

DYNAMICS AND STATISTICAL PHYSICS

DYNAMIK UND STATISTISCHE PHYSIK (DY)

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OVERVIEW OF INVITED TALKS AND SESSIONS

(lecture rooms HÜL 186 and SCH 251)

Plenary Talk

The plenary talk for division DY by Prof. Chan takes place Monday, 8:30, HSZ 01. The title of the talk is “Superfluidity in solid helium and solid hydrogen”. See the plenary section for the abstract.

Prize Talk

The prize talk (Max-Planck-Medaille) by Prof. Götze takes place Tuesday, 13:15, HSZ 04. The title of the talk is “Glassy Relaxation: a Paradigm for Condensed-Matter Dynamics”. See the plenary section for the abstract.

Invited Talks

DY 10.1	Mon	09:30	(HÜL 186)	Networks in Physics , <u>Maya Paczuski</u>
DY 12.7	Mon	12:30	(HÜL 186)	The scaling laws of human travel , <u>Dirk Brockmann</u> , Lars Hufnagel, Theo Geisel
DY 14.1	Mon	14:30	(HÜL 186)	Exploring out-of-equilibrium systems , <u>Luca Peliti</u>
DY 20.1	Tue	09:30	(HÜL 186)	Quantum Computer - dream and realization , <u>Rainer Blatt</u>
DY 28.1	Tue	09:30	(MÜL Elch)	Towards a Statistical Mechanics for Network Glasses , <u>Reimer Kühn</u> , Jort M. van Mourik, Martin Weigt, Annette Zippelius
DY 40.1	Thu	09:30	(HÜL 186)	Random polymers and depinning transitions , <u>Cecile Monthus</u> , Thomas Garel
DY 42.7	Thu	12:30	(HÜL 186)	Universal scaling behavior of non-equilibrium phase transitions , <u>Sven Lübeck</u>
DY 44.1	Thu	14:30	(HÜL 186)	Spin liquids: from frustrated magnets to quantum dimer models , <u>Frederic Mila</u>

Invited talks of the symposium Superfluidity

See section SYSF for the full program of the symposium.

SYSF 1.1	Mon	09:45	(HSZ 04)	Rotons and superfluidity , <u>Sebastien Balibar</u>
SYSF 1.2	Mon	10:15	(HSZ 04)	Disorder determined phase of the p-wave superfluid ^3He , <u>Igor Fomin</u>
SYSF 1.3	Mon	10:45	(HSZ 04)	From superfluids to vacuum of relativistic quantum fields , <u>Grigory Volovik</u>
SYSF 2.1	Mon	11:30	(HSZ 04)	High-Temperature Superfluidity in an Ultracold Fermi Gas , <u>Martin Zwierlein</u> , Jamil Abo-Shaeer, André Schirotzek, Christian Schunck, Wolfgang Ketterle
SYSF 2.2	Mon	12:00	(HSZ 04)	Superfluid regimes in strongly interacting Fermi gases , <u>Gora Shlyapnikov</u>
SYSF 2.3	Mon	12:30	(HSZ 04)	Bose-Einstein Condensation in a Disordered Potential , <u>Robert Graham</u>

Invited talks of the symposium Structure Formation and Self-Organization in non-equilibrium Systems

See section SYSS for the full program of the symposium.

SYSS 4.1	Fri	10:15	(HSZ 04)	Experiments on structure formation in complex continua , Ingo Rehberg , Christof Krülle, Reinhard Richter, Wolfgang Schöpf
SYSS 4.2	Fri	10:45	(HSZ 04)	Coarsening versus noncoarsening in nonequilibrium pattern forming systems , C. Misbah
SYSS 4.3	Fri	11:15	(HSZ 04)	About non-Boussinesq convection , H. Riecke
SYSS 4.4	Fri	11:45	(HSZ 04)	Self-organization and collective decision making in animal societies , Jean-Louis Deneubourg
SYSS 4.5	Fri	12:15	(HSZ 04)	Time-delayed feedback control of noise-induced patterns , Eckehard Schöll , Alexander Balanov, Johanne Hizanidis, Grischa Stegemann

Sessions

DY 10	Statistical Physics of Complex Networks I	Mon	09:30–11:00	HÜL 186	DY 10.1–10.5
DY 12	Statistical Physics of Complex Networks II	Mon	11:00–13:00	HÜL 186	DY 12.1–12.7
DY 14	Statistical Physics far from Thermal Equilibrium	Mon	14:30–16:15	HÜL 186	DY 14.1–14.6
DY 15	Quantum Chaos	Mon	15:00–17:00	SCH 251	DY 15.1–15.8
DY 16	Growth Processes and Surface Properties	Mon	16:15–18:15	HÜL 186	DY 16.1–16.8
DY 17	Superfluidity and Bose-Einstein-Condensation	Mon	17:15–18:00	SCH 251	DY 17.1–17.3
DY 20	Quantum Dynamics I	Tue	09:30–11:00	HÜL 186	DY 20.1–20.5
DY 21	Statistical Physics (general) I	Tue	10:00–11:45	SCH 251	DY 21.1–21.7
DY 22	Quantum Dynamics II	Tue	11:00–13:00	HÜL 186	DY 22.1–22.8
DY 23	Statistical Physics (general) II	Tue	11:45–13:15	SCH 251	DY 23.1–23.6
DY 24	Brownian Motion and Kinetic Theory I	Tue	14:30–16:15	HÜL 186	DY 24.1–24.7
DY 25	Granular Matter and Contact Dynamics I	Tue	14:30–16:30	SCH 251	DY 25.1–25.8
DY 26	Brownian Motion and Kinetic Theory II	Tue	16:15–18:15	HÜL 186	DY 26.1–26.8
DY 27	Granular Matter and Contact Dynamics II	Tue	16:30–18:00	SCH 251	DY 27.1–27.6
DY 28	Glass I (joint session with DF)	Tue	09:30–12:10	MÜL Elch	DY 28.1–28.7
DY 29	Glass II (joint session with DF)	Tue	14:30–16:10	MÜL Elch	DY 29.1–29.5
DY 34	Nonlinear Dynamics, Synchronization and Chaos I	Wed	14:30–16:15	HÜL 186	DY 34.1–34.7
DY 35	Ferro Fluids / Liquid Crystals	Wed	14:30–16:30	SCH 251	DY 35.1–35.8
DY 36	Nonlinear Dynamics, Synchronization and Chaos II	Wed	16:15–18:00	HÜL 186	DY 36.1–36.7
DY 38	Fluid Dynamics	Wed	16:45–18:00	SCH 251	DY 38.1–38.5
DY 40	Critical Phenomena and Phase Transitions I	Thu	09:30–11:00	HÜL 186	DY 40.1–40.5
DY 41	Dynamical Physics in Biological Systems	Thu	10:00–11:30	SCH 251	DY 41.1–41.6
DY 42	Critical Phenomena and Phase Transitions II	Thu	11:00–13:00	HÜL 186	DY 42.1–42.7
DY 43	Signals and neuronal Networks	Thu	11:30–12:45	SCH 251	DY 43.1–43.5
DY 44	Critical Phenomena and Phase Transitions III	Thu	14:30–16:00	HÜL 186	DY 44.1–44.5
DY 45	Soft Matter	Thu	14:30–16:00	SCH 251	DY 45.1–45.6
DY 46	Poster	Thu	16:00–18:00	P1	DY 46.1–46.133
DY 50	Lattice Dynamics and Non-Linear Excitations	Fri	10:15–11:30	HÜL 186	DY 50.1–50.5
DY 51	Non-Linear Stochastic Systems	Fri	11:30–13:30	HÜL 186	DY 51.1–51.8

Annual General Meeting of the Section Dynamics and Statistical Physics

Thu 18:30–19:30 HÜL 186

- Bericht
- Wahl eines neuen Sprechers
- Verschiedenes

Sessions

– Invited, Contributed Talks and Posters –

DY 10 Statistical Physics of Complex Networks I

Time: Monday 09:30–11:00

Room: HÜL 186

Invited Talk

DY 10.1 Mon 09:30 HÜL 186

Networks in Physics — ●MAYA PACZUSKI — Complexity Science Group, Department of Physics and Astronomy, University of Calgary, Canada

A fundamental problem in the physics of complex systems is to understand how qualitatively new behavior emerges from nonlinear interactions between large collections of constituents – be they particles, grains in a sand pile, species in a food chain, regulatory genes, or parts of the Earth’s crust. Recently complex networks have been recognized as cogent descriptions for social, biological and technological phenomena. Here I point out that they also play an important role in constructing sparse descriptions of ordinary physical systems, where the main degrees of freedom are nodes and their relevant interactions appear as links. These networks may self-organize into a complex critical state, with avalanches of all sizes. The specific examples I discuss here include our discovery of the scale free magnetic network in the solar corona, a SOC model for complex networks of interacting (magnetic flux) loops, and a network description of seismicity that uses only relations between events rather than properties of individual earthquakes to uncover the underlying spatiotemporal structure of seismicity.

DY 10.2 Mon 10:00 HÜL 186

Transient times and avalanche size distribution in the Olami-Feder-Christensen earthquake model — ●FELIX WISSEL and BARBARA DROSSEL — Institut f. Festkoerperphysik, Hochschulstrasse 8, 64287 Darmstadt

We present analytical and numerical results for the earthquake model by Olami, Feder and Christensen (OFC). First we discuss the transient time until the system is in the stationary state. By introducing the concept of effective sites and using a mean field ansatz for the toppling profile we explain the numerical data as function of the system size N and the coupling parameter α . In the limit $\alpha \rightarrow 0$, our calculation and our simulation data suggest that the transient time diverges as $T(N, \alpha) \sim \alpha^{-\nu} N^{\alpha-\mu}$ with exponents $\nu \simeq 0.5$ and $\mu > 0.5$. By analyzing the correlation function, we then find that the pattern of ”patches” (i.e., areas of similar force value) shows scaling behavior, and based on this result we argue that the avalanche size distribution in the thermodynamic limit of infinite system size is either a power law with α -dependent exponent τ or no power law at all. In any case, almost all topplings occur in the thermodynamic limit in avalanches of size one.

