems and reaction-diffusion systems.

DY 46.41 Thu 16:00 P1

Soliton ratchets in homogeneous nonlinear Klein-Gordon systems — •Luis Morales-Molina[1], Niurka Quintero[2], Angel Sanchez[3], and Franz Mertens[4] — [1]Max-Planck Institut f ür Physik Komplexer Systeme, 01187 Dresden, Germany — [2]Departamento de Fisica Aplicada I, E.U.P.,*Universidad de Sevilla, 41011 Sevilla, Spain — [3]Departamento de Matematicas, Universidad Carlos III de Madrid, 28911 Leganes, Madrid, Spain — [4]Physikalisches Institut, Universität Bayreuth, D-85440 Bayreuth, Germany

We study in detail the ratchet-like dynamics of topological solitons in homogeneous nonlinear Klein-Gordon systems driven by a bi-harmonic force. By using a collective coordinate approach with two degrees of freedom, namely the center of the soliton, $X(t)$, and its width, $l(t)$, we show, first, that energy is inhomogeneously pumped into the system, generating as result a directed motion; and, second, that the breaking of the time shift symmetry gives rise to a resonance mechanism that takes place whenever the width $l(t)$ oscillates with at least one frequency of the external ac force. In addition, we show that for the appearance of soliton ratchets, it is also neccesary to break the time-reversal symmetry. We analyze in detail the effects of dissipation in the system, calculating the average velocity of the soliton as a function of the ac force and the damping. We find current reversal phenomena depending on the parameter choice and discuss the important role played by the phases of the ac force. Our analytical calculations are confirmed by numerical simulations of the full partial differential equations of the sine-Gordon and ϕ^4 systems, which are seen to exhibit the same qualitative behavior.

DY 46.42 Thu 16:00 P1

Highly Efficient Laser Driving Mechanism for a Nano-Electromechanical Beam Resonator — •Daniel König and Jörg Kotthaus — LMU, Department für Physik, LS Prof. Kotthaus, Geschwister-Scholl-Platz 1, 80539 München

The relevance of nanoelectromechanical systems (NEMS) range from their applications as highly sensitive detectors, ultra small switches, and spin detectors to fundamental research [1,2,3]. As NEMS are continuously scaled down, they are starting to approach the quantum mechanical limit [4]. It is of particular interest to find efficient and reliable driving mechanisms of NEMS. Here we present an actuation mechanism, which relies upon the thermal induced deflection of a bi-metal strip after a laser excitation. The resonator is a bi-layer silicon-gold-system with the dimensions 10 μm, 200 nm, and 200 nm (length, width, height). The resonator is easily driven into the non-linear regime, where amplitudes up to 100 nm are reached at frequencies in the MHz range. For detecting the resonators response, the resonator is placed in a magnetic field of 12 Tesla at 4 Kelvin and the induced current due to its mechanical motion is measured with a lock-in technique.

[1] Ilic, Craighead et al., APL Vol 85, 13 (2004)
[2] J. E. Jang, S. N. Cha et al, APL 87, 163115 (2005)
[3] Rugar et al., Nature, Vol 430, 329 (2004)
[4] M. D. LaHaye et al., Science 304,74 (2004)

DY 46.43 Thu 16:00 P1

Pattern formation in nonlinear optical systems with feedback — •Guido Krüger and Rudolf Friedrich — Institute for Theoretical Physics University of Münster, Wilhelm.-Klemm-Str. 9, 48159 Münster

Optical systems are of growing interest in communication technology. Especially the combination of optical signals is a important task to produce optical switches.

In our study, we investigate two nonlinear Sodium vapor cells with feedback theoretically as well as numerically. The emerging patterns, which arise due to the nonlinearity and the feedback, will be presented and discussed (Hexagons, squares, stripes, honeycombs, labyrinthine, quasi-patterns and solitary structures). Furthermore our interest is to perform a logical operation with these two cells to check if it is possible to make a optical switch.

DY 46.44 Thu 16:00 P1

Hybrid model for investigating the role of Ca^{2+} buffers in intracellular Ca^{2+} dynamics — •Stefan Zeller[1], Martin Falcke[2], Sten Rüdiger[2], and Harald Engel[1] — [1]Institut für Theoretische Physik, TU-Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Abteilung Theorie SF5, Hahn-Meitner-Institut, Glienicker Str. 100, 14109 Berlin, Germany

We have modelled a four-component reaction-diffusion system with excitable elements, which are distributed inhomogeneously in a two-dimensional spatial domain. The source terms of the activator are spatially discrete and behave stochastically. With this model we investigate Ca^{2+} liberation through inositol 1,4,5-trisphosphate receptors which plays an universal role in cell regulation. Moreover, the specificity of cell signalling is achieved through the spatiotemporal patterning of Ca^{2+} signals.

Our interest is directed towards experiments [1] which have shown that mobile cytosolic Ca2+ buffers are modulating the coupling between the excitable elements. Surprisingly, a buffer with fast 'on-rates' should weaken the coupling but leads to more activation and a globalization of spatially uniform Ca^{2+} signals. To understand the role of the Ca^{2+} buffers for the Ca^{2+} dynamics in the cytosol, we perform adaptive numerical simulations of a hybrid stochastic and deterministic model.

[1] Sheila L. Dargan and Ian Parker, Buffer kinetics shape the spatiotemporal patterns of IP_3-evoked Ca^{2+} signals, J. Physiol (2003), **533.3**, pp.775-788

DY 46.45 Thu 16:00 P1

Monitored Control of Spiral Wave Cores along Arbitrary Trajectories — •Johannes Breuer, Vladimir S. Zykov, Harald Engel, and Eckehard Schöll — Technische Universität Berlin, Berlin, Germany

Controlling spatiotemporal patterns such as spiral waves in excitable media is interesting for various reasons. In particular, as many studies indicate, spiral waves are tightly connected to pathologic excitation modes in the heart muscle (ventricular tachycardia) and potentially related to migraine (spreading depression waves in neural tissue). Hitherto, feedback methods using the effect of resonant drift have proved to be a suitable means to control the motion of a spiral wave core[1, 2]. As an extension of these techniques we have developed a novel control algorithm that extracts the current phase and position of the spiral wave from a small number of detector signals and is thus capable of guiding the wave core along arbitrary prescribed trajectories.

[1] V. S. Zykov, G. Bordiougov, H. Brandtstädter, I. Gerdes, and H. Engel: Global Control of Spiral Wave Dynamics in an Excitable Domain of Circular and Elliptical Shape, Phys. Rev. Lett. 92(1), 018304 (2004)
[2] V. S. Zykov, and H. Engel: Feedback Control of Spiral Waves, Physica

D 199, 243 (2004)

DY 46.46 Thu 16:00 P1

Instabilities of spiral wave drift induced by a line–detector feedback — •Jan Schlesner, Vladimir Zykov, and Harald Engel — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Our experimental and numerical data show that a line–detector feedback can be efficiently used to induce a well-controlled spiral wave drift trough an excitable medium. To this aim a short excitability perturbation is applied globally each time a spiral wave front is tangent to the detector. However, the drift velocity is limited by instabilities which appear under high perturbation strengths or large time–delays in the feedback loop. A theory is developed that describes the spiral wave drift by a high–order iterative map, where the instabilities appear due to a Neimark bifurcation. Possible ways to suppress these instabilities are discussed.

DY 46.47 Thu 16:00 P1

Synchronization of a hierarchical ensemble of coupled excitable oscillators — •Cornelia Petrovic and Rudolf Friedrich — Institut für Theoretische Physik, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Str. 9, D-48149 Münster

Motivated by an experiment concerning the exothermic CO-oxidation on palladium supported catalyst (C.Ballandis, P.J.Plath, Journal of Non-Equilibrium Thermodynamics 25 3/4, 301 (2000)) we investigate a model for an ensemble of globally coupled nonlinear oscillators. These oscillators are relaxation oscillators with different frequencies showing various kinds of synchronization phenomena (from partial up to global synchronization). We focus on the emergence of selfaffine features in the temporal evolution of the system. In our contribution we shall present a detailed mathematical analysis of this system.

DY 46.48 Thu 16:00 P1

Simple dynamical systems with Preisach nonlinearity — •Sven Schubert, Roland Lange, and Günter Radons — Chemnitz University of Technology, 09107 Chemnitz

Many physical and technical systems such as shape memory alloys or certain friction models are characterized by a non-trivial hysteretic behavior, implying e.g. the appearance of nested sub-loops and a complex dependence on previous input events.

We study properties of output time series $\{y_n\}$ and the system memory behavior accrued from using a discrete Preisach-hysteresis transducer and logistic map input scenarios $\{x_n\}$. We demonstrate the sensitivity of the Preisach-hysteresis transducer to certain properties of the input time series which are usually not detected by standard time series analysis tools.

In addition we consider the iterates of the composition of a logistic map and a hysteresis transducer resulting in a *logistic Preisach-operator*. The aim is to gain a deeper understanding of dynamical systems with components showing complex hysteretic behavior. Our results show the appearance of fractal structures in dependence on the initial state and also a stabilizing influence of the hysteresis transducer.

DY 46.49 Thu 16:00 P1

Hydrodynamic Lyapunov modes and strong stochasticity threshold in Fermi-Pasta-Ulam models — •Hong-liu Yang and Günter Radons — Institute of Physics, Chemnitz University of Technology, D-09107 Chemnitz

The strong stochasticity threshold (SST) is characterized by a crossover of the system dynamics from weak to strong chaos with increasing the energy density ϵ. Correspondingly, the relaxation time to energy equipartition and the largest Lyapunov exponent exhibit different scaling behavior in the regimes below and beyond the threshold value. In this paper, we attempt to explore further changes in the energy density dependence of all Lyapunov exponents and of hydrodynamic Lyapunov modes (HLMs). In particular, we find that for the FPU-β and FPU-$\alpha\beta$ model the scaling of the energy density dependence of all Lyapunov exponents shows similar changes at SST as those of the largest Lyapunov exponent. This supports the point of view that the crossover in the system dynamics at SST reflects a global change in the geometric structure of the phase space. Furthermore, the FPU-β model is used as an example to show that HLMs exist in Hamiltonian lattice models with continuous symmetries. Numerical simulations demonstrate that there exist a smooth transition in Lyapunov vectors corresponding to the crossover in Lyapunov exponents at SST. In particular, our numerical results indicate that strong chaos is essential for the appearance of HLMs.

DY 46.50 Thu 16:00 P1

Interchange of Hopf bifurcation between super- and subcritical by using unstable time-delayed feedback control — •Chol-Ung Choe[1,2], Hiroyuki Shirahama[1,3], Klaus Höhne[1], and Hartmut Benner[1] — [1]Institut für Festkörperphysik, TU Darmstadt, Germany — [2]Department of Physics, University of Science, Pyongyang, DPR Korea — [3]Ehime University, Matsuyama, Japan

We show that robust nonlinear unstable time-delayed feedback control, which has successfully been used to control a torsionfree unstable periodic orbit, provides a tool to convert a subcritical Hopf bifurcation into a supercritical one and vice versa. We present experimental results on a van der Pol - like electronic oscillator showing a sub- or supercritical Hopf bifurcation. The application of the robust control changes the bifurcation type in a limited range of the bifurcation parameter of the circuit. This range can be extended by adopting half-period delay time. These results are supported by analytical theory and numerical simulations.

DY 46.51 Thu 16:00 P1

Phase-space correlations of chaotic eigenstates — •Holger Schanz — Max-Planck-Institut für Dynamik und Selbstorganisation und Fakultät für Physik, Universität Göttingen,*Bunsenstraße 10, D-37073 Göttingen, Germany

It is shown that the Husimi representations of chaotic eigenstates are strongly correlated along classical trajectories. These correlations extend across the whole system size and, unlike the corresponding eigenfunction correlations in configuration space, they persist in the semiclassical limit. A quantitative theory is developed on the basis of Gaussian wavepacket dynamics and random-matrix arguments. The role of symmetries is discussed for the example of time-reversal invariance.

DY 46.52 Thu 16:00 P1

Measurement of thermodynamic characteristics in small quantum systems — •Heiko Schröder and Günter Mahler — Universität Stuttgart, Institut für Theoretische Physik 1, Pfaffenwaldring 57, D-70550 Stuttgart

When considering smaller and smaller quantum systems, one would expect that a thermodynamic description of such systems should eventually fail. Surprisingly, even small quantum systems exhibit thermodynamical behaviour when in contact with an environment [1]. In this context, several ways of measuring the thermodynamic characteristics of small quantum systems are proposed and the problem of discriminating the degrees of freedom which contribute either to heat or to mechanical energy is addressed. This is done by an operational approach, considering simple quantum systems like harmonic oscillators connected to measurement devices.