DY 10.3 Mon 10:15 HÜL 186

Emergence of Hierarchical Structures in a Stochastic Network Model — ●MICHAEL KOENIG, STEFANO BATTISTON, and FRANK SCHWEITZER — Chair of Systems Design, ETH Zurich, CH-8092 Zurich, Switzerland

We investigate a network model governed by processes on two different time scales: The short time scale describes the eigendynamics of the nodes, a feature often neglected in network models. The long time scale describes the change of the network structure itself which represents the interactions between the nodes. Each node is characterized by a scalar variable, representing for example “size” or “output”, in a stochastic equation with auto-catalytic and hetero-catalytic growth terms. For the dynamics of the network, we consider different sets of rules for rewiring

the links according to the output of the nodes. For example, a rewiring of any link between two nodes is accepted iff this increases the output of both nodes. Starting from a random graph, the dynamics leads to a saturated state characterized by an optimized output of the system (Nash equilibrium). We find that this equilibrium structure corresponds to a hierarchy in the output distribution. Averaging over different network realizations, we further obtain power-law like behavior for other network variables, such as the distribution of links, clustering coefficients and the number and length of cycles in the network.

DY 10.4 Mon 10:30 HÜL 186

Maximum flow and topological structure of complex networks — ●DEOK-SUN LEE and HEIKO RIEGER — Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany

The problem of sending the maximum amount of flow q between two arbitrary nodes s and t of complex networks along links with unit capacity is studied, which is equivalent to determining the number of link-disjoint paths between s and t . The average of q over all node pairs with smaller degree k_{\min} is $\langle q \rangle_{k_{\min}} \simeq c k_{\min}$ for large k_{\min} with c a constant implying that the statistics of q is related to the degree distribution of the network. The disjoint paths between hub nodes are found to be distributed among the edge-biconnected links, and q can be estimated by the number of pairs of edge-biconnected links incident to the start and terminal node. The relative size of the giant edge-biconnected component of a network approximates to the coefficient c . The applicability of our results to real world networks is tested for the Internet at the autonomous system level.

DY 10.5 Mon 10:45 HÜL 186

Metropolis Public Transport: Network Topology and Vulnerability — ●CHRISTIAN VON FERBER^{1,2}, YURIJ HOLOVATCH^{3,4}, TARAS HOLOVATCH⁴, and VASYL PALCHYKOV⁴ — ¹Physikalisches Institut, Freiburg University — ²Complex Systems Research, Jagellonian University, Krakow — ³Institute for Condensed Matter Physics, Lviv, Ukraine — ⁴Ivan Franko National University of Lviv, Ukraine

We analyse the public transport (PT) networks of a number of major cities of the world. While the primary network topology is defined by a set of routes each servicing an ordered series of given stations, a number of different neighborhood relations may be defined both for the routes and the stations. E.g. one either defines two stations as neighbors whenever they are serviced by a common route or only if one station is the successor of the other in the series serviced by this route. The networks defined in this way display a number of distinguishing properties, the most striking being that often several routes proceed in parallel for a sequence of stations [1]. While other networks with real-world links like cables or neurons embedded in two or three dimensions often show similar features, these can be studied in detail in our present case. Previous studies of PT have mostly been restricted to much smaller networks and did not observe scale free behavior for which we find clear indications in the larger of the networks that we analyze. Our findings for the statistics as well as for relations between the topology and vulnerability of these networks are supported by simulations of an evolutionary model of PT networks that we propose. [1] C. von Ferber, Yu. Holovatch, and V. Palchykov, *Condens. Matter Phys.*8:225(2005)cond-mat/0501296

DY 12 Statistical Physics of Complex Networks II

Time: Monday 11:00–13:00

Room: HÜL 186

DY 12.1 Mon 11:00 HÜL 186

Universal dependence of inter-node distances in complex networks — •JANUSZ A. HOLYST, JULIAN SIENKIEWICZ, AGATA FRONCZAK, PIOTR FRONCZAK, and KRZYSZTOF SUCHECKI — Faculty of Physics, Warsaw University of Technology, Koszykowa 75, 00-662 Warszawa, Poland

We observe a universal scaling of internode distances in Erdős-Rényi random graphs, scale-free Barabási-Albert models, science collaboration networks, biological networks, Internet Autonomous Systems and public transport networks. The average shortest distance between two nodes of degrees k_i and k_j is equal to $\langle l_{ij} \rangle = A - B \log(k_i k_j)$. The scaling holds over several decades. We present a simple theory for the appearance of this scaling where parameters A and B depend on the mean value of a node degree $\langle k \rangle_{nn}$ calculated for the nearest neighbors and on network clustering coefficients. Corrections due to node degree-degree correlations are taken into account.

DY 12.2 Mon 11:15 HÜL 186

Scaling in analyzing and other critical Kauffman networks — •VIKTOR KAUFMAN, BARBARA DROSSEL, TAMARA MIHALJEV, and UTE PAUL — Institute of Condensed Matter Physics, TU Darmstadt

The application of methods of statistical physics supported by numerical simulations leads to an intuitive and at the same time quantitative understanding of critical Kauffman Random Boolean networks (RBNs) with two inputs per node in the limit of large system size. We study standard RBNs as well as the special case of analyzing RBNs, which were suggested to be suitable models for description of f.i. regulatory genetic networks. In the past few years unexpected results were found in such models. In particular we prove that analyzing networks do not have substantially shorter or less attractors than other critical networks. Further similar models can be studied using our approach.

DY 12.3 Mon 11:30 HÜL 186

Monte Carlo sampling of cycles in large networks — •KONSTANTIN KLEMM and PETER F. STADLER — Dept. of Bioinformatics, Leipzig University

An important characteristic of many complex networks is redundant wiring, which leads to the occurrence of cycles. Abundance of small cycles, in particular triangles, has been widely studied. Larger cycles with lengths up to system size have received much less attention due to the lack of efficient numerical tools. Here we present a Markov chain Monte Carlo algorithm that is able to sample cycles of all lengths with equal probability. By choosing length dependent (Boltzmann) weights the equilibrium distribution can be tuned to particularly long or short cycles.

As the main result for growing networks, we find that the dependence between network size N and typical cycle length is algebraic [1], $\langle h \rangle \propto N^\alpha$, with distinct values of α for different wiring rules. The Barabasi-Albert model has $\alpha = 1$. Other preferential and non-preferential attachment rules and the growing Internet graph yield $\alpha < 1$. [1] K. Klemm and P. F. Stadler, e-print cond-mat/0506493.

DY 12.4 Mon 11:45 HÜL 186

A Program Generating Homogeneous Random Graphs with Given Weights — •LESZEK BOGACZ¹, ZDZISLAW BURDA², WOLFHARD JANKE¹, and BARTŁOMIEJ WACLAW² — ¹Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11, 04109 Leipzig, Germany — ²Institute of Physics, Jagellonian University, Reymonta 4, 30-059 Krakow, Poland

We present a program package [1] which generates homogeneous random graphs with probabilities prescribed by the user. The statistical weight of a labeled graph α is given in the form $W(\alpha) = \prod_{i=1}^N p(q_i)$, where $p(q)$ is an arbitrary user function and q_i are the degrees of the graph nodes. The program can be used to generate two types of graphs (simple graphs and pseudo-graphs) from three types of ensembles (micro-

canonical, canonical and grand-canonical).

Its functionality will be explained in the talk with a few simple but characteristic examples.

[1] L. Bogacz, Z. Burda, W. Janke, and B. Wacław, cond-mat/0506330, to appear in Comp. Phys. Comm. (in print).

DY 12.5 Mon 12:00 HÜL 186

Coupled Multiplicative Stochastic Processes on Networks — •STEFANO BATTISTON — Chair of Systems Design, ETH Zurich, CH-8092 Zurich, Switzerland

We consider a system of coupled multiplicative stochastic process (MSP) with repulsive barrier, taking place on a network. We investigate by means of computer simulations the stationary distribution and the spatial correlations of such a system. While it is well known that a MPS with repulsive barrier produces a power law distribution, less attention has been drawn so far on the fact that even a weak local coupling destroys the power law and produces much less heterogeneous distributions. This fact raises an apparent contradiction because, several systems that can be described as strongly coupled MSP on a network, including some models of production networks, yet display power law distributions. A simple solution to such inconsistency is represented by asymmetric coupling. In this work we show that asymmetry allows both for strong coupling and power laws.

DY 12.6 Mon 12:15 HÜL 186

Statistical analysis of Polish public transport networks. — •JULIAN SIENKIEWICZ and JANUSZ A. HOLYST — Faculty of Physics, Warsaw University of Technology, Koszykowa 75, 00-662 Warszawa, Poland

We have analyzed Polish public transport networks of sizes ranging from $N = 152$ to $N = 2881$. Depending on the assumed definition of network topology the degree distribution can either follow a power law or can be described using an exponential function. Distributions of path lengths in all considered networks are given by asymmetric, unimodal functions. Clustering, assortativity coefficient and betweenness centrality are studied. All considered networks exhibit small world behavior and are hierarchically organized. We have observed a transition between dissortative small networks $N < 500$ and assortative large networks $N > 500$.

Invited Talk

DY 12.7 Mon 12:30 HÜL 186

The scaling laws of human travel — •DIRK BROCKMANN¹, LARS HUFNAGEL², and THEO GEISEL¹ — ¹MPIDS, Göttingen — ²KITP, UCSB, Santa Barbara, USA

In the light of increasing international trade, intensified human mobility and an imminent influenza A epidemic the knowledge of dynamical and statistical properties of human travel is of fundamental importance. Despite its crucial role, a quantitative assessment of these properties on geographical scales remains elusive and the assumption that humans disperse diffusively still prevails in models. I will report on a solid and quantitative assessment of human travelling statistics by analysing the circulation of bank notes in the United States. Based on a comprehensive dataset of over a million individual displacements we find that dispersal is anomalous in two ways. First, the distribution of travelling distances decays as a power law, indicating that trajectories of bank notes are reminiscent of scale free random walks known as Lévy flights. Secondly, the probability of remaining in a small, spatially confined region for a time T is dominated by algebraic tails which attenuate the superdiffusive spread. We show that human travel can be described mathematically on many spatiotemporal scales by a two parameter continuous time random walk model to a surprising accuracy and conclude that human travel on geographical scales is an ambivalent effectively superdiffusive process.

[1] Brockmann, D., L. Hufnagel, and T. Geisel, The scaling laws of human travel. Nature, 2006 (to be published).

[2] Hufnagel, L., D. Brockmann, and T. Geisel, Forecast and control of epidemics in a globalized world. PNAS, 2004. 101(42): p. 15124-15129.

DY 14 Statistical Physics far from Thermal Equilibrium

Time: Monday 14:30–16:15

Room: HÜL 186

Invited Talk

DY 14.1 Mon 14:30 HÜL 186

Exploring out-of-equilibrium systems — ●LUCA PELITI — Dipartimento di Scienze Fisiche and Unita' CNR-INFM, Universita' "Federico II", I-80126 Napoli (Italy)

I describe a new approach for the simulation of systems in a steady state out of equilibrium. The approach is inspired by the Diffusion Monte Carlo technique for the solution of the Schroedinger equation, and allows for the evaluation of the large deviation functional as a function of (spatially local or global) observables which are local in time. The method is illustrated with the current fluctuations of the Totally Asymmetric Exclusion Process and with the entropy production distribution of a driven Lorentz gas.

DY 14.2 Mon 15:00 HÜL 186

Entropy Production of a Single Two Level System. Experimental Proof of a Fluctuation Theorem — ●CARSTEN TIETZ¹, SEBASTIAN SCHULER¹, THOMAS SPECK², UDO SEIFERT², and JÖRG WRACHTRUP¹ — ¹3. Physikalisches Institut, Universität Stuttgart — ²II. Institut für Theoretische Physik, Universität Stuttgart

The entropy of small systems – e.g. from a single two-level-system (TLS) as used in this work – seems to be not obviously defined in Boltzmann's definition of entropy. Nonetheless, in the last decade the concept of entropy was expanded to entropy along single trajectories. So called fluctuation theorems valid for systems driven out from equilibrium quite generally relate the probability of entropy generation to entropy annihilation.

In this work we use the fluorescence trajectories of a single defect centre in diamond to experimentally determine the entropy along a trajectory of a single TLS driven out of equilibrium. We visualise the entropy evolution along a trajectory of the pure system and the entropy production of the surrounding medium, respectively. The total entropy obey several fluctuation theorems which relate the entropy producing trajectories to the entropy annihilating ones. We prove a Jarzynski like integral fluctuation theorem as well as the more general transient fluctuation theorem.

[1] S. Schuler, T. Speck, C. Tietz, J. Wrachtrup, U. Seifert Phys. Rev. Lett. 94, 180602 (2005).

DY 14.3 Mon 15:15 HÜL 186

Ageing without detailed balance: The bosonic contact and pair-contact processes — ●FLORIAN BAUMANN^{1,2}, MALTE HENKEL², MICHEL PLEIMLING¹, and JEAN RICHERT³ — ¹Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Germany — ²Laboratoire de Physique des Matériaux, Université Henri Poincaré Nancy I, France — ³Laboratoire de Physique Théorique, Université Louis Pasteur Strasbourg I, France

Ageing phenomena and scaling behaviour have been considered in many systems with detailed balance such as simple magnetic systems. Therefore it is an interesting question to extend these studies to systems without detailed balance, paradigmatic examples of which are reaction-diffusion systems. In these systems particles undergo diffusion on a lattice and in addition particle creation and annihilation occurs. In recent numerical investigations of a specific system of this type, dynamical scaling behaviour was found, and it turned out that an equality between two critical exponents, known from systems with detailed balance, does not hold true any more.

In order to shed more light on this, we look at two exactly solvable systems without detailed balance: The bosonic contact and pair-contact processes. Two-time quantities are computed in the scaling limit and ageing exponents and scaling function are determined. In particular we confirm the result that two mentioned critical exponents can indeed be different from each other.

[1] F. Baumann, M. Henkel, M. Pleimling, and J. Richert, J. Phys. A: Math. Gen. 38, 6623 (2005)

DY 14.4 Mon 15:30 HÜL 186

Reentrance during nonequilibrium relaxation — ●MICHEL PLEIMLING¹, LÁSZLÓ KÖRNYEI², and FERENC IGLÓI^{2,3} — ¹Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Germany — ²Institute for Theoretical Physics, Szeged University, Hungary — ³Research Institute for Solid State Physics and Optics Budapest, Hungary

In nonequilibrium critical dynamics the system under consideration is prepared in some initial state from which it is quenched to the critical temperature and then let to evolve in time according to the given dynamical rules. Generally one is interested in the relaxation of the magnetization and in the behavior of the autocorrelation function. In most of the studied cases the initial state is of two kinds: it is either the (completely) ordered one or the (completely) disordered one. In this talk we show that an intriguing reentrance in time is encountered in critical relaxation measurements which start from a non-trivial initial state given by a ground state of the random field Ising model. Competition between two different mechanisms, the dissolution of the compact cells forming the initial state and the usual domain growth, is responsible for this novel feature in nonequilibrium critical dynamics.

[1] L. Környei, M. Pleimling, and F. Iglói, cond-mat/0509372

DY 14.5 Mon 15:45 HÜL 186

Quantitative description of self-organised patterns in ac gas-discharge — ●HANS-GEORG PURWINS¹, LARS STOLLENWERK¹, SHALVA AMIRANASHVILI¹, and JEAN-PIERRE BOEUF² — ¹Institut für Angewandte Physik, Corrensstraße 2/4, 58239 Münster — ²CPAT, 118 route de Narbonne, 31 062 Toulouse Cedex, France

In this work we report on the experimental observation of the evolution of a filamentary pattern in a planar dielectric barrier gas-discharge system. The experimental results are described theoretically in terms of three variables: the electron and ion charge carrier concentration and the electric field. The corresponding set of equations consists of two equations of drift-diffusion type and the Poisson equation. This set of equations is solved numerically. Parameters and boundary conditions are taken from experiment. We find quantitative agreement between experiment and theory. This is the first time that a self-organised pattern in a planar gas-discharge system can be described theoretically in a quantitative manner.

DY 14.6 Mon 16:00 HÜL 186

What is hidden behind memory effects ? — ●K. MORAWETZ^{1,2} and P. LIPAVSKÝ³ — ¹Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — ²Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — ³Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 12116 Prague 2

The finite duration of the collisions in Fermionic systems as expressed by the retardation time in non-Markovian Levinson-type kinetic equations is discussed in the quasiclassical limit. We separate individual contributions included in the memory effect resulting in (i) off-shell tails of the Wigner distribution, (ii) renormalization of scattering rates and (iii) of the single-particle energy, (iv) collision delay and (v) related non-local corrections to the scattering integral. In this way we transform the Levinson equation into the Landau-Silin equation extended by the non-local corrections known from the theory of dense gases. The derived nonlocal kinetic equation unifies the Landau theory of quasiparticle transport with the classical kinetic theory of dense gases.

[1] K. Morawetz, P. Lipavský, and V. Špička, Ann. of Phys. 294, 134 (2001)

[2] P. Lipavský, K. Morawetz, and V. Špička, *Kinetic equation for strongly interacting dense Fermi systems*, Vol. 26,1 of *Annales de Physique* (EDP Sciences, Paris, 2001), ISBN: 2-86883-541-4.

DY 15 Quantum Chaos

Time: Monday 15:00–17:00

Room: SCH 251

DY 15.1 Mon 15:00 SCH 251

Fractal Classical Conductance Fluctuations — •HOLGER HENNING¹, RAGNAR FLEISCHMANN¹, and LARS HUFNAGEL² — ¹MPI for Dynamics and Self-Organization, Goettingen and Institute for Nonlinear Dynamics, University of Goettingen — ²Kavli Institute for Theoretical Physics, University of California, Santa Barbara

The coherent conductance through mesoscopic structures is well known to show reproducible fluctuations with the variation of an external parameter (e.g. a magnetic field). These fluctuations are caused by interference effects and can be described semiclassically. In systems with mixed regular and chaotic classical dynamics *fractal* conductance curves are found [1]. Experiments that study the transition from coherent to incoherent transport showing a change of the fractal dimension with the coherence-length [2], however, seemed to contradict the semiclassical theory of the fractal scaling.

We show that there is no contradiction but that the classical dynamics itself already leads to fractal conductance curves explaining the experimental observations. Moreover, we predict fractal classical conductance fluctuations not only in systems with mixed phase space but in purely chaotic systems.

[1] R. Ketzmerick, Phys. Rev. B, 54, 10841

[2] A.P. Micolich et al., Phys. Rev. Lett., 87, 036802

DY 15.2 Mon 15:15 SCH 251

From irregular subthreshold oscillations to intermittent spiking: canard explosion for a chaotic attractor — •MICHAEL ZAKS, XAVIER SAILER, and LUTZ SCHIMANSKY-GEIER — Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin

In a deterministic model of a neuron with one fast and two slow variables, we observe the crisis of a chaotic attractor: a minute parameter variation causes the strong abrupt (albeit continuous) increase of the amplitude of irregular oscillations. In contrast to conventional types of attractor crises, this phenomenon owes to separation of characteristic timescales; it is related to the motion of the system in the phase space along the repelling part of the slow surface. In contrast to the conventional canard explosion, the transition is experienced not by a single limit cycle but by the attracting chaotic set. For the discussed model the crisis marks the transition from the state of chaotic subthreshold oscillations to the regime of intermittent chaotic spiking. Similar phenomena have been recovered in collective dynamics of large ensembles of globally coupled slow-fast stochastic oscillators.

DY 15.3 Mon 15:30 SCH 251

Microwave Billiards with broken Time Reversal Symmetry — •FLORIAN SCHÄFER — TU Darmstadt, Institut für Kernphysik, Schlossgartenstrasse 9, 64289 Darmstadt

The effect of a broken time reversal symmetry on the principle of detailed balance has been studied in microwave resonators. This is the first time where resonance shapes of isolated and nearly degenerated resonances were analyzed with respect to their behaviour under time reversal. A model was developed to describe the violation of detailed balance in the nearly degenerated case and was successfully tested on the available data.

This work is supported by the DFG within SFB 634.