[1] J. Gemmer, M. Michel, G. Mahler. Quantum Thermodynamics, LNP 657, Springer 2004

DY 46.53 Thu 16:00 P1

Model studies on quantum fluctuation theorems — •Jens Teifel and Günter Mahler — Universität Stuttgart, Institut für Theoretische Physik 1, Pfaffenwaldring 57//IV, 70550 Stuttgart, Germany

If an external force acts on a thermodynamic system on a finite time scale, it may be driven out of equilibrium. The Jarzynski relation, a classical fluctuation theorem, connects the work performed on a system and the difference of the free energy of the initial and final state respectively. A quantum analogue has been established by S. Mukamel [1]. Here we study simple models of quantum thermodynamic systems; their unitary evolution during the externally driven process as well as the variance and distribution of work is examined.

[1] Phys. Rev. Lett. 90, 170604 (2003)

DY 46.54 Thu 16:00 P1

Transport Phenomena in 1-D spin chains — •Pedro Vidal, Günter Mahler, and Mathias Michel — 1. Institut für Theoretische Physik, Universität Stuttgart

We study transport in a 1-D quantum spin chain by solving the Schrödinger equation. Because of the integrability of our models, and thus their conservation laws, we can analyse the system in a closed form in subspaces of our Hilbert space. Local quantities are defined via the coarse graining of our system and the "diffusion" behavior of these observables is calculated analyticaly or numerically, depending on the complexity of the sub-Hilbert space. We find evidence for a non experimental

1/t decay for the local coarse grained observables such as the local energy.

DY 46.55 Thu 16:00 P1

Quantum relaxation in two-level systems under influence of a stationary $1/f^{\alpha}$ noise — •Igor Goychuk and Peter Hänggi — Institut für Physik, Universität Augsburg, Germany

We investigate relaxation in quantum two-levels systems under the influence of stationary $1/f^{\alpha}$ noises. The renewal model of two-state non-Markovian processes with finite mean residence time but diverging variance of the residence time distribution is considered. Applying the general theory developed in [1], we obtained exact analytical solution of the considered quantum relaxation problem in the Laplace domain [2]. Performing both asymptotical analysis and precise numerical inversion to the time domain we show that for a broad range of parameters the relaxation can be mostly single-exponential ending, however, with a heavy $1/t^{1-\alpha}$ tail ($0 < \alpha < 1$). For α close to one, this creates impression of a nonequilibrium residual magnetization, i.e. relaxation to a nonequilibrium steady state on a numerically (or might be also physically) accessible time-scale.

[1] I. Goychuk, Phys. Rev. E **70**, 016109 (2004); I. Goychuk and P. Hänggi, Adv. Phys. **54** (2005) (in press).
[2] I. Goychuk and P. Hänggi, Chem. Phys. (2006) (in press).

DY 46.56 Thu 16:00 P1

Adsorption isotherms and isosteric heat of monoatomic gas adsorbed on closed-end single-wall carbon nano-bundles — •Igor Poltavsky, Tatiana Antsygina, and Konstantin Chishko — B. Verkin Institute for Low Temperature Physics and Engineering, 47 Lenin Ave., Kharkov 61103, Ukraine

Adsorption isotherms and isosteric heats of monoatomic gas adsorbed on outer and inner surfaces of closed-end single-wall carbon nanotube bundles have been investigated theoretically. An original model to describe such a system was developed. The used approach is based on account of equilibrium conditions among three subsystems: a quasi-one-dimensional (so called "three-chain") subsystem formed by atoms in grooves on the outer surface, a two-dimensional (2D) monolayer on the outer surface and a one-dimensional subsystem formed by atoms adsorbed in interstitial channels. To describe the three-chain subsystem we took into account interactions between the nearest and second nearest neighbors in all three chains. Since we are interested in the coverage range where the formation of the monolayer just begins we treated the 2D subsystem as an ideal gas.

The adsorption isotherms and isosteric heat were calculated for different values of substrate binding energies and interparticle interaction parameters. Theoretical results are in good agreement with the experimental data. For real systems (helium and methane) we obtained the binding energies for adsorption in various positions. We also found the coverage ranges for which the adsorption into one of the above-mentioned subsystems prevails.

DY 46.57 Thu 16:00 P1

Effects of carrier gas and different thermostats in molecular dynamics simulations of vapor-liquid nucleation — •Jan Wedekind[1], David Reguera[2], and Reinhard Strey[1] — [1]Institut für Physikalische Chemie, Universität zu Köln, Luxemburger Str. 116, D-50939 Köln, Germany — [2]Departament de Física Fonamental, Facultat de Física, Universitat de Barcelona, Martí i Franquès, 1, 08028-Barcelona, Spain

Nucleation is the first step in most first-order phase transitions such as condensation. As an activated process, it is highly sensitive to small changes in temperature leading to differences in nucleation rates of up to several orders of magnitude. In molecular dynamics (MD) simulations it is not a trivial task to keep the temperature constant. One way is to directly thermostat the vapor itself. However, this may lead to an undesirable change of the temperature of a condensing cluster. Another approach mimicing the experiment is to thermostat the condensable species through their collisions with a carrier gas. We investigated the influence of a carrier gas in a MD simulation of nucleation of Lennard-Jones argon. We simulated a system at two different supersaturations without and with three different concentrations of carrier gas. Each simulation was repeated up to 1000 times yielding a previously unmatched accuracy of the statistics. It turns out that the choice of thermostat does not have a significant influence on the results of argon nucleation, even though this result may not be generalized to any kind of nucleation system or nucleating species.

DY 46.58 Thu 16:00 P1

Phase-Ordering and Ageing Phenomena in q-State Potts Models with q = 3 and 8 — •Eric Lorenz and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11, 04109 Leipzig, Germany

Dynamical properties of Potts models with $q = 3$ and $q = 8$ are studied during phase-ordering through numerical simulations with a non-conserved order parameter. The systems are quenched from a highly disordered state ($T_1 = \infty$) into the ferromagnetic phase($T_2 \approx \frac{1}{2}T_c$) whereafter the dynamical self-similarity of phase-ordering shows up. Tied with this process is the phenomenon of ageing, i.e. the breaking of time-translational invariance. To reveal ageing in the considered systems, two-time quantities such as the autocorrelation $A(t, s)$, autoresponse $R(t, s)$ and spatiotemporal response $R(t, s; r)$ are measured and compared with scaling functions predicted from local scale invariance.

DY 46.59 Thu 16:00 P1

Mechanisms involved in the formation and dynamics of dissipative solitons — •Hendrik U. Bödeker, Shalva Amiranashvili, and Hans-Georg Purwins — Westfälische Wilhelms-Universität Münster, Institut für Angewandte Physik, Corrensstr. 2/4, 48149 Münster

Dissipative solitons appear as a generic structure in a large variety of dissipative, spatially extended nonlinear systems. As they are strongly nonlinear structures with high amplitude that are usually generated in subcritical bifurcations, their formation cannot be understood in terms of a perturbation approach. Consequently, a systematic understanding of the mechanisms of soliton formation and stabilization is still lacking. On this poster, we will give an overview on these mechanisms we found in different systems allowing for the formation of dissipative solitons, with particular emphasis on our new results in reaction-diffusion systems. Furthermore, different types of destabilization of stationary dissipative solitons leading to dynamical phenomena are discussed.

DY 46.60 Thu 16:00 P1

Two particles with bistable coupling on a ratchet — •Jörg Menche[1,2] and Lutz Schimansky-Geier[1] — [1]Humboldt Universität zu Berlin — [2]Universität Leipzig

We study the motion of two Brownian particles coupled by a bistable potential on a periodically rocked ratchet. Bistable coupling symmetrizes the two particles and admits a richer dynamics that cannot be found with linear coupling or a single particle. Depending on the coupling strength and the equilibrium distance we find different step patterns and current reversals. We present numerical results and compare them with analytical solutions in limiting cases of adiabatically slow rocking and of rigid coupling.

DY 46.61 Thu 16:00 P1

Kinetic Lattice Gas Models in Nanofluidics — •Carlo Dotti, Mihail Popescu, Andrea Gambassi, and Siegfried Dietrich — Max Planck Institut fuer Metallforschung, Stuttgart

While hydrodynamics is reasonably well understood at normal scales, it is not expected to work when one or more sizes of the liquid film are comparable to the atomic size. In those cases the discrete character of both the liquid and substrate is expected to play a crucial role, requiring fundamentally different theoretical description for both the equilibrium and the non-equilibrium situation. Understanding the dynamics of nanofluidics is crucial to build reliable micro and nano-devices which can be useful in various industrial and scientific applications. My main goal is to investigate nano-fluidics phenomena, focusing on non-equilibrium aspects, employing both analytical and numerical techniques.

DY 46.62 Thu 16:00 P1

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

We investigate the structural and elastic properties of two dimensional colloidal systems via Monte-Carlo Simulations. The colloidal systems of interest were modelled by hard disk systems. Simulations in the NPT- and NVT-Ensemble were carried out in order to analyse lattice formation in binary mixtures. The elastic properties of these systems were calculated using a fluctuation method by S. Sengupta et.al [1]. In this context we also examined the influence of quenched impurities on the elastic properties of a mono disperse hard disk system [2][3]. Another point of

interest is the influence of external laser fields on these colloidal crystals. Simulations of a $S_1(AB)$ lattice under the influence of a commensurable, spatially periodic, external laser field show domain formation processes that are absent in the field free case.

[1] S. Sengupta, P. Nielaba, M. Rao and K. Binder,Phys. Rev. E **61**, pp. 1072 (2000)
[2] K. Franzrahe et. al., Comp. Phys. Commun. **169**,pp 197-202 (2005)
[3] P. Nielaba, K. Binder, C. Chaudhuri, K. Franzrahe, P. Henseler, M. Lohrer, A. Ricci, S. Sengupta, W. Strepp, J. Phys.: Condens. Matter **16**, S4115-S4136 (2004)

DY 46.63 Thu 16:00 P1

Modern Methods in Protein Simulations — •Christoph Junghans[1,2] and Ulrich H.E. Hansmann[2] — [1]Institut für Theoretische Physik, Universität Leipzig — [2]Computational Biology and Biophysics, John von Neumann Institute for Computing, Forschungszentrum Jülich

The aim of this work [1] is to study the behaviour of four advanced Monte Carlo methods in protein simulations employing a realistic ECEPP/3-based all-atom model. The implementation is based on the open source package SMMP [2]. The techniques applied were multicanonical Monte Carlo [3], parallel tempering [4], Wang-Landau sampling [5] and simulated tempering [6]. They all exhibit good properties for the high-temperature and -energy region, but still have ergodicity problems in the low-energy region due to the size of the conformation space and the rough free-energy landscape.

[1] C. Junghans, in Technical Report IB-2005-13, R. Esser (Ed.), John von Neumann Institute for Computing, J/"ulich, 2004.
[2] F. Eisenmenger, U.H.E. Hansmann, S. Hayryan and C.-K. Hu, Comp. Phys. Comm. **138** (2001) 192.
[3] B.A. Berg and T. Neuhaus, Phys. Rev. Lett. **68** (1992) 9.
[4] K. Hukushima and K. Nemoto, Jour. Phys. Soc. (Jap.) **65** (1996) 1604.
[5] F. Wang and D.P. Landau, Phys Rev. E **64** (2001) 056101.
[6] E. Marinari and G. Parisi, Europhys. Lett. **19** (1992) 451.

DY 46.64 Thu 16:00 P1

Fractional calculus applied to the ion dynamics in porous matter — •Dean Korošak[1], Bruno Cvikl[1,2], Renata Jecl[1], Janja Kramer[1], and Anita Prapotnik Brdnik[1] — [1]University of Maribor, Faculty of Civil Engineering, Chair for Applied Physics, Smetanova 17, 2000 Maribor Slovenia — [2]J. Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

We present the application of fractional calculus in the analysis of the measured dielectric response of the clay-water system which exhibits anomalus features in its low frequency part.

The conductivity spectra for samples with higher water content are shown to collapse to a single master curve when appropriately rescaled. The frequency dependence of the conductivity is shown to follow the power-law with the exponent n=0,67 before reaching the frequency-independent part. It is argued that the observed conductivity dispersion is a consequence of the anomalously diffusing ions in the clay-water system. It is however a non-trivial task to determine the correct underlying diffusion process since different dynamic processes yield the same mean square time dependence as for instance do fractional Brownian motion and fractal time process. The fractional Langevin equation is used to describe the stochastic dynamics of the single ion connecting the power-law exponent of the observed conductivity dispersion to the order of the fractional derivative in the fractional Langevin equation.