DY 15.4 Mon 15:45 SCH 251

Spectral properties of mushroom billiards — •THOMAS FRIEDRICH — Schlossgartenstraße 9, 64289 Darmstadt

In 2001 Bunimovich proposed a family of billiards shaped like mushrooms as a generalization of the well studied stadium billiard. The classical phase space of mushroom billiards is well separated into regular and chaotic regions with no KAM islands. We investigated the quantum properties of mushroom billiards experimentally using superconducting microwave cavities by measuring frequency spectra and wave functions. In the measured spectra a supershell structure was observed which, as could be shown, is due to the interference of short periodic orbits of comparable length. Their influences become also visible in the nearest neighbour distance distribution of resonance frequencies. We succeeded in separating the eigenmodes of the mushroom billiard into regular and chaotic modes following Poissonian and GOE statistics, respectively. With those

subsets of modes dynamic tunneling between the two phase space regions was observed in terms of field distributions and frequency shifts. We thus found that the spectral properties of mushroom billiards are mainly governed by shell structures and dynamic tunneling. This work has been supported by DFG within SFB 634.

DY 15.5 Mon 16:00 SCH 251

Vortex and anti-vortex correlations in open microwave billiards — •RUVEN HÖHMANN, ULRICH KUHL, YOUNG-HEE KIM, MICHAEL BARTH, and HANS-JÜRGEN STÖCKMANN — Fachbereich Physik der Philipps-Universität Marburg

In quasi-two-dimensional microwave resonators there is a one-to-one correspondence between the Poynting vector and the probability current density in the corresponding quantum-mechanical system. This has been used to study the flow patterns through an open microwave billiard with particular emphasis to vortices and anti-vortices. Vortices correspond to nodal points of the complex wave function and anti-vortices to the hyperbolic points of the flow. Various pair correlation functions of vortices and anti-vortices, as well as distributions of nearest neighbor distances are investigated. The results are interpreted in terms of the random plane wave model [1,2].

[1] M. Berry, M. Dennis, Proc. R. Soc. Lond. A 456, 2059 (2000). [2] A. Saichev et al., Phys. Rev. E 64, 036222 (2001).

DY 15.6 Mon 16:15 SCH 251

Randomization of time-evolved wave-packets in chaotic quantum systems — •NIKOLAI HLUBEK and ARND BÄCKER — Institut für Theoretische Physik, TU Dresden, 01062 Dresden

The time-evolution of initially localized wave-packets is studied for the case of quantum billiards with classically chaotic dynamics. For large times one expects that the wave-packet resembles a random wave. This implies that the intensity distribution is an exponential, which is confirmed by our results. In contrast to stationary states, we demonstrate that the spatial autocorrelation is different from the usual Bessel function behaviour. Of particular interest is the time-scale for which the randomization sets in. It turns out that this is much smaller than the Heisenberg time and we investigate its relation to the Ehrenfest time.

DY 15.7 Mon 16:30 SCH 251

Dynamical tunneling in a mixed phase space — •LARS SCHILLING, ARND BÄCKER, ROLAND KETZMERICK, and STEFFEN LÖCK — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

The phase space of mixed systems consists of regular islands that are dynamically separated from the chaotic sea. Quantum mechanically these phase space regions are connected by dynamical tunneling. We derive a formula predicting dynamical tunneling rates of regular states to the chaotic sea. Agreement with numerics for kicked systems with resonance-free islands will be presented.

DY 15.8 Mon 16:45 SCH 251

Description of optical microresonators: When rays suffice — •MARTINA HENTSCHEL — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg — ATR Wave Engineering Laboratories, 2-2-2 Hikaridai, Kyoto 619-0228, Japan

Optical microresonators are interesting not only as model systems in the field of quantum chaos but also as components of future communication devices. This raises the question to what extent, based on the concept of ray-wave correspondence, the simple ray model can be deployed in application-oriented problems. It is well-known that for small size parameters (below approximately 500) semiclassical corrections, namely the Goos-Hänchen and Fresnel filtering effects, become important and potentially spoil ray model predictions. However, for large size parameters (above 1000, say) the ray model should suffice. The high capability of the ray model in this regime is confirmed and illustrated by various examples. We explain, for instance, a neat experiment in which a quadrupolar glass fiber showed a filter characteristics for specific setup geometries. Ray simulations reveal that this effect resulted from multiple beam interference that is possible in a limited parameter range around the conditions met in experiment.

DY 16 Growth Processes and Surface Properties

Time: Monday 16:15–18:15

Room: HÜL 186

DY 16.1 Mon 16:15 HÜL 186

Crack Propagation as a Free Boundary Problem — ●DENIS PILIPENKO, ROBERT SPATSCHKEK, EFIM BRENER, and HEINER MUELLER-KRUMBHAAR — Institut fuer Festkoerperforschung, Forschungszentrum 52425 Juelich

We demonstrate a macroscopic theory of fracture in the spirit of nonequilibrium growth processes in pattern formation. The theory is based only on the dynamical theory of elasticity, surface energy and elastically induced phase transitions between a hard and a soft solid phase. Alternatively, crack growth can be described by surface diffusion along the crack. Although it is commonly believed that crack growth is dictated by the microscopic details in the vicinity of the tip, and despite the simplicity of our continuum theory, it predicts many important features of fracture. Among them is the limitation of the steady state growth velocity to values appreciably below the Rayleigh speed (the speed of sound) and tip blunting. We present a multipole expansion technique to solve numerically the problem of steady state growth in a very efficient way, using a sharp interface description of the propagating crack front. The results are discussed and compared to phase field simulations.

DY 16.2 Mon 16:30 HÜL 186

Phase Field Modeling of Crack Propagation — ●ROBERT SPATSCHKEK, CLEMENS MUELLER-GUGENBERGER, EFIM BRENER, and HEINER MUELLER-KRUMBHAAR — Institut fuer Festkoerperforschung, Forschungszentrum 52425 Juelich

The phenomenon of fracture is of extraordinary relevance for our life. Cracks occur on all scales from nano- to kilometers, from tiny microcracks in material failure to the geological scales of earthquakes. Therefore, it is not surprising that a full modeling of rupture requires to separate a whole hierarchy of lengthscales, from the detailed structure of the tip region to the macroscopic scale of stress relaxation. Obviously, this leads to enormous numerical calculations. We present a simple theory that describes the entire fracture process in the framework of a macroscopic continuum theory of pattern formation, based only on the dynamical elasticity and phase transition dynamics. A phase field model is employed to solve the equations numerically on massively parallel computers with many hundreds of processors. We discuss predictions, limitations and possible extensions to the model.

DY 16.3 Mon 16:45 HÜL 186

Effect of a forced flow on dendritic solidification — ●THOMAS FISCHALECK and KLAUS KASSNER — Otto-von-Guericke-Universität Magdeburg, FNW/ITP, PF 4120, 39016 Magdeburg

The effects of convective flow on dendritic crystal growth and pattern formation have been an active research topic for many years, but have not been fully understood on the theoretical side. This is mainly because the governing equations are considerably more complicated than without flow and microscopic solvability theory, successfully describing a single free crystal growing into its quiescent supercooled melt, is no longer applicable in its original formulation.

Introducing an asymptotic decomposition scheme to nonlinear solvability theory we substantially extend the range of this concept and present a new approach to dendritic growth phenomena based on a free boundary formulation. This technique is demonstrated for dendritic growth in a forced potential flow.

DY 16.4 Mon 17:00 HÜL 186

KMC simulations of sintering nano-clusters including grain boundaries in 3D — ●MARTIN FENDRICH, RUSLAN ZINETULLIN, and DIETRICH E. WOLF — Institut der Physik, Universität Duisburg-Essen, Campus Duisburg, Germany

Thermal sintering processes of two nano-clusters are simulated using the Kinetic Monte-Carlo (KMC) method. 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 the two particles in contact. The simulations show that the qualitative sintering process may be divided into two stages. In the first stage a fast reorientation of the grains takes place leading to special classes of mutual torsions with misorienta-

tion angles between 0 and $\approx 80^\circ$. The frequencies in which orientations of the characteristic classes occur can be understood in terms of a coherent site lattice analysis. The evolution of the cluster's shape and the duration of the subsequent coalescence stage strongly depends on the adopted orientation of the grains.

DY 16.5 Mon 17:15 HÜL 186

Simulation of binary alloy cluster growth: Segregation, exchange processes, magnetic interactions and magnetic field effects — ●MARIO EINAX¹, STEFAN HEINRICHS¹, PHILIPP MAASS², and WOLFGANG DIETERICH¹ — ¹Fachbereich Physik, Universität Konstanz, D-78457 Konstanz — ²Institut für Physik, Technische Universität Ilmenau, D-98684 Ilmenau

We present detailed kinetic Monte Carlo (KMC) simulations of growing nanoclusters on a weakly interacting substrate within a fcc-type binary alloy model. This model is designed to describe recent molecular beam epitaxy experiments on CoPt₃ nanoclusters that develop perpendicular magnetic anisotropy (PMA) [1]. As a consequence of Pt surface segregation (driven by exchange processes) and cluster shape we find a growth-induced structural anisotropy, located near the cluster surface, which is compatible with experimentally observed magnetic properties [2]. Analytic approaches are discussed to clarify the competition between the incoming flux and surface equilibration processes leading to kinetically limited surface segregation.

In a second step our model is generalized to include an external magnetic field in the growth direction, which is found to induce bulk structural anisotropy favorable for PMA. Moreover, magnetic interactions are shown to have a significant influence on the bulk transition temperature for the onset of L1₂-ordering [3].

[1] M. Albrecht et al., Europhys. Lett. **56**, 884 (2001)

[2] S. Heinrichs et al., cond-mat/0510196

[3] M. Einax et al., to be published

DY 16.6 Mon 17:30 HÜL 186

Surface processes during low energy ion bombardment of glassy metallic thin films — ●SEBASTIAN VAUTH and S. G. MAYR — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Thin glassy metallic Zr₆₅Al_{7.5}Cu_{27.5} films are prepared by cocondensing the three components by electron beam evaporation under UHV conditions. After that the sample is irradiated in situ with keV-Kr⁺-ions and the surface topographies are analyzed by scanning tunneling microscopy (STM) with respect to structure formation and smoothing. The studies are performed as a function of irradiation conditions, viz. ion energy and fluence. The STM data are numerically analyzed by calculating the root mean square roughness and spectral power densities to track down the underlying surface mechanisms of structure formation. To get insight on a microscopic level we perform molecular dynamics (MD) simulations of glassy CuTi and Si films. We investigate temperature activated processes in comparison with processes caused by ion bombardment. To model the experimental results on a mesoscopic level we make use of stochastic rate equations describing the surface morphology. In similarity to equations to model film growth we develop an equation for irradiation based on our experimental and MD data. This work is financially supported by the DFG Sonderforschungsbereich 602, TP B3.

DY 16.7 Mon 17:45 HÜL 186

The isotropic-nematic interface in suspensions of platelets — ●TANJA SCHILLING¹, PAUL VAN DER SCHOOT², and DAVID VAN DER BEEK³ — ¹Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz, Staudinger Weg 7, Germany — ²Eindhoven University of Technology, Applied Physics, PO Box 513, 5600 MB Eindhoven, The Netherlands — ³Van 't Hoff Laboratory for Physical and Colloid Chemistry, Utrecht University, 3584 CH Utrecht, The Netherlands

Suspensions of plate-like particles phase separate into an isotropic and a nematic phase at sufficiently high concentrations. The reasons for this are identical to those for the formation of a nematic phase in suspensions in rod-like colloids: a strongly anisotropic excluded-volume interaction between the particles favours parallel alignment. However, there is a crucial difference between the nematic ordering of rods and platelets: Rods

may be quantitatively understood at the level of second virial theory whereas this is not the case for platelets. Presumably this is the reason why in the theoretical literature so much more emphasis has been on nematics of rods than on that of platelets. Also, experimentally it seems to be easier to suppress gelled states in rod dispersions than in plate ones. Recently, however, significant progress in the experimental study of suspensions of platelets has been made, making it timely to consider the issue in more detail.

We present a combined theoretical, simulational and experimental study of the isotropic-nematic interface. In particular, we show that its interfacial tension can be extracted from the capillary rise of the interface without knowledge of the elastic constants of the nematic phase.

DY 16.8 Mon 18:00 HÜL 186

Heat capacity of quasi-one-dimensional atomic adsorbates deposited in the grooves of carbon nanotube bundles — ●KONSTANTIN CHISHKO, TATIANA ANTSYGINA, and IGOR POLTAVSKY — B. Verkin Institute for Low Temperature Physics and Engineering, 47 Lenin Ave., Kharkov 61103, Ukraine

The model taking into account both the formation of one-dimensional (1D) condensate at the bottom of the external grooves on carbon nanotube bundles and also the promotion of two secondary 1D chains over primary one (three-chain quasi-one-dimensional structure) is developed to describe the thermodynamics of rare gas adsorption on the nanobundle surface. The Gibbs free energy and the heat capacity of the system under study have been obtained within a universal lattice gas approach using both two-time Green functions and transfer matrix methods with regard to interparticle interactions in the primary and secondary chains. So, the model is adequate for treatment of a rather wide range of coverages on the initial stage of deposition. The heat capacity has been found as functions of both temperature T and low-dimensional adsorbate density n_{ads} at different values of interparticle energies and the interaction energy between adsorbed atoms and the substrate nanobundle. As a function of n_{ads} , the heat capacity demonstrates non-monotonic behavior with peaks localized near $n_{ads} \simeq 1$ and $n_{ads} \simeq 3$ which correspond to completed occupation of the positions in the primary and secondary chains. The height and width of the peaks are determined by the magnitudes of the interaction energies in the system. All the effects predicted by the theory are accessible for the experimental observation.

DY 17 Superfluidity and Bose-Einstein-Condensation

Time: Monday 17:15–18:00

Room: SCH 251

DY 17.1 Mon 17:15 SCH 251

Bose-Einstein Condensate in Trapped Systems from a Canonical Point of View — ●KONSTANTIN GLAUM¹, HAGEN KLEINERT¹, and AXEL PELSTER² — ¹Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — ²Fachbereich Physik, Universität Duisburg-Essen, Universitätsstraße 5, 45117 Essen, Germany

We develop a perturbative path integral approach for calculating a recursion relation for the partition function of a fixed number N of weakly interacting bosons in different trap configurations. After performing a chain resummation of the perturbative result, we discuss how a two-particle δ -interaction influences the behaviour of the thermodynamic quantities near the quasi-critical point. Furthermore, we show that the heat capacity and the number of particles in the ground state, which defines the quasi-condensate, approach their thermodynamic limits uniformly for all temperatures.

DY 17.2 Mon 17:30 SCH 251

Emergence of superfluidity in the dynamics of a Bose-Einstein condensate in a parabolic lattice — ●JOACHIM BRAND¹ and ANDREY KOLOVSKY^{1,2} — ¹Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany — ²Kirensky Institute of Physics, 660036 Krasnoyarsk, Russia

The dynamics of a Bose-Einstein condensate is studied in a combined periodic plus harmonic external potential. The emergence and break-

down of superfluid transport in this system is analysed from a nonlinear-dynamics point of view. Unexpected regimes of stable collective dipole and Bloch oscillations are identified and explained in terms of quantum mechanical and classical pendulum models[1]. The theoretical analysis is supported by full numerical solutions of the discrete and continuous nonlinear Schrödinger equation.

[1] J. Brand and A. R. Kolovsky. E-print cond-mat/0412549

DY 17.3 Mon 17:45 SCH 251

Parametric Bose-Hubbard Hamiltonians and Structural Analysis of Eigenstates in the Chaotic Regime — ●MORITZ HILLER^{1,2}, TSAMPIKOS KOTTOS^{1,3}, and THEO GEISEL^{1,2} — ¹Max-Planck-Institut für Dynamik und Selbstorganisation, Bunsenstr. 10, D-37073 Göttingen, Germany — ²Fakultät für Physik, Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — ³Department of Physics, Wesleyan University, Middletown, CT-06459, USA

We consider a family of chaotic Bose-Hubbard Hamiltonians (BHH) parameterized by the coupling strength k between neighboring sites. As k increases, the eigenstates undergo changes which are reflected in the structure of the Local Density of States. We analyze these changes both numerically and analytically, using perturbative and semiclassical methods. The outcome of our studies is relevant to a vast number of experimental realizations of Bose-Hubbard Hamiltonians, like condensate systems in optical lattices and atom lasers.

DY 20 Quantum Dynamics I

Time: Tuesday 09:30–11:00

Room: HÜL 186

Invited Talk

DY 20.1 Tue 09:30 HÜL 186

Quantum Computer - dream and realization — ●RAINER BLATT — Technikerstrasse 25 A-6020 Innsbruck — Institut für Experimentalphysik, University of Innsbruck

Computational operations always rely on real physical processes, which are data input, data representation in a memory, data manipulation using algorithms and finally, the data output. With conventional computers all the processes are classical processes and can be described accordingly. Theoretically, it is known for several years now that certain computations could be processed much more efficiently using quantum mechanical operations. This requires the implementation of quantum bits (qubits), quantum registers and quantum gates and the development of quantum algorithms. Several approaches for the implementation of quantum computers will be presented, with special emphasis on the ion storage techniques. Experimental realizations of quantum registers and quantum gate operations using strings of trapped ions in a linear Paul trap will be discussed. With a small ion-trap quantum computer based on two and three trapped Ca⁺ ions as qubits we have generated in a pre-programmed way specific quantum states. In particular, entangled

states of two particles, i.e. Bell states, and of three particles, i.e. GHZ and W states, were generated using an algorithmic procedure. With a tomographic method, these states were subsequently analysed and the respective entanglement was characterized using various entanglement measures. With Bell states as a resource, entangled states are applied for teleportation and improved precision measurements.

DY 20.2 Tue 10:00 HÜL 186

Thermal and Nonthermal Relaxation in Spin Environments — ●HARRY SCHMIDT and GÜNTER MAHLER — Institut für Theoretische Physik 1, Universität Stuttgart

We investigate a small quantum system (the “central system”, typically a spin-1/2 particle), coupled to a large environment. The environments considered typically also consist of many spin-1/2 particles. Though large, the environment is not treated by a reservoir approximation but is modeled explicitly and the time evolution of the total system is treated exactly.

We are interested in the equilibrium state of the central system after relaxation from a product state. If the environment is initially in a

thermal state with a given temperature and the central system relaxes to a thermal state with the same temperature, the relaxation process is called “canonical” or “thermal”. Here we show that not all types of environments exhibit such a canonical relaxation. In particular, we present a method to quantitatively distinguish systems showing canonical relaxation from those that do not. This method is applied to spin environments with and without internal interaction showing a qualitative change in the relaxation behavior due to the interaction.

[1] Schmidt, Mahler: PRE **72**, 016117 (2005)

DY 20.3 Tue 10:15 HÜL 186

Thermal aspects of small spin systems — ●MARKUS HENRICH and GÜNTER MAHLER — 1. Institut für Theoretische Physik, Universität Stuttgart

With upcoming of nano-technologies there is more and more interest also in thermodynamic properties of nano- and mesoscopic systems. Numerically most accessible are small spin systems. These systems, when combined with appropriate baths, can show interesting thermal properties. Here we investigate spin systems with a Heisenberg interaction coupled to one or two baths under different local conditions. We show how these conditions influence the steady state of the spin system. In addition, for thermal equilibrium we compare different master-equation approaches with the exact Schroedinger-evolution [1].

[1] M. Henrich et al, “Global and local relaxation of a spin-chain under exact Schroedinger and master equation dynamics”, Phys. Rev. E **72**, 026104 (2005)

DY 20.4 Tue 10:30 HÜL 186

Statistical Dynamics in Closed Quantum Systems? — ●CHRISTIAN BARTSCH and JOCHEN GEMMER — Physics Department, University of Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

The time evolution of closed finite quantum systems is strictly given by the Schrödinger equation which itself yields only completely reversible dynamics. Nevertheless, there are calculations by HAM (Hilbert Space Average Method) suggesting that under certain conditions statistical behaviour of appropriate variables can evolve in such systems. For certain classes of few particle systems the numerical solution of the time-dependent Schrödinger equation has been compared with those predictions. The occurrence of statistical dynamics has been analyzed especially with respect to the spatial structure of the potentials which the particles encounter.