[1] R. Hilfer, Phys. Rev. B vol 44, 1991, pp. 60-75.
[2] E. Lutz, Phys. Rev. E vol 64, 2001, 051106.

DY 46.65 Thu 16:00 P1

Dynamics of glass-forming liquids in soft confinement — •Maria Mayorova[1], Reiner Zorn[1], Dieter Richter[1], and Bernhard Frick[2] — [1]IFF, FZJ, Germany — [2]ILL, Grenoble, France

Effect of soft confinement (microemulsion) on the dynamics of viscous propylene glycol (PG) near its glass transition temperature is investigated.

To determine the size of PG core and its polydispersity measurements by neutron small-angle scattering were performed. The data were fitted by a model combining a Schultz distribution of spheres with a Percus-Yevick type structure factor. This fit displays an value of averaged PG core radius about 0,86 nm.

Elastic scans being obtained with a backscattering (BS) spectrometer reveal a temperature region of crystallization in case of confined PG (heating branch). An earlier onset of glass transition of confined PG could be detected from comparison of the mean square displacement for bulk and confined PG.

Fast dynamic processes (Boson peak (Bp)) were observed with time-of-flight (TOF) spectrometer. There is a clearly visible Bp in the case of bulk PG. For confined PG it is suppressed. As Bp for PG in hard confinement displays just opposite behavior, this suppression can be interpretated as a result of extremely small size of PG core or soft confinement. The data obtained on TOF and BS spectrometers have been combined by Fourier transform. The comparison of scattering function behavior for bulk and confined PG provides information that in the case of confined PG the α relaxation is more stretched.

DY 46.66 Thu 16:00 P1

Ordering of a 2D colloidal system in a 1D quasicrystalline potential — •Michael Schmiedeberg and Holger Stark — Universität Konstanz, Fachbereich Physik, D-78457 Konstanz

Using the Landau-Alexander-McTague theory, Das and Krishnamurthy proposed that quasicrystalline order can be induced in a two-dimensional charge-stabilized colloidal system by a one-dimensional optical lattice consisting of modulations with wave vectors $q_0\tau$ and q_0/τ. Here, τ is the number of the golden mean and q_0 is the position of the first peak in the direct correlation function of the colloidal system in the liquid phase [1]. Our Monte Carlo simulations, however, demonstrate that such a stable two-dimensional quasicrystalline ordering of the colloids does not exist. We only find stable solid phases of trigonal and rhombic symmetry. Using a more careful implementation of the Landau-Alexander-McTague theory, we calculate a complete phase diagram consistent with the results of our simulations. The system also exhibits a new mechanism of laser-induced melting that relaxes strain in the rhombic phase induced by the optical lattice. Therefore, we find laser-induced melting for all temperatures in contrast to the same phenomenon governed by fluctuations [2].

[1] C. Das and H.R. Krishnamurthy, Phys. Rev. B **58**, R5889 (1998)
[2] L. Radzihovsky, E. Frey, D.R. Nelson, Phys. Rev. E **63**, 031503 (2001)

DY 46.67 Thu 16:00 P1

Adsorption of random correlated copolymer: the Morita approximation — •Alexey Polotsky[1,2], Andreas Degenhard[1], and Friederike Schmid[1] — [1]Fakultät für Physik, Universität Bielefeld, Universitätsstraße 25, D-33615 Bielefeld, Germany — [2]Sérvice de Physique de l'Etat Condensé CEA Saclay, F-91191 Gif-sur-Yvette Cedex, France

A single ideal random copolymer chain with correlations in the monomer sequence, which adsorbs onto an impenetrable planar surface, is considered within a lattice model. The average over the quenched disorder is approximated by a constrained annealed approximation introduced by T. Morita in 1964 [1], whereas the sum over polymer conformations is carried out with the help of the generating function technique (in the grand canonical ensemble). With this combined approach, different conformational characteristics of the adsorbed chain are obtained. These calculations are also supplemented with direct numerical lattice computations averaged over many realisations of random sequence with the given statistics. The comparison of the results obtained in two different ways allows us to make a conclusion about the accuracy and applicability of the Morita approximation for the random copolymers with different degree of correlations and different types of nonadsorbing monomers (neutral or repelling from the surface).

[1] T. Morita. J. Math. Phys. **5**, 1401, (1964)

DY 46.68 Thu 16:00 P1

Shear-driven gelation in two dimensions — •Daniel Rings[1], Kajetan Bentele[2], and Klaus Kroy[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Vor dem Hospitaltore 1, D-04103 Leipzig — [2]Abteilung Theoretische Physik (SF5), Hahn-Meitner-Institut Berlin, Glienicker Str. 100, D-14109 Berlin

Cluster aggregation and gelation under shear flow are studied by off-lattice molecular dynamics simulation of a colloidal suspension. The two dimensional model of sticky hard disks includes rotations of the growing clusters induced by the constant shear rate of the solvent. We are studying the liquid-gel phase transition characterized by a jammed state of the system after a finite time depending on the particles' volume fraction. The fractal structure of the spanning cluster is analyzed and interpreted in terms of a crossover from kinetic aggregation to percolation theory.

Finite size effects in confined geometries are also considered.

DY 46.69 Thu 16:00 P1

Transport of Colloids in Micro-Channels — •Peter Henseler and Peter Nielaba — Department of Physics, University of Konstanz, D-78457 Konstanz

We carried out non-equilibrium computer simulations in order to investigate the transport of classical particles through channels of various configurations. The particles are driven by externally applied potential gradients. In the corresponding experiment [1] on superparamagnetic colloidal particles this is achieved by tilting the microchannel, so that the particles are driven by the gravitational field. Two different computational methods were used to match to the experimental situation: On the one hand we performed a Molecular Dynamics simulation in combination with a Nosé-Hoover thermostat and on the other hand we did a Langevin Dynamics simulation. Hydrodynamic interactions of the particles were neglected. We will present a comparison of simulation results of both methods and with the experiment on the occurring structures in dependence of the inclination, the strength of the pair interaction between particles and the channel geometry. We will also report on the flow behavior of the particles in the micro-channel.
[1] M. Köppl, A. Erbe and P. Leiderer, University of Konstanz, private communication

DY 46.70 Thu 16:00 P1

Like-charged rods at zero temperature — •Axel Arnold[1] and Christian Holm[2] — [1]FOM Institute for Atomic and Molecular Physics, Kruislaan 407, 1098 SJ Amsterdam, The Netherlands — [2]Frankfurt Institute for Advanced Studies, Max von Laue-Str. 1, D-60438 Frankfurt a. M.

It is well known that charged polymers can attract in the presences of multivalent counterions. This effect has been confirmed by a large number of computer simulations, and experiments have shown that DNA, a stiff, highly negatively charged polyelectrolyte, can be condensed by multivalent counterions. This correlation–induced attraction is for instance believed to be important for the compaction of DNA inside viral capsids. Here the DNA is idealized as an infinitely long, charged rod.

We investigate the attraction of like–charged rods in the presence of counterions using the strong coupling theory of R. Netz. We present results for the equilibrium distance of the rods at infinite counterion–coupling and the particle distribution. These results are in good agreement with numerical simulations. Our results show that the degree of agreement between the simulations at finite coupling and the theory can be characterized by a single parameter γ_{RB}.

In the case of zero temperature, one finds under certain circumstances flat configurations, in which all charges are located in the rod–rod plane. The energetically optimal configuration and its stability are determined analytically, which depends on only one parameter γ_z, similar to γ_{RB}. These findings are in good agreement with results from computer simulations.

DY 46.71 Thu 16:00 P1

Conductivity Measurements on Water in Oil Microemulsions — •Robert Wipf, Thomas Blochowiscz, Gustav Nyström, and Bernd Stühn — Institute of Condensed Matter Physics, Technical University Darmstadt, D-64289 Darmstadt

Water-in-oil microemulsions are thermodynamically stable mixtures of waterdroplets in a continuous oil phase. The water droplets are stabilized by a monomolecular surfactant layer. Surfactant molecules have a polar, hydrophilic headgroup and an apolar, lipophilic tail. The investigated microemulsion consists of water and decane with sodium bis(2-ethylhexyl)sulfosuccinate (AOT) as surfactant. Structure and dynamics of this system is well characterized by small-angle-X-ray and dynamic light scattering measurements. The conductivity of such systems shows a steep increase with volume fraction of droplets or temperature increasing over a certain critical value. This behavior can be attributed to a dynamic percolation phenomenon.[1]

Adding an amphiphilic triblock copolymer to a microemulsion leads to an interconnection of the droplets and thus to generation of a transient network. Here we will present our conductivity measurements on pure microemulsions and microemulsions containing polymer. We performed frequency and temperature dependent measurements in a range of $15°C$ to $35\circ C$ and 10^{-2}Hz to 10^{6}Hz respectively. First we characterized the percolation transition in pure microemulsions. Then we investigated the influence of increasing polymer content on the ion transport and relaxation in the microemulsion was investigated.
[1] H. Kataoka et al.: J. Phys. Chem. B 2003, 107, 12542-12548

DY 46.72 Thu 16:00 P1

Colloidal 2d-transport in restricted geometrie — •Michael Köppl , Artur Erbe, and Paul Leiderer — Universität Konstanz, FB Physik, Universitätsstr. 10, 78467 Konstanz

Colloidal particles can be used as model systems for the behavior of atomic or nanometer scale sized objects. Thermal energies of the particles in solution are of the same order of magnitudes as typical interparticle interactions. This leads to mesoscopic behavior. On the other hand, classical systems like cars on a motorway or pedestrians on a walkway can be modelled as well. In this work we study the transport of colloidal particles (4.7 μm in diameter) through narrow constrictions on the scale of $60 - 100$ μm. The behavior of these systems shows similarities to current transport in mesoscopic wires or electron transport on Helium surfaces. We create additional potential barriers by application of focused light fields (laser tweezing or repulsion of the particles by the light fields) on the particle ensemble. Transport through these barriers can be tuned by changing the interparticle interactions and the height of the potential barriers. We typically use superparamagnetic particles in our experiments. Thus the interactions between the particles depend quadratically on an externally applied magnetic field for low fields. An increase in magnetic field leads to a change form a liquid phase to a crystalline phase. The influence of this change on the transport behavior of the system is studied in detail.

DY 46.73 Thu 16:00 P1

Relaxation dynamics of gelling polymers — •Alice von der Heydt[1], Henning Löwe[2], Peter Müller[1,3], and Annette Zippelius[1] — [1]Institut f. Theoretische Physik, Universität Göttingen, Germany — [2]Eidgen. Institut f. Schnee- und Lawinenforschung SLF, Davos, Switzerland — [3]Fakultät f. Mathematik, Universität Bielefeld, Germany

Frequency-dependent dielectric relaxation of a gelling macromolecular liquid was investigated within Rouse dynamics for a macroscopic model network with quenched disorder: random permanent *polar* crosslinks of concentration c were drawn from a bond percolation ensemble. Disorder-averages with respect to the ensemble of crosslinks and uncorrelated dipole orientations yield the generic dielectric susceptibility $\chi_c(\omega)$ in terms of the ensemble-averaged density of eigenvalues $D_c(\gamma)$ or the resolvent of the network's connectivity matrix Γ. When approaching the c-driven sol-gel transition at the critical concentration $c_{\rm crit}$, the growing impact of small relaxation rates is clearly visible in $\chi_c(\omega)$: A crossover in the low-frequency domain from asymptotic Debye behavior at small c to e.g. a cusp for $\mathrm{Re}\,\chi_c(\omega)$ at $\omega = 0$ and criticality can be deduced from the known scaling of $D_c(\gamma)$. For a mean field ensemble, the critical change in the exponents is confirmed by an approach which does not assume scaling. In this case the frequency dependence can be obtained via the resolvent of Γ by numerically solving an exact integral equation which arises in the replica formulation of the disorder average [1].