DY 20.5 Tue 10:45 HÜL 186

Ultrafast electron dynamics in thin metal films — ●GIOVANNI MANFREDI and PAUL-ANTOINE HERVIEUX — GONLO-IPCMS, 23 rue du Loess, BP 43, F-67034 Strasbourg, France

Self-consistent simulations of the ultrafast electron dynamics in thin metal films were performed using both semiclassical (Vlasov) and quantum (Wigner) phase-space models. Numerical results showed that: (i) heat transport is ballistic and occurs at a velocity close to the Fermi speed; (ii) after the excitation energy has been absorbed by the film, slow nonlinear oscillations appear, with a period proportional to the film thickness, which are attributed to nonequilibrium electrons bouncing back and forth on the film surfaces. These effects are robust and are not suppressed by electron-electron or electron-ion collisions.

When an oscillatory laser field is applied to the film, the field energy is partially absorbed by the electron gas. Maximum absorption occurs when the period of the external field matches the period of the nonlinear oscillations, which, for sodium films, lies in the infrared range. Possible experimental implementations are discussed.

DY 21 Statistical Physics (general) I

Time: Tuesday 10:00–11:45

Room: SCH 251

DY 21.1 Tue 10:00 SCH 251

Multiscale simulations of micro-structure selection in binary alloy solidification — ●HEIKE EMMERICH¹ and MATTHIAS JURGK² — ¹RWTH Aachen, Computational Materials Engineering, Center for Computational Engineering Science (CCES), Institute of Minerals Engineering (GHI), Mauerstrasse 5, 52064 Aachen — ²Max-Planck-Institut für Physics of Complex Systems, Noethnitzerstr. 38, 01187 Dresden

We demonstrate that the competition of dendritic crystals in a solidifying sample gives rise to two qualitatively different micro-structure solutions depending on the density ρ of crystals in the melt. Here we show for the first time, that there is a non-steady transition from one to the other. The precise ρ -dependence of the transition point is determined by the Biot number. Our investigation is based on a scaling analysis for the tip velocity of the dendritic crystals, which we assume to be aligned in an array and to be coupled via the transport of heat. We develop our analytical solutions based upon the asymptotic Kruskal-Segur reduction to a differential equation in the complex plane. It is supported by numerical simulations of a multiscale model of alloy growth. On the one hand this solution can be used to improve the accuracy of applied solidification simulations. On the other hand it yields additional insight in the universality of diffusion limited crystal growth in the presence of competing micro-structures.

DY 21.2 Tue 10:15 SCH 251

Coupled Phase Field/Monte Carlo Simulation for Heterogeneous Crystallization Kinetics — ●JÜRGEN HUBERT and HEIKE EMMERICH — RWTH Aachen, Computational Materials Engineering, Center for Computational Engineering Science (CCES), Institute of Minerals Engineering (GHI), Mauerstrasse 5, 52064 Aachen*

Phase field models are a now well established and rapidly growing section within the field of modeling the evolution phase transitions. Among other things they can be used for the simulation of nano crystallization processes, grain growth and heterogeneous nucleation. By combining the phase field method with Monte Carlo Algorithms, the evolution of the crystal orientation can be described with only a slight increase in the necessary computing power.

This entry will show new expansions of existing models, as well as

the possibilities and challenges of grain growth simulations with a large number of different crystal orientations.

DY 21.3 Tue 10:30 SCH 251

Size effects in molecular dynamics simulations of nucleation — ●JAN WEDEKIND¹, DAVID REGUERA², and REINHARD STREY¹ — ¹Institut für Physikalische Chemie, Universität zu Köln, Luxemburger Str. 116, D-50939 Köln, Germany — ²Universitat de Barcelona, Departament de Física Fonamental, Facultat de Física, Universitat de Barcelona, Martí i Franquès, 1, 08028-Barcelona, Spain

Most molecular dynamics (MD) simulations of vapor-liquid nucleation are performed in a closed, canonical NVT -system. Under these conditions the vapor pressure and thus the supersaturation change during the condensation and growth of a droplet due to the fixed total number of molecules N . Furthermore, the feasibility of observing a nucleation event may depend significantly on the size of the system at hand. We investigate the potential importance of finite size effects in MD simulations of nucleation in the framework of the modified liquid drop model (MLD) [1,2] and the implications of our investigations on the results reported in the literature. Furthermore we show with comparatively simple calculations how it is possible to estimate the system size in terms of N or similarly V , beyond which corrections due to size effects become negligible. By optimizing the system parameters it is possible to save valuable calculation time and extend the range of supersaturations attainable by simulations by several orders of magnitude.

[1] C. L. Weakliem and H. Reiss, J. Chem. Phys. **99** (7), 5374 (1993).

[2] D. Reguera, R. K. Bowles, Y. Dijkstraev, and H. Reiss, J. Chem. Phys. **118** (1), 340 (2003).

DY 21.4 Tue 10:45 SCH 251

Hole crystallization in semiconductors — ●MICHAEL BONITZ¹, VLADIMIR FILINOV², and HOLGER FEHSKE³ — ¹Institut für Theoretische Physik and Astrophysics, University Kiel, Leibnizstr. 15, 24098 Kiel — ²Institute for High Energy Density, Russian Academy of Sciences, Izhorskay 13/19, Moscow 127412, Russia — ³Institute of Physics, University Greifswald, 17487 Greifswald

Electrons and holes in a solid are normally delocalized over the crystal

lattice. However, it has been speculated [1,2] that, for a sufficiently large mass ratio $M = m_h/m_e$, hole localization and even crystallization should be possible. We present a theoretical analysis of the conditions of hole crystallization which yields a critical mass ratio M of about 80 and predictions of the possible density and temperature range. We also discuss the close relation of the hole crystals to ion crystals in classical plasmas and in ultradense stellar objects such as White Dwarfs and neutron stars.

A phase diagram of Coulomb crystals in electron-hole plasmas which is applicable to generic plasmas with two charge components is presented. The analytical results are confirmed by extensive first principle path integral Monte Carlo simulations which cover the transition from an excitonic gas to a hole crystal embedded into a Fermi gas of electrons.

- [1] B.I. Halperin, and T.M. Rice, Rev. Mod. Phys. 40, 755 (1968);
- [2] A.A. Abrikosov, J. Less-Comm. Metals 62, 451 (1978);
- [3] M. Bonitz, V.S. Filinov, V.E. Fortov, P.R. Levashov, and H. Fehske, Phys. Rev. Lett. (2005), accepted

DY 21.5 Tue 11:00 SCH 251

Mesoscopic fluctuations and intermittency in aging dynamics — ●PAOLO SIBANI — Fysisk Institut, SDU, Campusvej 55, DK5230 Odense M

Mesoscopic aging systems are characterized by large intermittent noise fluctuations. In a *record dynamics* scenario [P. Sibani and J. Dall, Europhys. Lett. 64, 2003] these events, or quakes, are treated as a Poisson process with average $\alpha \ln(1 + t/t_w)$, where t is the observation time, t_w is the age and α is a parameter. Assuming for simplicity that quakes constitute the only source of de-correlation, we present a model for the probability density function (PDF) of the configuration autocorrelation function. Beside α , the model has the average quake size $1/q$ as a parameter. The model autocorrelation PDF has a Gumbel-like shape, which approaches a Gaussian for large t/t_w and becomes sharply peaked in the thermodynamic limit. Its average and variance, which are given analytically, depend on t/t_w as a power-law and a power-law with a logarithmic

correction, respectively. Most predictions are in good agreement with recent data from the literature and with the simulations of the Edwards-Anderson spin glass carried out as a test.

DY 21.6 Tue 11:15 SCH 251

Lineabatic treatment of periodically driven stochastic systems — ●MYKHAYLO EVSTIGNEEV and PETER REIMANN — Universität Bielefeld, Unversitätsstr. 25, 33615 Bielefeld

A periodically driven noisy system in the limit of long times is considered. To deduce its asymptotic time-periodic probability distribution, two approaches are commonly used: adiabatic theory, valid if driving is very slow, and linear response theory, applicable when driving is weak. A novel approximation scheme - the lineabatic approximation - is introduced, which combines these two approaches to yield the driven probability distribution even when driving is moderately strong and fast, so that both linear response and adiabatic approximations break down. The accuracy of the lineabatic scheme is discussed based on specific examples.

DY 21.7 Tue 11:30 SCH 251

A connection between an exactly soluble stochastic control problem and a nonlinear reaction-diffusion equation — ●ROGER FILLIGER¹, MAX OLIVIER HONGLER², and LUDWIG STREIT¹ — ¹CCM, Universidade da Madeira, Portugal — ²IPR, EPF-Lausanne, Switzerland

We present an exactly soluble optimal stochastic control problem involving a diffusive two-state random evolution process and connect it to a non-linear reaction-diffusion type of equation by using the technique of logarithmic transformations. The work generalizes the recently established connection between a discrete two velocities, non-linear Boltzmann equation and the optimal control of a two-state random evolution process. We further show that the cost structure associated to the control problem is connected to the large deviations probabilities of the uncontrolled dynamics.

DY 22 Quantum Dynamics II

Time: Tuesday 11:00–13:00

Room: HÜL 186

DY 22.1 Tue 11:00 HÜL 186

“Hermite” states in the quantum interaction of vortices — ●ALEXEY ROMANOV, CHUKBAR KONSTANTIN, and ZABURDAEV VASILY — Russian Research Center ‘Kurchatov Institute’, pl. Kurchatova 1, 123182 Moscow

In this paper, we consider transition from classical dynamics of vortices to quantum. Problem of two identical cinematic vortices (each vortex produce 2d velocity field with current function $\psi(|\mathbf{r}|)$) reduces to the Hamiltonian system with Hamilton function $H(q, p) = \psi(\sqrt{q^2 + p^2})$ ($q=x$, $p=y$). We perform transition to quantum vortices dynamic according to the standard rule: $q \rightarrow q, p \rightarrow -i\hbar \frac{\partial}{\partial q}$. Now we start to solve quantum problem with Hamilton operator $\hat{H} = \hat{\psi}(\sqrt{\hat{r}^2})$, $\hat{r}^2 = -\hbar^2 \partial^2 / \partial q^2 + q^2$. Operator \hat{r}^2 corresponds to quantum oscillator with Hermite eigenfunction, and eigenvalue spectrum $(1, 3, \dots, 2n+1)$. So Hamiltonian \hat{H} , which describes dynamic of quantum vortex, has Hermite eigenfunctions and eigenvalue spectrum: $\psi(\sqrt{2n+1})$. Quantum oscillator has, so called, coherent states, which is stable during quantum evolution. Vortex Hamiltonian doesn’t have such states, because of dispersion of angular frequency. Also we consider transition for system with anisotropic current function $\psi = A \frac{x^2 - y^2}{(x^2 + y^2)^2}$.

DY 22.2 Tue 11:15 HÜL 186

The limited validity of the Kubo formula for thermal conduction. — ●JOCHEN GEMMER¹, ROBIN STEINGEWEG¹, and MATHIAS MICHEL² — ¹Physics Department, University of Osnabrück, Barbarastr. 7, 49069 Osnabrück — ²Institute of Theoretical Physics I, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

The Kubo formula describes a current as a response to an external field. In the case of heat conduction there is no such external field. We analyze why and to what extend it is nevertheless justified to describe heat conduction in modular quantum systems by the Kubo formula. “Modular” we call systems that may be described as consisting of weakly coupled identical subsystems. We explain in what sense this description applies to a large class of systems. Furthermore, we numerically evaluate the Kubo

formula for some finite modular systems. We compare the results with data obtained from the direct numerical solution of the corresponding time-dependent Schroedinger equation.

- [1] Michel et al. *Phys. Rev. Lett.*, **95**, 180602 (2005)

DY 22.3 Tue 11:30 HÜL 186

Relevance of the electronic environment for the neutron scattering behavior of protons — ●TYNO ABDUL-REDAH^{1,2}, ARIS C. CHATZIDIMITRIOU-DREISMANN³, and MATTHIAS KRZYSTYNIAK³ — ¹ISIS Facility, Rutherford Appleton Laboratory, UK. — ²School of Physical Sciences, The University of Kent at Canterbury, Canterbury, UK. — ³Inst. f. Chemie, TU Berlin, Berlin, Germany.

A large number of neutron Compton scattering (NCS) experiments on hydrogen containing materials like liquid water, metal hydrogen systems and organic compounds has been reported on where a striking effect of a strong neutron proton scattering cross section shortfall has been found (for an overview, see [1]). This effect - which has been very recently confirmed using electron-proton Compton scattering on organic polymers [2] - was attributed to the existence of short lived protonic quantum entanglement and/or to the breakdown of the Born-Oppenheimer approximation during the scattering process. Recent NCS experiments on various metal hydrogen systems strongly indicate the relevance of the electronic environment surrounding the proton. Concretely, changing the electronic charge density around or the bonding conditions of the protons leads to different cross section anomalies in those materials. It is concluded that the electronic environment determines the decoherence process of the protons thus leading to these different anomalous shortfalls.

- [1] T. Abdul-Redah et al., Neutron News 15 (2004) 14.
- [2] C. A. C.-Dreismann et al., Phys. Rev. Lett. 91 (2003) 057403.
- [3] T. Abdul-Redah et al., J. Alloys Compd. (2005), in press.

DY 22.4 Tue 11:45 HÜL 186

Novel sampling approaches for complex ensembles in ab-initio molecular dynamics — ●JOCHEN SCHMIDT^{1,2}, DANIEL SEBASTIANI¹, and CHRISTOPHER J. MUNDY² — ¹Max Plank Institute for Polymer Research, Mainz — ²Lawrence Livermore National Laboratory, Livermore CA, USA

Computer simulations using ab-initio approaches are a very important and widely used tool to study the microscopic behaviour of gases, liquids and solids. The traditional simulation of an NVE-ensemble does not reflect the usual experimental setup, where temperature and pressure are monitored. Besides this, there is an extensive interest in studying properties as a function of these quantities. Therefore the simulation of an NPT-ensemble is crucial. We present the implementation of constant pressure calculations in the highly parallel DFT-code QUICKSTEP, which is a part of the CP2K program package, using a mixed Gaussian and Plane Waves approach (GPW) [1]. This enables the application of our method to extended systems. Further, we use a recently developed method to simulate shock wave propagation in condensed matter, which allows the investigation of shock compression with ab-initio methods [2]. Both theoretical background and first applications will be presented.

[1] VandeVondele J., Krack M., Mohamed F., et al., Computer Physics Communications 167, 103 (2005)

[2] Reed E. J., Fried L. E. and Joannopoulos J. D., Phys. Rev. Lett. 90, 235503 (2003)

DY 22.5 Tue 12:00 HÜL 186

Normal transport behaviour in one-dimensional chaotic quantum systems — ●ROBIN STEINIGEWEG and JOCHEN GEMMER — Physics Department, University of Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

We investigate the transport behaviour of several one-dimensional (1D) quantum systems neither modelling heat baths nor using standard methods as the Kubo formula for heat conduction. Instead we numerically solve the corresponding time-dependent Schrödinger equation for various initial states and model parameters. It turns out that within the parameter range where normal transport occurs, that is, Fourier's law applies the nearest neighbour spacing distribution (NNLSD), $P(s)$, can be well described by a Wigner distribution. Amongst others we also investigate a spin system, namely a $s = 1/2$ Heisenberg chain in an external magnetic field B . Since this integrable system has a Poisson-like distribution $P(s)$ and does not show normal transport, we allow (small) local variations B_μ from the mean field B . As a consequence the distribution $P(s)$ becomes Wigner-like and normal transport occurs. This result reaffirms the assumption that normal transport behavior of 1D quantum systems is associated with a Wigner-like NNLSD.

DY 22.6 Tue 12:15 HÜL 186

Fourier's Law from Schrödinger Dynamics — ●MATHIAS MICHEL¹, JOCHEN GEMMER², and GÜNTER MAHLER¹ — ¹Institut für Theoretische Physik I, Universität Stuttgart — ²Fachbereich Physik, Universität Osnabrück

The relationship between microscopic and macroscopic levels of description has challenged physicists for centuries and in many branches of research. In this talk we demonstrate that a class of closed quantum systems gives rise to diffusive behavior (normal heat conduction, see [1]) on a mesoscopic level while the microscopic dynamics is governed by the respective Schrödinger equation only. The key to understanding such qualitative differences is not just the mere system size but rather the complete or reduced description as dictated by observation. For example, quantum thermodynamics [2] has been able to show that a partition of a closed quantum system into a small part of interest and a large environment will typically lead to thermal equilibrium properties with respect to the small part. In the same spirit, heat conduction and Fourier's law emerge from closed system quantum dynamics under appropriate coarse-graining in real space! Such a behavior may show up already in surprisingly small composite quantum objects.

[1] M. Michel et al., Phys. Rev. Lett. **95**, 180602 (2005)

[2] J. Gemmer et al., Quantum Thermodynamics, Springer (2004)

DY 22.7 Tue 12:30 HÜL 186

Effective quantum potentials — ●C. OLBRICH¹ and K. MORAWETZ^{1,2} — ¹Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — ²Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

An exact correspondence is established between a N -body classical interacting system and a $N - 1$ -body quantum system with respect to the partition function [1]. The resulting hermitian quantum-potential is a $N - 1$ -body one. Inversely the Kelbg potential is reproduced which describes quantum systems at a quasi-classical level. Such quantum potential allows to simulate quantum effects within the classical molecular dynamics reproducing the quantum correlation energy. We present a simple procedure to construct such effective quantum potentials for any temperature and density and present simulation results for the conductivity in quasi two-dimensional systems.

[1] K. Morawetz; Phys. Rev. E 66 (2001) 022103

DY 22.8 Tue 12:45 HÜL 186

Continuous time quantum walks in phase space — ●OLIVER MÜLKEN — Institut für Physik, Universität Freiburg

We formulate continuous time quantum walks (CTQW) in a discrete quantum mechanical phase space. We define and calculate the Wigner function (WF) and its marginal distributions for CTQWs on circles of arbitrary length N . The WF of the CTQW shows characteristic features in phase space. Revivals of the probability distributions found for continuous and for discrete quantum carpets do manifest themselves as characteristic patterns in phase space.

\Zitat{1}{arXiv: quant-ph/0509141}

DY 23 Statistical Physics (general) II

Time: Tuesday 11:45–13:15

Room: SCH 251

DY 23.1 Tue 11:45 SCH 251

Strong disorder fixed point in the dissipative random transverse field Ising model — ●GREGORY SCHEHR and HEIKO RIEGER — Theoretische Physik, Universität Saarbrücken

We study the zero temperature equilibrium properties of the random transverse Ising model (RTFIM) where each spin is coupled to an ohmic bath of harmonic oscillators. We propose a real space renormalization group (RG) procedure that we then study numerically. We determine the phase diagram and the critical exponents, which are found to be independent of the dissipative strength. In addition we find some indication for a diverging dynamical exponent when approaching the transition, suggesting that the critical behavior is governed by a new infinite randomness fixed point, with "activated" scaling.

DY 23.2 Tue 12:00 SCH 251

Small Scale Anisotropy in Lagrangian Turbulence — ●EBERHARD BODENSCHATZ^{1,2}, NICHOLAS OUELLETTE², HAITAO XU², and MICKAEL BURGOIN² — ¹MPI for Dynamics and Self-Organization, Goettingen — ²Cornell University, Ithaca, NY

Intense turbulence is generally assumed to be statistically isotropic at small length and time scales regardless of the symmetries of the large scale flow. We have studied the effects of large scale anisotropy on small scale turbulent fluctuations via the second order Lagrangian velocity structure function and the Lagrangian velocity spectrum in an intensely turbulent laboratory flow using three dimensional optical particle tracking. We find that the asymmetries of the large scale flow are reflected in small scale statistical quantities, though with no change of the scaling exponents. In addition, we present new measurements of the Lagrangian structure function scaling constant S_{C_0} , which is of central importance to stochastic turbulence models as well as to the understanding of turbulent pair dispersion and scalar mixing, from both the structure function

and the spectrum, and the two measurements are shown to agree. The scaling of \mathcal{C}_0 with the turbulence level is also investigated, and found to be in agreement with an existing model.