[1] K. Broderix, T. Aspelmeier, A. K. Hartmann and A. Zippelius, Phys. Rev. E **64** (2001), 021404

DY 46.74 Thu 16:00 P1

Computer Simulation of Stochastic Dynamics in Hard-Sphere Systems — •Thomas Voigtmann[1], Cristiano De Michele[2], and Antonio Scala[2] — [1]University of Edinburgh, U.K. — [2]Universita di Roma "La Sapienza", Italy

The hard-sphere system, and derived systems like the square-well system (hard spheres with added square-well attraction) are useful models for understanding the dynamics of soft condensed matter. There, one is interested in their stochastic dynamics, i.e. the many-body Langevin equation with step-wise discontinuous pair potentials. Computer simulation (called Stochastic Dynamics, or Brownian Dynamics in the limit of vanishing inertial terms) is a helpful tool to gain insight here. But conventional algorithms are restricted to smooth potentials, where one can discretize the equations using some small time step. Hard spheres, on the other hand, need to be simulated with an event-driven algorithm; but this method does not work a priori for Brownian dynamics. Monte-Carlo-inspired schemes exist, but they have potential problems arising from the occurence of overlapping particles. We discuss a method to implement Brownian Dynamics and Stochastic Dynamics in hard spheres based on an event-driven algorithm. The accuracy of this method is assessed, and we discuss extensions to square-well systems and external forces, that are not easily achieved with previous methods.

DY 46.75 Thu 16:00 P1

Application of new chain growth algorithms for lattice polymers — •Thomas Vogel, Michael Bachmann, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11, 04109 Leipzig

We apply recently developed enhancements of the Pruned Enriched Rosenbluth Method (PERM) [1], namely the Multicanonical Chain-Growth Algorithm [2] and the Flat Histogram Method [3], to polymers and peptides on lattices.

The multicanonical version is based on the idea to sample temperature-independently the complete energy space of polymer conformations. It enables, for example, the determination of the density of states within one simulation run for hydrophobic-polar (HP) proteins.

The flat histogram version follows a similar strategy from a micro-canonical view of the problem and was used so far for studies of long interacting self-avoiding walks (ISAWs).

We apply both algorithms to interacting self-avoiding walks as well as to HP proteins to compare the behaviour of the two versions and, of course, to get new results for statistical properties of polymers and peptides.

[1] P. Grassberger, Phys. Rev. E **56** (1997) 3682.
[2] M. Bachmann and W. Janke, Phys. Rev. Lett. **91** (2003) 208105.
[3] T. Prellberg and J. Krawczyk, Phys. Rev. Lett. **92** (2004) 120602.

DY 46.76 Thu 16:00 P1

Comparing Thermodynamics of the AB Protein Model in Monte Carlo and Molecular Dynamics Simulations — •Jakob Schluttig, Michael Bachmann, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11, 04109 Leipzig, Germany

There are two big classes of computer simulations, which are extensively employed to study protein folding: Monte Carlo and Molecular Dynamics simulations. However, it is not clear whether the results of these different types of simulations are really comparable, since the dynamics of the employed algorithms is significantly different. Unlike Monte Carlo, Molecular Dynamics in its simplest form leaves the total energy of a system constant. Therefore, the concept of temperature has to be introduced by thermostat algorithms, which extend the simulation to the canonical ensemble. Over the years, a variety of such thermostat methods has been developed, as well as sophisticated improvements of the original Monte Carlo Metropolis techniques. In this work, the outcome of carefully adjusted Molecular Dynamics and Monte Carlo simulations is thoroughly compared for a simple coarse-grained hydrophobic-polar heteropolymer model and the statistical significance is verified.

DY 46.77 Thu 16:00 P1

Folding Channels for Coarse-grained Heteropolymer Models — •Stefan Schnabel, Michael Bachmann, and Wolfhard Janke — Institut für Theoretische Physik Universität Leipzig Augustusplatz 10/11 04109 Leipzig

Applying multicanonical simulations we investigated off-lattice heteropolymers by using versions of the AB model [1,2], being off-lattice models for heteropolymers. The heteropolymers consist of hydrophobic (A) and hydrophilic (B) monomers. Their energy is obtained from specific Lennard-Jones potentials between nonbonded pairs of these monomers in addition to the chain's bending and torsional energy. In particular, AA contacts are favored to allow the formation of a hydrophobic core. Beside the investigation of the heteropolymer's thermodynamical quantities like heat capacity and radius of gyration we study the folding channels in the free-energy landscape by comparing the equilibrium conformations with the folded state in terms of a structural overlap parameter [3]. The investigations of the state-space shapes show a great variety according to different monomer sequences.

[1] F. H. Stillinger, T. Head-Gordon, and C. L. Hirshfeld, Phys. Rev. E 48, 1469 (1993).
[2] A. Irbäck, C. Peterson, F. Potthast, and O. Sommelius, J. Chem. Phys. 107, 273 (1997).
[3] M. Bachmann, H. Arkın, and W. Janke, Phys. Rev. E 71, 31906 (2005).

DY 46.78 Thu 16:00 P1

A simple spin model for investigating molecular recognition — •Hans Behringer, Andreas Degenhard, and Friederike Schmid — Fakultät für Physik, Universität Bielefeld, D-33615 Bielefeld

Biological systems such as the immune system rely on the ability of biomolecules to specifically recognise each other. Molecular recognition can be viewed as the ability of a biomolecule to interact preferentially with a particular target molecule among a vast variety of different but chemically similar rival molecules. In this talk equilibrium aspects of molecular recognition are investigated using simple spin models for the recognition process of two rigid biomolecules consisting of different types of subunits. To this end, a two-stage approach is adopted. First the structure of the target molecule is fixed and learned by a probe molecule. This design step, which might be considered to mimic natural evolution, results in an ensemble of probe sequences. In a second step the recognition ability of the designed probe ensemble with respect to the chosen target sequence is tested by comparing the free energy of association with the previously fixed target structure and a different competing structure. Particular attention is paid to the appearance of mis-recognitions, and to the effect of additional constraints in the design step on the recognition ability of the designed probe ensemble. In addition, the influence of cooperative effects accompanying the association of the target biomolecule and the probe molecules is investigated.

DY 46.79 Thu 16:00 P1

Age-Dependence of Correlations and Quasi-Periodicities in Heart Rate and Respiration during Sleep — •Aicko Yves Schumann[1], Jan W. Kantelhardt[1], and Thomas Penzel[2] — [1]Fachbereich Physik und Zentrum für Computational Nanoscience, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — [2]Klinikum für Innere Medizin, Klinikum der Universität Marburg, 35033 Marburg (Lahn)

In order to characterize the autonomic regulation in the human cardiovascular system we employ Detrended Fluctuation Analysis (DFA) and Phase Rectified Signal Averaging (PRSA). We study the age and sex dependence of the scaling behaviour of ECG (heartbeat intervals) and respiration (inspiration and expiration intervals) from 116 healty subjects during sleep. Sleep minimizes physical and mental disturbances which camouflage the intrinsic autonomous variabilities of interrest. Since sleep itself is not homogeneous we distinguish between REM and non-REM (light and deep) sleep stages and investigate their interrelation with ECG and respiration by comparing long-term correlations and additional quasi-periodicities. The results might be used to detect sleep stages based on ECG and respiration instead of more complicated brain recordings or to identify anomalous autonomic regulation in patients.

DY 46.80 Thu 16:00 P1

Formation of species diversity due to self-organized criticality — •K. Morawetz[1,2], N. Amecke[1], R. Radünz[1], M. Döring[1], and M. Schreiber[1] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

The occurrence of species diversity due to a change in environmental conditions is simulated by a slight modification of the Bak-Sneppen model. We find that the forced separation of individuals leads to a separation of mutation probabilities and consequently to a bifurcation of the specie.

DY 46.81 Thu 16:00 P1

Thermodynamics and Folding Kinetics of Coarse-Grained Protein Models — •Anna Kallias, Wolfhard Janke, and Michael Bachmann — Institut für Theoretische Physik, Universität Leipzig

We investigate three-dimensional off-lattice, coarse-grained models for proteins. Different interactions between monomers lead to three different formulations, the AB [1], the GAB and a Gō-like model. Contact maps give information on the structure of ground states, which have been found using the ELP algorithm introduced in Ref. [2]. Secondary structure patterns known from real proteins can be recognised. Parallel tempering Metropolis simulations are used for thermodynamic investigations. For example conformational transitions and free energy landscapes of the different models are compared. The free-energy landscapes are measured as functions of the overlap with the native state using different overlap definitions. The coarse-grained variant of the Gō model is found to behave similarly to its standard all-atom formulation. Folding and unfolding kinetics are investigated including the visualisation of single folding processes as well as measurements of the average folding behaviour, as for example Chevron plots.

[1] F. A. Stillinger and T. Head-Gordon, Phys. Rev. E **52**,3, 1995.
[2] U. H. E. Hansmann and L. T. Wille, Phys. Rev. Lett. **88**,6, 2002.

DY 46.82 Thu 16:00 P1

Signal Detection in Comodulated Noise — •Michael Buschermöhle, Ulrike Feudel, Jesko L. Verhey, and Jan A. Freund — Carl-von-Ossietzky Universität Oldenburg

Many natural sounds share the property of having common amplitude modulations across different frequency regions. Examples of these kinds of sounds are the masking noises used for experiments concerning comodulation detection differences (CDD) and comodulation masking release (CMR). Typical stimuli for these experiments consist of one or more masking noise bands and a signal that is either a pure tone or a noise band as well. Previous research in humans and other vertebrates has shown that in CDD and CMR experiments signal detection thresholds vary depending on the correlation structure of the envelopes of the constituting noise bands. We propose a simple model that is capable of reproducing important features of psychophysical signal detection thresholds in response to CDD and CMR stimuli. The model is based solely on peripheral processing and has the following stages: frequency filtering, envelope extraction, compression, and computation of the temporal average. Signal detection is realized by registering changes in the mean compressed envelope of the filtered stimulus. Many aspects of CMR and CDD can be accounted for by this largely analytically tractable model.

DY 46.83 Thu 16:00 P1

ON NUCLEATION-AND-GROWTH STRATEGIES IN MODEL BIOPOLYMER SYSTEMS — •NATALIA KRUSZEWSKA and ADAM GADOMSKI — U.T.A. BYDGOSZCZ, INST. MATHS & PHYS., AL. KALISKIEGO 7, PL-85796 BYDGOSZCZ

We are dealing with nucleation-and-growth strategies based on the self-avoiding random walk (SARW). We investigate some below mentioned dynamic effects by means of a Monte Carlo simulation in a discrete two-dimensional space, using periodic boundary conditions. The dynamics is set up by the well-known HP model.
The effects of interest are the following:
(i) estimation of the optimal number of SARW monomers forming a stable nucleus; (ii) influence of inter- vs intra-chain effects on the formation of the stable nucleus; (iii) role of (optimal) temperature in the formations of nuclei; (iv) observation on how does the excluded-volume effect propagate through both nucleation and growth stages of the process
[1] J. Łuczka et al.: Phys. Rev. E **51**, 5762 (1995).

The growth stages will be examined while the optimal nuclei formed are at some fixed as well as variable positions. As a consequence, either a network of SARWs or a cluster-cluster assemblage will be formed.
The strategies revealed by realization of points (i)-(iv) above, can lead to better understanding of soft-matter aggregations such as biopolymer or colloid
[2] A. Gadomski et al.: Chem. Phys. **310**, 153 (2005).

DY 46.84 Thu 16:00 P1

Statistical Studies of Complex Systems: A Random Matrix Approach — •Pragya Shukla — Department of PHysics, IIT Kharagpur-721302, West Bengal, India

In general, the physical systems are quite complex in nature. Our approximate knowledge of the complicated interactions in these systems manifests itself by a randomization of various generators of the dynamics. The operators associated with wave dynamics e.g Hamiltonian, electromagnetic waves in a microwave cavity, or signals in a brain can therefore be modeled by random matrices.

The choice of a suitable random matrix model of a complex system is very sensitive to the nature of its complexity. The statistical analysis of various complex systems requires, therefore, a thorough probing of a wide range of random matrix ensembles which is not an easy task. It is highly desirable, if possible, to identify a common mathematcal structure among all the ensembles and analyze it to gain information about the ensemble-properties. Our successful search in this direction leads to Dyson's Brownian motion model as the common base. This also reveals the deep level of universality hidden underneath the world of complex sysetms.

DY 46.85 Thu 16:00 P1

CONTINUOUS TIME QUANTUM WALKS ON TWO-DIMENSIONAL NETWORKS — •Antonio Volta, Oliver Mülken, and Alexander Blumen — Theoretische Polymerphysik, Universität Freiburg, Hermann Herder Straße 3, 79104 Freiburg, Germany

We present a description of the quantum mechanical transport by continuous time quantum walks (CTQWs) on networks topologically equivalent to two-dimensional lattices. The quantum transport topic increased recently its importance because of the development of quantum information theory and the application to potential quantum computers. We provide results for CTQW on discrete tori, cylinders and finite squares. The propagation is described by the Schrödinger equation. In the case of finite square lattices, by placing at time t=0 the excitation in one corner, one observes a very fast transport to the opposite one via the diagonal. The long time average of the transition probability distribution shows, for some special lattice sizes, asymmetric features. We also pay attention to the probability to be still or again at the initial site. We provide, for the quantum mechanical case, a lower bound which for some geometries is rather close to the exact, numerical result. The lower bound depends only on the eigenvalue spectrum of the Hamiltonian, which can be obtained analytically for our structures, by applying methods from solid state and polymer physics.
[1] O. Mülken, A. Volta, A. Blumen, Phys. Rev. A 72 (2005) 042334

DY 46.86 Thu 16:00 P1

The influence of different updating methods on the dynamics of Kauffman networks — •Florian Greil and Barbara Drossel — Institut für Festkörperphysik, Technische Universität Darmstadt

We consider the influence of different updating schemes on the dynamics of random Boolean networks. The standard synchronous updating rule, which is usually chosen, is compared with stochastic and deterministic asynchronous rules. For the asynchronous stochastic update and certain types of asynchronous deterministic update, the number of attractors in a critical Boolean network grows like a power law with the system size. The mean size of the attractors increases as a stretched exponential. This is in strong contrast to the synchronous case.

DY 46.87 Thu 16:00 P1

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

Boolean networks with canalizing functions are used to model gene regulatory networks. In order to understand how such structures could have evolved, we simulate evolution of a boolean network with canalizing functions, where mutations change the connections and the functions of the nodes. One fitness criterion is for example the robustness of the network against small perturbations. We explore the fitness landscape of these systems by performing an adaptive walk and we keep track of changes in attractor length and of the occurring mutations.

DY 46.88 Thu 16:00 P1

Optical Localization in Networks with High Clustering — •Jan W. Kantelhardt[1], Richard Berkovits[2], and Shlomo Havlin[2] — [1]Fachbereich Physik und Zentrum für Computational Nanoscience, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — [2]Minerva Center and Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel

We study quantum localization-delocalization phase transitions in complex optical fiber networks with different topology, characterized by homogeneous and scale-free degree distributions and different levels of clustering (frequency of triadic closure). We find that strong clustering induces a transition to a localized optical phase similar to the Anderson transition induced by disorder in electronic quantum systems and determine the corresponding phase diagramms. Clustering in complex networks represents an additional degree of freedom that is comparable with dimensionality in lattices.

DY 46.89 Thu 16:00 P1

Scaling in critical random Boolean networks with different connectivity and different choice of update functions — •Tamara Mihaljev, Barbara Drossel, and Viktor Kaufman — Institut für Festkörperphysik, Technische Universität Darmstadt

The Kauffman model describes a system of randomly connected nodes with dynamics based on Boolean update functions. Though it is a simple model, it exhibits very complex behaviour for "critical" parameter values at the boundary between a frozen and a disordered phase, and is therefore used for studies of real network problems. We consider here the general class of critical Kauffman networks with different number of inputs per node and different distributions of Boolean functions. By defining and analyzing two different stochastic processes we derive mostly analytically

the scaling behaviour of the number of nonfrozen and relevant nodes in these networks in the thermodynamic limit. Our results show that only a finite number of relevant nodes have more than one relevant input. It follows that for every class of critical Kauffman networks all relevant components apart from a finite number are simple loops and that the mean number and length of attractors increases faster than any power law with network size.

DY 46.90 Thu 16:00 P1

Stability of attractors under noisy delays in Boolean networks — •Konstantin Klemm[1] and Stefan Bornholdt[2] — [1]Dept. of Bioinformatics, University of Leipzig, Germany — [2]Institute for Theoretical Physics, University of Bremen, Germany

Boolean networks at the critical point have been discussed for many years as, e.g., scaling of number of attractors with system size. Recently it was found that this number scales superpolynomially with system size, contrary to a common earlier expectation of sublinear scaling. We here point out that these results are obtained using deterministic synchronous update, which limits their significance for biological systems where noise is omnipresent.

We check the stability of the attractors when the assumption of synchronous update is relaxed. The synchrony in the model is perturbed by slightly accelerating or decelerating the update of a subset of units. This set of perturbations is motivated by the noisy delay time with which a biological switch responds to a changing input. An attractor is called stable if after any such perturbation synchrony is regained. In random Boolean networks at the critical point, the number of stable attractors grows sublinearly with increasing system size [1]. Thus in large systems almost all attractors considered earlier are artefacts arising from the synchronous clocking mode.

[1] K. Klemm and S. Bornholdt, Phys. Rev. E (R), in press (2005), e-print cond-mat/0411102

DY 46.91 Thu 16:00 P1

Spin glass models with Lévy-distributed couplings — •Steffen Hohn and Andreas Engel — Carl-von-Ossietzky Universität, 26111 Oldenburg, Germany

A mean-field model for spin glasses is studied in which the distribution of coupling strengths has long tails, $P(J) \sim 1/|J|^{(1+\alpha)}$ for large $|J|$. The transition temperature T_c to the spin glass phase and the temperature T_{AT} signalling the breakdown of replica symmetry are determined numerically for various values of α using finite size scaling. Moreover the distribution of local magnetic fields for temperatures between T_c and T_{AT} is determined. The results are checked against a novel application of the replica trick to these systems.

DY 46.92 Thu 16:00 P1

Gas Flow through Nanopores: An Access to Gas Transport at Huge Knudsen Numbers — •Simon Grüner, Klaus Knorr, and Patrick Huber — Technische Physik, Universität des Saarlandes, 66123 Saarbrücken, Germany

We present helium gas flow experiments on a silicon membrane which is permeated by a bundle of parallel, tubular channels of 10 nanometer diameter. Such a membrane geometry allows us to study gas flows for Knudsen numbers, Kn, over four orders of magnitude, from 1-10000 (Kn refers to the ratio of the mean free path to the tube diameter). Already at Kn approx 0.1 a breakdown of continuum-like behavior is expected and, indeed, the helium flow in our system disagrees with the Hagen-Poiseuille prediction. In fact, our observations rather indicate a Knudsen diffusion-like gas transport.

DY 46.93 Thu 16:00 P1

Rupture dynamics of thin liquid films — •Frank Müller and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg; Institut für Experimentelle Physik

Thin liquid films show a characteristic rupture dynamics. After the equilibriumshape is appropriately disturbed (e.g. by piercing), a hole grows with edges propagating driven by the surface tension of the liquid. The dynamics of such films was first described by Rayleigh in the early 20$^{\text{th}}$ century. Corresponding experiments have been reported on plane soap films and catenoids (e.g. Ranz et al. 1959 and Cryer et al. 1992). It was found that the velocity of the edge of the hole differs with approximately 10 % from values calculated by Rayleigh, who disregarded dissipation. We study the dynamics of smectic liquid crystal films with particular focus on catenoid shaped films. A high-speed camera (more than 10.000 fps) is used for the recording of the rupture process.

DY 46.94 Thu 16:00 P1

Particle accumulation in laminar flow — •Michael Schindler, Marcin Kostur, Peter Talkner, and Peter Hänggi — Institut für Physik, Universität Augsburg

For most applications of microfluidic flows the transport properties of immersed particles are of decisive relevance. Small particles moving in flow fields with small velocity gradients can be described as point-like. They undergo an advective motion superimposed by Brownian motion, which finally leads to a uniform particle distribution. Non-uniformity may only result from the finite extension of the particles.

We will discuss two effects leading to particle accumulation. In the first case the boundary leads to a non-uniform distribution of small spherical particles. The second mechanism is based on the coupling of translational and rotational motion for asymmetric objects and may lead to a spatial separation of chiral particles in conveniently chosen flow fields.

[1] Z. Guttenberg *et al.*, *Flow profiling of a surface acoustic wave nanopump*, Phys. Rev. E **70**, 056311 (2004)
[2] M. Kostur, M. Schindler, P. Talkner and P. Hänggi, *Chiral separation in microflows*, (submitted)

DY 46.95 Thu 16:00 P1

Statistical properties of a point vortex model for twodimensional turbulence — •Oliver Kamps and Rudolf Friedrich — Institute of Theoretical Physics, Wilhelm-Klemm-Str. 9 48149 Münster

Starting from a point-vortex description of a forced twodimensional flow we investigate the statistical properties of the lagrangian and eulerian fluid dynamics. In our numerical investigations we focus on the probability distribution functions for the velocity increments of the vortex particles. We compare the results with direct numerical simulations of the two dimensional Navier-Stokes equation.

DY 46.96 Thu 16:00 P1

A Truncated System for Taylor-Couette Flow in Finite Gaps — •Hans-Reinhard Berger — Technische Universität, Institut für Physik, D-09107 Chemnitz

The Taylor-Couette flow of viscous fluids is examined by a low-dimensional truncated expansion using trigonometric functions. The influence of gap width between the cylinders is included up to second order in the gap width. By comparing the results for the critical Taylor number obtained from the series expansion with numerical results from linear stability calculation of the original hydrodynamic equations, the truncation is validated with an error of less than two percent. It is found that increasing gap width has a stabilizing influence on the laminar flow compared with results of the small-gap approximation. The results of the stability analysis of the truncated system of ordinary differential equations describe well the transition from laminar to Taylor-vortex flow, but no further bifurcations to more complex flows are found. The reason for this behaviour is assumed to be due to the omission of non-axisymmetric disturbances.

DY 46.97 Thu 16:00 P1

Statistical properties of Lagrangian particles in vortical structures — •M. Wilczek and R. Friedrich — Institut für Theoretische Physik, Wilhelm-Klemm-Str. 10, 48149 Münster

It is well known that turbulent velocity fields contain coherent structures. A common assumption is that intermittency in the velocity signal is caused by these structures.

Therefore it is interesting to examine the evolution of a single Lagrangian particle in a random sequence of coherent vortices. For the special case of a sequence of Burgers vortices we obtain statistical properties, e.g. probability density functions for the velocity increments.

DY 46.98 Thu 16:00 P1

Wetting Transitions at the Free Surface of Binary Liquids studied by Faraday Waves — •Stephan Gier[1,2], Andriy Kityk[3], Christian Wagner[1], and Patrick Huber[2] — [1]Experimentalphysik, Universität des Saarlandes, D-66041 Saarbrücken — [2]Technische Physik, Universität des Saarlandes, D-66041 Saarbrücken — [3]Institute for Computer Science, Technical University of Czestochowa, PL-42200 Czestochowa

We present measurements on standing surface waves at the free surface of two binary liquids (pentane/water and methanol/cyclohexane) as a function of temperature, T, and molar fraction, x, of one component.

The critical acceleration, a_c and the wave number, k_c, for surface waves exhibit distinct changes upon variation of T and x that can be related to surface wetting transitions. Thus we demonstrate that Faraday surface waves allow visualizing and examining on a *macroscopic* scale rheological changes triggered by modifications of the *microscopic* surface structure of liquids.

DY 46.99 Thu 16:00 P1

Time-Delayed Feedback Control of Stochastic Growth Equations — •Michael Block and Eckehard Schöll — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

Various growth phenoma in general, and especially crystal growth, can be described by continuous stochastic differential equations. Utilizing a forward-backward Euler algorithm we solve various growth equations in 1+1 and 2+1 dimensions. The focus is on the exponents describing the time-evolution of a surface: the growth exponent, the roughness exponent and the dynamic exponent, where only two of those are independent. We apply two different time-delayed feedback control methods to the stochastic growth equations with the aim of controlling the surface roughness. Different coupling schemes of the control force are investigated and compared. In particular, we propose a digital control scheme and a differential control scheme, where the difference between the desired growth exponent and the actual local growth exponent enters into the control force in a digital or differential way, respectively. These schemes are applied to the Kardar-Parisi-Zhang equation and the so called MBE (Molecular Beam Epitaxy) equation. It is shown that the growth exponent β, and thus the temporal evolution of the rms surface roughness, can be adjusted within certain ranges. Limitations of those control schemes are investigated in detail.

DY 46.100 Thu 16:00 P1

Distribution of extremes in the fluctuations of two-dimensional equilibrium interfaces — •Deok-Sun Lee — Theoretische Physik, Universität des Saarlandes,* 66041 Saarbrücken, Germany

We investigate the statistics of the maximal fluctuation of two-dimensional Gaussian interfaces. Its relation to the entropic repulsion between rigid walls and a confined interface is used to derive the average maximal fluctuation $\langle m \rangle \sim \sqrt{2/(\pi K)}\,\ln N$ and the asymptotic behavior of the whole distribution $P(m) \sim N^2\, e^{-(\text{const})\, N^2 e^{-\sqrt{2\pi K}\, m} - \sqrt{2\pi K}\, m}$ for m finite with N^2 and K the interface size and tension, respectively. The standardized form of $P(m)$ does not depend on N or K, but shows a good agreement with Gumbel's first asymptote distribution with a particular non-integer parameter. The effects of the correlations among individual fluctuations on the extreme value statistics are discussed in our findings.

DY 46.101 Thu 16:00 P1

Simulation of heteroepitaxial growth and surface alloy formation — •Sebastian Weber[1], Michael Biehl[2], Thorsten Volkmann[1], and Miroslav Kotrla[3] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg — [2]Institute for Mathematics and Computing Science, University of Groningen, P.O. Box 800, NL-9700 AV Groningen — [3]Institute of Physics, Academy of Sciences of the Czech Republic, Prague

We study the hetero-epitaxial growth of an fcc(111) crystal surface, in which the lattice spacing of adsorbate materials differ from that of the substrate. We employ off-lattice equilibrium and kinetic Monte Carlo simulations based on simple model interactions with a Lennard Jones pair potential between the particle species. Emphasis is on the formation of monolayers of binary adsorbates with a nontrivial composition profile. One important aspect is the formation of nano-structured surface alloys and the dependence on growth temperature and lattice mismatch.

DY 46.102 Thu 16:00 P1

Simulation of heteroepitaxial growth and misfit dislocations — •Markus Walther[1], Michael Biehl[2], Florian Much[1], and Christian Vey[1] — [1]Institut für Theoretische Physik und Astrophysik, Sonderforschungsbereich 410, Universität Würzburg, Am Hubland, D-97074 Würzburg — [2]Institute for Mathematics and Computing Science, University of Groningen, P.O. Box 800, NL-9700 AV Groningen

The atomistic simulation of strain effects in heteroepitaxial systems requires the development of off-lattice models which allow for continuous positions of the particles. We present the results of Kinetic Monte Carlo simulations of heteroepitaxial growth where the particle interactions are described by simple pair-potentials, e.g. Lennard-Jones potential in (1+1) dimensions. The lattice spacing of adsorbate materials differs from that of the substrate. The misfit induces compressive or tensile strain in the initial pseudomorphic film, resulting in the appearance of misfit dislocations in thick films and for large misfits that also affect the subsequent growth. For small misfits the adsorbate aggregates in three dimensional structures upon a pseudomorphic wetting layer in the so-called Stranski Krastanov growth mode.

DY 46.103 Thu 16:00 P1

KMC simulations of thermally sintering nano-clusters in 3D — •Martin Fendrich, Ruslan Zinetullin, Frank Westerhoff, and Dietrich E. Wolf — Institut der Physik, Universität Duisburg-Essen, Campus Duisburg, Germany

A C++ code is developed in order to simulate the thermal sintering process of nano-particles using the kinetic Monte-Carlo method (KMC). For the sintering time of two different sized particles we obtained the power law $\tau \propto R^4$ with the reduced radius $(R_1^{-1} + R_2^{-1})^{-1}$, which means that the relaxation time is dominated by the smaller particle. We proved the existence of a capillary instability of crystalline nano-wires having a length-to-width ratio of 8.8 of the resulting fragments. The time needed for separation of the wires turned out to be $\propto R^{4\pm0.2}$. By letting two independent fcc-lattices interpenetrate each other and allowing atoms to exchange between them, a grain boundary is modeled. We developed a hybrid simulation scheme combining the atomistic KMC method with a numerical integration of the equations of motion for two particles in contact. The qualitative sintering process may be divided into two stages. A fast reorientation of the grains takes place leading to special classes of mutual torsions with misorientation angles between 0 and $\approx 80°$. These classes can be understood in terms of a coherent site lattice analysis. This is followed by a long coalescence stage.

DY 46.104 Thu 16:00 P1

Computer Simulation of Binary Crystal Growth from Solution — •Felix Kalischewski and Andreas Heuer — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität, 48149 Münster

We investigate the interface dynamics and equilibrium properties governing epitaxial growth of binary crystals from solution.

First, we focus on jump rates of single particles between characteristic sites by means of a lattice-free Monte-Carlo model using the Lennard-Jones (12,6)-potential. Relatively fast transitions (e.g. surface-diffusion) can be analyzed by direct "observation". Rates of rather slow processes (e.g. ad/desorption, step-diffusion) are determined based on the free energy of their path in an Eyring-like fashion.

The exploration of equilibrium properties requires larger systems, thus a faster hdp/fcc-lattice simulation employing nearest-neighbor interactions is applied. We specifically investigate the combined solubility of the end-members depending on the crystal composition. We observe a behavior in general agreement with the Lippmann-diagrams. Deviations from the ideal solid solution are discussed.

These results provide the microscopic basis for models describing oscillatory zoning in binary solid solutions.

DY 46.105 Thu 16:00 P1

Ripple formation under shearing — •C.A. Krülle[1], A. Wierschem[2], N. Aksel[2], and I. Rehberg[1] — [1]Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth — [2]Technische Mechanik und Strömungsmechanik, Universität Bayreuth, D-95440 Bayreuth

Our understanding of the formation of ripples and dunes in the desert or at the beach can be regarded as a paradigm for a nonequilibrium process which can be treated with modern methods of nonlinear dynamics and structure formation. The main goals of our interdisciplinary project, which combines methods and expertises of fluid mechanics and experimental physics, are (i) the detailed experimental investigation of the complex interactions between the driving fluid and the granular bed, (ii) to clarify the question, whether turbulent currents are necessary for ripple formation, and (iii) the validation of continuum models with our experimental data.

DY 46.106 Thu 16:00 P1

Optimized computer algorithm for the simulation of densely packed spheres with arbitrary size distribution — •Antje Elsner[1,2], Helmut Hermann[1], and Dietrich Stoyan[2] — [1]Institute for Solid State and Materials research, IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Institute of Stochastics, Freiberg University of Mining and Technology, D-09596 Freiberg, Germany

Random dense packed spheres are a widely applicable model to simulate structures. There are different approaches to get dense packed systems. One of them is the so called force biased algorithm. A system of spheres is densified by stepwise rearrangement of sphere centres and recalculation of diameters. Some ways to optimize this algorithm are explained, especially the optimization of the virtual interaction forces between spheres during the packing process. It is demonstrated how systems with arbitrary size distributions can be optimized under different constraints.

DY 46.107 Thu 16:00 P1

Quantum paste: a model granulate wetted by superfluid Helium — •Masoud Sohaili and Stephan Herminghaus — MPI for Dynamics and Self-Organization, Bunsenstr. 10, D-37073 Göttingen, Germany

The dynamic properties of a dry granulate change dramatically upon addition of liquid, due to the formation of capillary bridges between mutually adjacent grains in the pile. The relative contribution of the surface tension and the viscosity of the liquid to this effect is still unclear. We have therefore set up an experiment to observe fluidization of a model granulate which is wetted by liquid Helium. The latter looses its classical viscosity at the superfluid transition temperature of 2.17 K. By comparing its properties above and below this temperature, it is possible to extract the effect of viscosity upon the dynamic properties of the granular pile.

DY 46.108 Thu 16:00 P1

Unclustering transition in wet granular matter — •Axel Fingerle and Stephan Herminghaus — MPI for Dynamics and Self-Organization, Bunsenstr. 10, 37073 Göttingen, Germnay

In earlier studies of free cooling of dry granular matter in one dimension, the aggregation of mass in clusters was found to be a monotonic process in time. We demonstrate analytically and by extensive simulations that the clustering of dense *wet* granular matter is not monotone but undergoes a sharp unclustering transition. We put forward a mean field theory for wet granular matter far from thermal equilibrium using the Minimal Capillary Model [S. Herminghaus, *Adv. Phys.*, **54**, 221 (2005)] and point out that wet granular matter belongs to the class of dissipative piecewise Hamiltonian systems, which is discussed in the context of recent fluctuation theorems.

DY 46.109 Thu 16:00 P1

Liquid Bridges in Wet Granular Systems: Networks and Clusters — •Mario Scheel, Stephan Herminghaus, and Ralf Seemann — MPI for Dynamics and Self-Organization, Bunsenstr. 10, D-37073 Göttingen, Germany

The properties of a dry granulate change dramatically when small amounts of liquid are added. This is due to capillary bridges forming between mutually adjacent grains in the pile, which exert an attractive force by virtue of the surface tension of the liquid. As more liquid is added, the liquid forms clusters, and the stability of the pile is reduced. Although the tensile strength of wet granulates can be roughly estimated from the capillary forces, a quantitative theory of the mechanical properties of granulate requires a detailed understanding of the topology of the complex network of capillary bridges and clusters. We have determined the macroscopic properties of model granulates with vertical agitation experiments, and the microscopic geometry of the distribution of liquid via x-ray microtomography. Transitions from capillary bridges to clusters as well as percolation can be clearly identified.

DY 46.110 Thu 16:00 P1

Switching via quantum activation: a parametrically modulated oscillator — •Michael Marthaler[1] and Mark Dykman[2] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe, Germany — [2]Michigan State University, Department of Physics and Astronomy, East Lansing, MI 48824, USA

We study switching between period-two states of an underdamped quantum oscillator modulated at nearly twice its natural frequency. For all temperatures and parameter values switching is determined by diffusion over oscillator quasienergy, provided the relaxation rate exceeds the rate of interstate tunneling. The diffusion has quantum origin and accompanies relaxation to the stable state. We find the semiclassical distribution over quasienergy. For $T = 0$, where the system has detailed balance, this distribution differs from the distribution for $T \to 0$; the $T = 0$ distribution is also destroyed by small dephasing of the oscillator. The characteristic quantum activation energy of switching displays a characteristic dependence on temperature and scaling behavior near the bifurcation point where period doubling occurs.

DY 46.111 Thu 16:00 P1

Clusters of oriented dipolar particles under shear. — •Stefan Fruhner and Siegfried Hess — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Germany

A fluid of oriented dipolar colloidal particles is considered as realized either in magneto-rheological fluids [1] or in inverted ferro-fluids. The dynamics of clusters of three particles is analysed by solving the equations of motion supplemented by a Gaussian thermostat. The short range order and the effect of an imposed shear flow is studied. The regarded particles interact by a dipole-dipole potential. A long range effective potential is added to keep them close to each other. One observes the formation of chains. The effect of the variation of the dipole strength parameter and the temperature on the process of chain-forming is studied. A simple shear flow is introduced which results in a disturbance of the cluster. Contributions to the shear stress and normal stress differences as well as the dependence of the viscosity on the dipole-dipole interaction and on the shear rate are analysed.

[1]M.Kröger, P.Ilg and S. Hess, J. Phys.: Condens. Matter 15(2003) S1403-S1423

DY 46.112 Thu 16:00 P1

Shear-thickening and Shear-thinning behaviour in nonlinear Maxwell model Fluids. — •Bastian Arlt and Siegfried Hess — Institut für Theoretische Physik, Technische Universität, Hardenbergstraße 36, Berlin, D-10623, Germany

A generalization of the Maxwell model where the relaxation is associated with a modification of the rheological model introduced by O. Hess, Ch. Goddard and S. Hess [1] is considered. The nonlinear Maxwell model equation involves the derivative of a potential function with respect to the stress tensor. In [1] terms up to the 4^{th} order were used. Here an alternative potential with terms up to 6^{th} order is studied. Consequences of the model, in particular the shear stress, the first and second normal stress difference are presented for a plane Couette flow. Shear thinning, shear thickening and also the occurence of a yield stress are found. The transient and the dynamic behaviour of the components of the shear stress tensor are presented.

[1] O. Hess, Ch. Goddard, S. Hess: *From Shear-Thickening and Periodic Flow Behavior to Rheo-Chaos in Nonlinear Maxwell-Model Fluids*, Physica A (2005)

DY 46.113 Thu 16:00 P1

Dynamic dielectric polarization of tumbling nematic liquid crystals — •Stefan Grandner, Sebastian Heidenreich, Sabine Klapp, and Siegfried Hess — Institut für theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

The orientation of a tumbling nematic liquid crystal shows a time dependent response in a stationary Couette flow. This behavior can be described by a nonlinear inhomogeneous relaxation equation for the alignment tensor [1]. Different types of periodic behavior referred to as tumbling, wagging, kayaking tumbling and kayaking wagging have been identified. Even chaotic solutions are found [2]. Here, we consider a liquid crystal consisting of particles with an electric dipole moment. The coupling between the alignment tensor and the electric polarization is taken into account in an extended Landau-de Gennes potential. The microscopic origin of these terms is analysed. The resulting dynamic equations are solved and the physical consequences for the time dependence of the electric polarization of a streaming tumbling nematic are discussed.

[1] S. Hess, Z. Naturforsch. 30a, 728, 1224 (1975)
[2] G. Rienäcker, M. Kröger and S. Hess, Phys. Rev. E 66, 040702(R) (2002)

DY 46.114 Thu 16:00 P1

Traveling patterns in rotating magnetic fields — •Katharina Schatz, Robert Krauss, Reinhard Richter, and Ingo Rehberg — Experimentalphysik 5, Universität Bayreuth, D-95440 Bayreuth, Germany

Recently we have demonstrated, that a magnetic field rotating on the free surface of a ferrofluid layer can induce considerable fluid motion towards the direction the field is rolling. This effect can be utilized for a magnetic pump, which can drive a flow even in small geometries, where a mechanical driving of the flow is not possible. In our contribution we demonstrate that the pump is still working if a constant magnetic field is superimposed on the rotating one. This enables us to drive a periodic pattern of Rosensweig peaks by means of a rotating field. The traveling velocity of the pattern is measured for different values of the rotation amplitude and frequency.

[1] Robert Krauß, Bert Reimann, Reinhard Richter, and Ingo Rehberg, Appl. Phys. Lett. **86** 024102-1 (2005).

DY 46.115 Thu 16:00 P1

Preventing the Rayleigh-Taylor instability in ferrofluids — •Dirk Rannacher and Andreas Engel — Carl-von-Ossietzky Universität, 26111 Oldenburg, Germany

Whenever a dense, heavy fluid is layered on a light fluid the plane interface between the two immiscible fluids becomes unstable, the denser fluid moves down under the influence of the gravitational force and the lighter fluid is displaced upwards. This instability is called the Rayleigh-Taylor instability.

We consider a system of two superimposed, immiscible, viscous fluids with densities ρ_1 for the lower and $\rho_2 > \rho_1$ for the upper fluid, where the upper one is a ferrofluid.

Ferrofluids are stable suspensions of magnetic particles and a suitable liquid carrier. A magnetic field **H** stabilizes a flat surface of a ferrofluid by suppressing surface modulations when the magnetic field is parallel to the wave vector **k** of this modulation [1]. Consequently to stabilize a two dimensional surface a rotating magnetic field is proposed.

A linear stability analysis shows, that the instability of a two dimensional flat interface between a ferrofluid and a non-magnetic fluid can be stabilized by a parallel, rotating magnetic field.

[1] R. E. Rosensweig, Ferrohydrodynamics, (Cambridge University Press, Cambridge, 1985)

DY 46.116 Thu 16:00 P1

Equilibrium Properties of a Bidispersed Ferrofluid with Chain Aggregates: Theory and Computer Simulations — •Christian Holm[1,2], Sofia Kantorovich[3], Alexei O. Ivanov[3], and E.S. Pyanzina[3] — [1]Frankfurt Institute for Advanced Studies (FIAS) Johann Wolfgang Goethe University, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany — [2]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz, Germany — [3]Urals State University, Lenin av, 51, Ekaterinburg, 620083, Russia

The presence of chains, formed due to the magnetic dipole-dipole interaction, leads to strong deviations of magnetization curve from the Langevine curve for ideal superparamagnetic gas. Here we compare simulational results for a bidisperse ferrofluid (Ref. [2]) with the theoretical model (bidisperse ferrofluid with chains) predictions (Ref. [3]). We find for a small concentration of the large particle that the magnetization behavior is close to the one given by the modified mean field approach. For higher concentration of large particles there is a considerable growth in the initial susceptibility. The latter cannot be described in terms of homogeneous ferrocolloids. Using the results of Ref [1,3] we built a bidisperse model and calculated magnetic and structural quantities of the bidisperse fluid of Ref. [2]. The theoretical results are in excellent quantitative agreement with the ones of computer simulations.

[1] V.S. Mendelev, A.O. Ivanov, Physical Review E 70, 051502 (2004)
[2] Z. Wang, C. Holm, Physical Review E 68, 041401 (2003)
[3] S.S.Kantorovich, A.O. Ivanov, Physical Review E 70, 021401 (2004)

DY 46.117 Thu 16:00 P1

Ageing at surfaces: The semi-infinite spherical model — •Florian Baumann[1,2] and Michel Pleimling[1] — [1]Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Germany — [2]Laboratoire de Physique des Matériaux, Université Henri Poincaré Nancy I, France

Ageing phenomena have been considered in many translationally invariant systems. An interesting question is to see what happens if we introduce a spatial surface. In the past [1] numerical investigations were done on this question, and it turned out that surface ageing exponents, surface scaling functions and a surface fluctuation-dissipation ratio can reasonably be defined in close analogy to the bulk case.

Here we aim at adding some exact results to the discussion by considering the semi-infinite kinetic spherical model [2]. We do this for both Dirichlet and Neumann boundary conditions at the surface, which corresponds to the ordinary transition and special transition point respectively. We compute the exact results for the two-time surface correlation and response functions in the dynamical scaling regime as well as the surface fluctuation-dissipation ratio. The results for the critical exponents are in line with previously found scaling relations connecting them to static exponents. We also study the low-temperature phase of this model. Our results show that for Dirichlet boundary conditions the value of the non-equilibrium surface exponent b_1 does not vanish, in contrast to the usual bulk value of systems undergoing phase ordering.

[1] M. Pleimling, Phys. Rev. B **70**, 104401 (2004)
[2] F. Baumann and M. Pleimling, cond-mat/0509064

DY 46.118 Thu 16:00 P1

Quantum Monte Carlo Study of Dimerized Heisenberg Models — •Sandro Wenzel, Leszek Bogacz, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11, 04109 Leipzig

In this contribution we study two-dimensional anti-ferromagnetic dimerized Heisenberg systems such as the $J - J'$ model [1] given by the Hamiltonian

$$\hat{H} = J \sum_{\langle i,j \rangle_1} \hat{\mathbf{S}}_i \hat{\mathbf{S}}_j + J' \sum_{\langle i,j \rangle_2} \hat{\mathbf{S}}_i \hat{\mathbf{S}}_j - h \sum_i \hat{\mathbf{S}}_i^z \,, \qquad (1)$$

for $S = 1/2$ and generalisations thereof [2]. Here, $\langle i,j \rangle_1$ and $\langle i,j \rangle_2$ denote two different kinds of nearest neighbour bonds that are distributed on the square lattice in a regular fashion.

Such models play an important role in the study of quantum effects in low-dimensional magnetic systems. The focus of our research will be on the ground state phase diagram ($T \to 0$) and the magnetization properties for $h > 0$. We will present results of our investigations of the model by means of the Stochastic Series Expansion [3] (SSE) Quantum Monte Carlo scheme. Finally, we compare our findings with approximate theoretical results obtained for the $J - J'$ model in [1].

[1] S.E. Krüger, J. Richter, J. Schulenberg, D.J.J. Farnell, and R.F. Bishop, Phys. Rev. B **61** (2000) 14607.
[2] M. Matsumoto, C. Yasuda, S. Todo, and H. Takayama, Phys. Rev. B **65** (2001) 014407.
[3] O.F. Syljuasen and A.W. Sandvik, Phys. Rev. E **66** (2002) 046701.

DY 46.119 Thu 16:00 P1

Series expansions for percolation and bond-diluted Ising models on Z^D — •Meik Hellmund[1] and Wolfhard Janke[2] — [1]Mathematisches Institut, Universität Leipzig — [2]Institut für Theoretische Physik, Universität Leipzig

We derive high-temperature series expansions for the free energy and the susceptibility of random-bond q-state Potts models on hypercubic lattices using a star-graph expansion technique.

For the case of the Ising ($q = 2$) model, disordered by quenched bond dilution, a detailed analysis of the influence of the disorder on the second-order phase transition (change in critical temperature and exponent γ) is presented for 3, 4 and 5 dimensions.

In the pure (no disorder) case we obtain series for the free energy and susceptibility with explicit q- and D-dependence up to order 17 (arbitrary D) and 19 ($D \leq 5$), resp. This allows us to analyze bond percolation ($q \to 1$) and tree percolation ($q \to 0$) and obtain critical exponents in various dimensions.

DY 46.120 Thu 16:00 P1

Molecular dynamics simulations of argon nucleation — •Jan Wedekind[1], David Reguera[2], and Reinhard Strey[1] — [1]Institut für Physikalische Chemie, Universität zu Köln, Luxemburger Str. 116, D-50939 Köln, Germany — [2]Departament de Física Fonamental, Facultat de Física, Universitat de Barcelona, Martí i Franquès, 1, 08028-Barcelona, Spain

The properties of noble gases like argon are well known experimentally and can be adequately described using a Lennard-Jones potential. This potential is in turn comparatively easy to use in more elaborate

nucleation theories and simulations. Thus, noble gases are ideal to test different theoretical approaches. It was assumed that classical nucleation theory (CNT) describes an almost ideal substance like argon much better than e.g. water [1]. Yet, recent experiments on argon nucleation show enormous deviations from CNT of up to 26 orders of magnitude [3]. We carried out MD simulations of vapor-liquid argon nucleation to investigate if these results are confirmed. Five different supersaturations were simulated at five temperatures similar to the experiment. Each set consists of up to 1000 simulation runs for better statistics. The nucleation rate isotherms yield the critical cluster size n^* based on thermodynamic arguments. Also, we introduce a new approach based on rate theory to analyze the results. Thus, we can also determine n^* directly from the kinetics without thermodynamical considerations. We compare these results with experiment and different theories.

[1] Wölk, Strey, J Phys Chem B 105, 11683 (2001)
[2] Iland, Dissertation, Universität zu Köln, 2004

DY 46.121 Thu 16:00 P1

Non-Markovian Persistence in the diluted Ising model at criticality — •Gregory Schehr[1] and Raja Paul[2] — [1]Theoretische Physik, Universität Saarbrücken — [2]BIOMS, IWR, Ruprecht-Karls-University Heidelberg,

We investigate global persistence properties for the non-equilibrium critical dynamics of the randomly diluted Ising model. The disorder averaged persistence probability $\bar{P}_c(t)$ of the global magnetization is found to decay algebraically with an exponent θ_c that we compute analytically in a dimensional expansion in $d = 4 - \epsilon$. Corrections to Markov process are found to occur already at one loop order and θ_c is thus a novel exponent characterizing this disordered critical point. Our result is thoroughly compared with Monte Carlo simulations in $d = 3$, which also include a measurement of the initial slip exponent. Taking carefully into account corrections to scaling, θ_c is found to be a universal exponent, independent of the dilution factor p along the critical line at $T_c(p)$, and in good agreement with our one loop calculation.

DY 46.122 Thu 16:00 P1

Effect of weak disorder on the ground state of uniaxial dipolar spin systems in the upper critical dimension — •A. V. Klopper[1,2], U. K. Rössler[2], and R.L. Stamps[1] — [1]School of Physics, University of Western Australia, Perth, Austalia — [2]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Extensive Monte Carlo simulations are used to investigate the stability of the ferromagnetic ground state in 3D systems of Ising dipoles with added quenched disorder modelled by short-range direct $+/-J$ exchange couplings. The uniaxial dipolar spins are arranged on face centered cubic lattices with periodic boundary conditions. These systems model the collective ferromagnetic order due to classical dipole-dipole interactions observed in various densely packed arrays of dipoles. Finite-size scaling relations for the pure dipolar ferromagnetic system have been derived by a renormalization group calculation. These functions include logarithmic corrections to the expected mean field behaviour since the system is in its upper critical dimension. Scaled data confirm the validity of the finite-size scaling description and results are compared with subsequent analysis of weakly disordered systems [1]. A disorder-temperature phase diagram displays the preservation of the ferromagnetic ground state with the addition of small amounts of disorder. Stronger disorder destroys the ferromagnetic ground state. Different scenarios for the structure of the phase diagram and the critical properties of disordered systems are discussed.

[1] A.V. Klopper et al., cond-mat/0509751.

DY 46.123 Thu 16:00 P1

Phase diagrams of the mixed-spin Ising model on the decorated square lattice — •Jozef Strecka, Lucia Canova, and Jan Dely — Department of Theoretical Physics and Astrophysics, Faculty of Science, P. J. Safarik University, 040 01 Kosice, Slovakia

Generalized version of decoration-iteration transformation is used in order to establish a mapping correspondence between the mixed-spin Ising model on the decorated square lattice and respectively, a simple spin-1/2 Ising model on the anisotropic square lattice solved by Onsager several years ago [1]. Even if horizontal bonds of the decorated square lattice are occupied by different spins as the vertical ones, this mapping procedure enables to obtain exact results for phase diagrams as well as all basic thermodynamic quantities such as Gibbs free energy, magnetization, specific heat, etc.

Within the framework of this mapping, we will investigate in particular the phase diagrams depending basically on the single-ion anisotropy strength acting on the higher-spin sites. It turns out that the system under investigation may exhibit very rich and unexpected critical behaviour, which strongly depends on the spin quantum number of decorating sites. In addition, a detailed analysis of the temperature dependence of the total magnetization will be accomplished for the ferrimagnetic version of the model system, since the ferrimagnetic spin systems often exhibit manifold temperature dependences of the total magnetization.

[1] L. Onsager, Phys. Rev. 65 (1944) 117.

DY 46.124 Thu 16:00 P1

Weak universality, bicritical points and reentrant transitions of the mixed-spin Ising model on the union jack lattice — •Lucia Canova, Jan Dely, and Jozef Strecka — Department of Theoretical Physics and Astrophysics, Faculty of Science, P. J. Safarik University, 040 01 Kosice, Slovakia

The mixed spin-1/2 and spin-S (S>1/2) Ising model on the union jack (centered square) lattice is solved by establishing a mapping correspondence with the uniform eight-vertex model by following the procedure worked out previously by Lipowski and Horiguchi [1]. It is shown that the model under investigation becomes exactly soluble as a free-fermion eight-vertex model [2] when the parameter of uniaxial single-ion anisotropy tends to infinity. Under this restriction, the critical points are characterized by critical exponents from the standard Ising universality class. In a certain subspace of interaction parameters, which corresponds to a coexistence surface between two ordered phases, the model becomes exactly soluble as a symmetric zero-field eight-vertex model [3]. This surface is bounded by a line of bicritical points, which have interaction-dependent critical exponents that satisfy a weak universality hypothesis [4]. In the rest of the parameter space, the free-fermion approximation [2] is used in order to estimate the criticality of the model system.

[1] A. Lipowski, T. Horiguchi, J. Phys. A: Math. Gen. 28 (1995) L261.
[2] C. Fan and F. Y. Wu, Phys. Rev. B 2 (1970) 723.
[3] R. J.Baxter, Exactly solved models in statistical mechanics (Academic Press, New York, 1982).
[4] M. Suzuki, Progr. Theor. Phys. 51 (1974) 1992

DY 46.125 Thu 16:00 P1

Excitations and percolation phenomena in 3D random field Ising magnets — •Martin Zumsande and Alexander K. Hartmann — University of Göttingen, Institute for Theoretical Physics, Friedrich-Hund-Platz 1, 37077 Göttingen

The ground-state structure of the three-dimensional Gaussian random field Ising magnet (RFIM) is known to show a rich behaviour, especially since there occurs a disorder-driven phase transition in 3D. For small random fields the 3D RFIM is ferromagnetic, at high fields the spins align with the random fields leading to a paramagnetic phase. We compute ground states of very large systems ($L \approx 100^3$ spins) using a mapping of the problem to the maximum-flow minimum-cut problem of graph theory which can be solved by efficient algorithms.

We create small excitations by freezing one spin of the system opposite to its ground state direction and recalculating the ground state. Doing this, we generate clusters that have a maximum extension at criticality where the correlation length diverges. We numerically determine geometrical and energetical properties of these clusters.

We also study percolation properties of the ground state at different random fields. There is a transition from the ferromagnetic phase where one spin direction percolates to the paramagnetic phase, where both of them do. We determine the properties of the percolation transition of this and related types of percolation and discuss the influence of the phase transition on this.

DY 46.126 Thu 16:00 P1

Internal dynamics and complex motion of nonlinear excitations in a highly dispersive near-discrete medium — •Oksana Charkina and Mikhail Bogdan — B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, 47 Lenin Ave., Kharkov 61103, Ukraine

The strong spatial dispersion in crystals can change drastically dynamic properties of nonlinear excitations. A typical example of the excitations in an imperfect lattice is a dislocation, which can be considered as a soliton (kink) of the Frenkel-Kontorova model. In the system with the strong dispersion solitons exhibit a complex intrinsic structure with internal degrees of freedom. To succeed in analytical description of the novel effect a fourth-order spatio-temporal derivative is added to the

usual sine-Gordon equation. This approach allows us to find exactly a total spectrum of linear excitations of the kink. It consists of a discrete set of frequencies of internal modes and a single band spectrum of continuum waves. It is shown analytically and numerically that a translational motion of a single soliton in the dispersive system is accompanied by exciting its internal dynamics and creation of the breather state, and by generation of the radiation. It is demonstrated that a fast motion of two identical solitons leads to a formation of the bound soliton complex, which is stable and can move radiationlessly in the highly dispersive sine-Gordon system.

DY 46.127 Thu 16:00 P1

Features of phonon densities of some FCC metals — •Elena V. Manzhelii, Igor A. Gospodarev, Vladimor O. Kruglov, and Sergey Feodosyev — B.Verkin ILTPE NAS of Ukraine 47 Lenin Ave., Kharkov 61103 , UKRAINE

The behavior of the phonon densities near the Van Hove singularities has been investigated using the force constants of the interatomic interaction that were obtained from experimental results for elastic constants [1]. The calculation was performed by the Jacobian matrix method, which permitted us to analyze the contribution to the spectral densities from the phonons propagating in all directions (not in the high-symmetry ones). This procedure enabled us to detect an additional singularity in some metals, such as Cu, Au and Al. The singularity was detected near the upper edge of the continuum spectrum band and was due to the nonmonotonous character of the dispersion curves and the maximum frequency inside the Brillouin zone. Such singularity is absent in some metals (e.g. Ag). The relaxation of the force constants at the sample boundaries (surfaces, ribs, apexes) has been investigated.

1. S.B. Feodsyev, I.A. Gospodarev, V.O. Kruglov, E.V. Manzhelii, Condensed Matter Division, SIYI41, Prague 2004.

DY 46.128 Thu 16:00 P1

LOCAL VIBRATIONS TRANSFORMATION INTO IMPURITY — •Sergey B. Feodosyev, Igor A. Gospodarev, Vladimir I. Grishaev, Arnold M. Kosevich, Alexandr V. Kotlyar, Vladimir O. Kruglov, Elena V. Manzhelii, and Eugenii S. Syrkin — B.Verkin Institute for Low Temperature Physics and Engineering NAS of Ukraine 47 Lenin Ave., Kharkov 61103 , UKRAINE

The phonon densities of disordered solid solutions with varied concentration of light substitutional impurity characterized by mass defect above the threshold value for formation of a local vibration are calculated by Jacoby-matrix technique. The transformation such a discrete vibration level into impurity zone with increasing impurity content is studied. It is shown that an increase of impurity concentration gives rise to broadening of basic local level accompanied by occurrence of additional peaks on the phonon density. They are attributed to the impurity configurations appeared at finite concentrations and two first moments of their spectral densities sufficiently differ from those of isolated defect. The calculations were performed for both the solutions of isotope impurity in FCC-lattice with central interaction of near neighbors, and solid solutions of aluminum in silver.

DY 46.129 Thu 16:00 P1

LOCAL VIBRATIONS OF LIGHT SUBCTITUTIONAL IMPURITIES INTRODUCED INTO MICROCONTACT — •Oleksandr Kotlyar, Sergey Feodosyev, Igor Gospodarev, Vladimir Grishaev, Arnold Kosevich, and Elena Manzhelii — B.Verkin Institute for Low Temperature Physics and Engineering NAS of Ukraine, 47 Lenin ave., Kharkov Ukraine

The spectral phonon densities of light impurity atoms introduced into differ positions of microcontact are calculated by Jacoby-matrix technique. It is shown that frequencies of local vibrations (LVs) caused by availability of impurity atom near boundaries of a sample (surfaces, ribs and apexes) or in the neighborhood of the other impurities may be well described within the frames of the two-moment-model, as we called it, as well as the LVs of isolated impurity in the depth of crystal volume [1]. Therefore, for different LVs of atoms located in the non- equivalent crystal positions the frequencies of the local vibrations coincide with high precision if two first moments of their spectral densities coincide too. That is why practically full distortion of the crystal regularity in the disposition of boundary atoms does not cause merging of the discrete local levels into a single impurity zone. Out of the strip of the quasi-continuous phonon spectrum only a few very sharp peaks which are precisely separated one from another.

1.O.V.Kotlyar, S.B.Feodosyev, Low Temp. Phys, 32, N3 (2006)

DY 46.130 Thu 16:00 P1

Coherent phonon avalanches in ruby — •L. G. Tilstra, A. F. M. Arts, and H. W. de Wijn — Debye Institute, Department of Physics and Astronomy, Utrecht University, P.O. Box 80.000, 3508 TA Utrecht, The Netherlands

Coherent phonons are generated by stimulated emission in a single crystal of dilute ruby at 1.4 K, and subsequently seen to propagate through the crystal. The "hot" medium is the metastable $\overline{E}(^2E)$ doublet split in a magnetic field, whose levels are connected by a one-phonon transition. The doublet is population inverted by pulsed selective optical excitation into its upper level, and the ensuing stimulated phonon emission is detected via the accelerated growth of the lower level's population by the use of luminescence. The coherence is established by comparison with the predictions from a set of Bloch equations [1] designed to describe a strain wave coupled to a nonequilibrium spin system.

For longer crystals, in which the hot zone has a limited extent, the crystal surfaces act as mirrors, and the generated phonon beam passes repeatedly through the hot zone, much like in an optical laser. The phonon beam is amplified upon each pass until the population inversion becomes exhausted. Both the divergence and the frequency spread of the beam have been studied.

[1] L. G. Tilstra, A. F. M. Arts, and H. W. de Wijn, Phys. Rev. B **68**, 144302 (2003).

DY 46.131 Thu 16:00 P1

Trapping of discrete solitons by defects in nonlinear waveguide arrays — •Rodrigo Vicencio and Luis Morales — Max-Planck-Institut für Physik Komplexer Systeme

We study the trapping process of moving discrete solitons by linear and nonlinear impurities embedded in a one-dimensional nonlinear cubic array. We show that there exist optimal values for the strength of the impurity and for the angle where a strong trapping is obtained. We introduce a criterion for studying scattering dynamics of localized waves in nonlinear extended systems, where trapping of energy takes place.

DY 46.132 Thu 16:00 P1

Discrete soliton mobility in two-dimensional waveguide arrays with — •Rodrigo Vicencio[1] and Magnus Johansson[1,2,3] — [1]Max-Planck-Institut für Physik Komplexer Systeme — [2]Department of Physics, Chemistry and Biology (IFM), Linköping — [3]University of Kalmar, Department of Chemistry and Biomedical

We address the issue of mobility of localized modes in two-dimensional nonlinear Schrödinger lattices with saturable nonlinearity. This describes e.g. discrete spatial solitons in a tight-binding approximation of two-dimensional optical waveguide arrays made from photorefractive crystals. We discuss numerically obtained exact stationary solutions and their stability, focussing on three different solution families with peaks at one, two, and four neighboring sites, respectively. When varying the power, there is a repeated exchange of stability between these three solutions, with symmetry-broken families of connecting intermediate stationary solutions appearing at the bifurcation points. When the nonlinearity parameter is not too large, we observe good mobility, and a well defined Peierls-Nabarro barrier measuring the minimum energy necessary for rendering a stable stationary solution mobile.

DY 46.133 Thu 16:00 P1

Guest-host interaction of deuterated THF molecules in clathrate hydrates — •Beata Walasek and Rudolf Feile — Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt

Recent investigations on molecular vibrations of tetrahydrofurane (THF) as guest molecule in the hydrate cages of the THF-clathrate hydrate revealed an inequivalent influence of the surrounding water molecules on two characteristic vibrations (C-C-C-C stretches and C-O-C stretch) compared to the THF molecule in liquid THF-water solution.

We have performed Raman scattering experiments on deuterated tetrahydrofurane (THF-d8) molecules in liquid THF-d8, in liquid mixtures of THF-d8 with H_2O/D_2O, and THF-d8-H_2O/D_2O-clathrates. The results give a more detailed knowledge about molecular vibrations of the fivefold ring of four carbon atoms and one oxygen atom and the THF-d8 interaction with H2O/D2O. Additionally, we get a more clear picture

about the low temperature anomalies observed in THF-clathrates.