DY 23.3 Tue 12:15 SCH 251

The order-disorder transition in the Coulomb glass lattice model — ●ARNULF MÖBIUS and ULRICH RÖSSLER — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Phase transitions in the Coulomb glass have been under controversial debate for two decades, from first numerical studies to recent analytical theory [1]. Here we numerically investigate lattices half-filled with localised particles interacting via the long-range Coulomb potential. For zero static disorder and finite temperature T , order-disorder transitions are observed for dimensions $d = 2$ and 3 . Surprisingly, the critical properties are consistent with the Ising model with short-range interaction [2].

To study the influence of static disorder at $T = 0$, we developed an efficient procedure for the ground state search. It combines branch-and-bound type algorithms for complex relaxation steps, thermal cycling, flooding local minima, relaxation of cluster excitations, and renormalisation. Thus ground states of samples of up to 12^3 sites are found with high probability. Studying 2d and 3d lattices with a random on-site potential, rectangularly distributed between $-B/2$ and $B/2$, we observed an order-disorder transition for $d = 3$. Using finite-size scaling, we obtained $B_c = 0.375 \pm 0.015$ as critical disorder strength for lattice constant 1. This value exceeds the result of the nonlinear screening theory [1] by a factor of roughly 2. However, for $d = 2$, already arbitrarily small disorder seems to destroy the ordered phase.

[1] S. Pankov, V. Dobrosavljevic, Phys. Rev. Lett. **94**, 049402 (2005).

[2] A. Möbius, U.K. Rößler, cond-mat/0309001.

DY 23.4 Tue 12:30 SCH 251

Multi-Channel Transport in Disordered Medium under Generic Scattering Conditions: A Transfer Matrix Approach — ●PRAGYA SHUKLA — Department of physics, IIT Kharagpur-721302, West Bengal, India

A variety of transport properties can be formulated in terms of the eigenvalues of transmission matrix of the region. The knowledge of the statistical behavior of transmission eigenvalues is therefore very useful in the statistical analysis of transport properties. This motivates us to study the joint probability distribution of transmission eigenvalues. Previous attempts in this direction have resulted in the well-known DMPK equation which describes the statistical evolution of transmission eigenvalues with respect to changing length of the medium. Various assumptions made in its derivation, however, restrict its applicability to quasi

one dimensional systems or under specific scattering conditions. As the transport properties are also sensitive to other system parameters besides length e.g., boundary conditions, disorder strength and dimensionality, a generalization of DMPK equation for higher dimensions and under generic scattering conditions is required. The talk discusses our results obtained in this direction. Our results show that the evolution of transmission eigenvalues, due to changes in various physical parameters in a disordered region of arbitrary dimensions, is governed by a single complexity parameter; this implies a deep level of universality of transport phenomena through a wide range of disordered regions.

DY 23.5 Tue 12:45 SCH 251

Application of Zhangs Square Root Law and Herding to Financial Markets — ●WAGNER FRIEDRICH — Institut für Theoretische Physik, Universität Kiel, Leibnizstr.15, D-24098 Kiel

We apply an asymmetric version of Kirman's herding model to volatile financial markets. In the relation between returns and agent concentration we use the square root law proposed by Zhang. This can be derived by extending the idea of a critical mean field theory suggested by Plerou et al. We show that this model is equivalent to the so called 3/2-model of stochastic volatility. The description of the unconditional distribution for the absolute returns is in good agreement with the DAX independent whether one uses the square root or a conventional linear relation. Only the statistic of extreme events prefers the former. The description of the autocorrelations are in much better agreement for the square root law. The volatility clusters are described by a scaling law for the distribution of returns conditional to the value at the previous day in good agreement with the data.

DY 23.6 Tue 13:00 SCH 251

The inverse scattering problem of traffic flow — ●MARTIN TREIBER, ARNE KESTING, and DIRK HELBIG — Technische Universität Dresden

We discuss one-dimensional stochastic driven multi-particle systems with asymmetric next-neighbour interactions such as traffic flow. Based on a Fokker-Planck approach, it is possible to approximatively calculate the stationary velocity and distance distributions among the elements (driver-vehicle units) as a function of the generalized interaction potential. The results relate to the ones known from Random Matrix Theory.

In this contribution, we propose a method to treat the inverse problem, i.e., determining the generalized interaction potential, the acceleration function, and the strength of the stochastic force from empirical single-vehicle data. We apply the method to data from a Dutch freeway and compare the resulting empirical acceleration function with that of popular car-following models.

DY 24 Brownian Motion and Kinetic Theory I

Time: Tuesday 14:30–16:15

Room: HÜL 186

DY 24.1 Tue 14:30 HÜL 186

Balancing between source and target - a novel kind of fractional Fokker-Planck operator — ●VITALY BELIK, DIRK BROCKMANN, and THEO GEISEL — MPI für Dynamik und Selbstorganisation, Göttingen

Based on the recently introduced concept of topological superdiffusion we introduce a novel kind of fractional Fokker-Planck operator for random motion in inhomogeneous environments which incorporates the relative impact of the source and target location of an underlying random walk. We show that the dynamics in weak inhomogeneities exhibits distinct regimes of attenuation and enhancement. The operator can be constructed in two ways: with non-normalized Boltzmann-like probability density (a), which corresponds to some common physical systems, such as hetero-polymers, and normalized one (b), which naturally arises in population dynamical systems. We show that in the limit of ordinary diffusion an increase in the target influence slows down the process in either case. Surprisingly, a superdiffusive process may either be slowed down or enhanced with increasing target influence, in contrast with the common belief that external quenched disorder generally attenuates dispersion. As our theory obeys ordinary Gibbs-Boltzmann thermodynamics we believe that it will facilitate the understanding of a number of anomalous transport phenomena in fields such as intracellular transport and dispersal phenomena in ecological systems.

DY 24.2 Tue 14:45 HÜL 186

Diffusion in disordered fractals — ●JANETT BALG, DO HOANG NGOC ANH, KARL HEINZ HOFFMANN, STEFFEN SEEGER, and SUJATA TARAFDAR — Institut für Physik, Technische Universität Chemnitz - D-09107 Chemnitz, Germany

Diffusion in disordered media shows anomalous behavior for certain length scales. In order to model anomalous diffusion random-walks on regular fractals were usually used. Here we study disordered fractals in an attempt to capture the random nature of the disordered material by randomly mixing different Sierpinski carpet generators. In particular, we investigate the diffusion on the resulting fractals by random-walk simulations and exact enumeration. We find that the random-walk exponent d_w shows a strong dependence on the mixture composition. Beyond that we consider the influence of external fields on the movement of the diffusing particles.

DY 24.3 Tue 15:00 HÜL 186

Dissipative spin ratchets — ●DARIO BERCIoux, MILENA GRIFONI, and KLAUS RICHTER — Institut für Theoretische Physik, Universität Regensburg, Germany

Spin ratchets [1] are a novel class of ratchet systems [2] based on the spin inversion asymmetry induced by spin-orbit interaction in confined structures. For such systems, it has been shown that it is possible to

generate, under the influence of an unbiased driving force, a net spin current different from zero without additional charge current.

In this contribution we present results with respect to the influence of an external environment coupled with the spin ratchet. We approximate the spin ratchet with an effective two-band tight-binding Hamiltonian in presence of spin-orbit interaction. The environment is represented by a bath of harmonic excitations bilinearly coupled to the particle position [3]. All the calculations are done in the framework of the real-time path integral technique [3].

[1] A. Pfund, D. Bercioux, and K. Richter in preparation.

[2] P. Reimann, *Phys. Rep.* **361**, 57 (2002).

[3] U. Weiss, *Quantum dissipative systems*, World Scientific, 2001

DY 24.4 Tue 15:15 HÜL 186

Effective Approximations of First Passage Time Distributions of Non-Markovian Processes — •TATJANA VERECHTCHAGUINA, IGOR M. SOKOLOV, and LUTZ SCHIMANSKY-GEIER — Institut für Physik, Humboldt Universität zu Berlin, 12489 Berlin

Motivated by the dynamics of resonant neurons we discuss the properties of the first passage time (FPT) densities for nonmarkovian differentiable random processes. We start from an exact expression for the FPT density in terms of an infinite series of integrals over joint densities of level crossings, and consider different approximations based on truncation or on approximate summation of this series. Thus, the first few terms of the series give good approximations for the FPT density on short times. For rapidly decaying correlations the decoupling approximations perform well in the whole time domain.

As an example we consider resonate-and-fire neurons representing stochastic underdamped or moderately damped harmonic oscillators driven by white Gaussian or by Ornstein-Uhlenbeck noise. We show, that approximations reproduce all qualitative different structures of the FPT densities: from monomodal to multimodal densities with decaying peaks. The approximations work for the systems of whatever dimension and are especially effective for the processes with narrow spectral density, exactly when markovian approximations fail.

DY 24.5 Tue 15:30 HÜL 186

Entropic transport in symmetric tubes — •POORNACHANDRA S. BURADA, GERHARD SCHMID, and PETER HÄNGGI — Institut für Physik, Universität Augsburg

We study the transport of biased Brownian particles in symmetric tubes in two and three dimensions with periodically varying cross-section. Bottlenecks which produce entropic barriers hinder the motion of the particles and exhibit peculiar characteristics in the transport behavior which are different from that taking place in systems with energy barriers [1]. The constrained dynamics is responsible for an existence of a scaling regime for the particle current and the diffusion coefficient in terms of the ratio between the work done to the particles and thermal energy. Our findings, genuine of the entropic nature of the barriers, can be used in the control of transport through quasi-one dimensional structures, such as pores, ion channels and zeolites, in which irregularities of the boundaries may induce entropic effects. The kinetic description of

the dynamic quantities have been developed within an analytic approach [2] and corroborated by simulations.

[1] P. Reimann, C. Van den Broeck, H. Linke, P. Hänggi, J.M. Rubi, and A. Pérez-Madrid *Phys. Rev. Lett.* **87**, 010602 (2001).

[2] D. Reguera and J.M. Rubi, *Phys. Rev. E* **64**, 061106 (2001).

DY 24.6 Tue 15:45 HÜL 186

High-efficiency Deterministic Josephson Vortex Ratchet — •EDWARD GOLDOBIN¹, MARKUS BECK¹, MANFRED NEUHAUS², MICHAEL SIEGEL², REINHOLD KLEINER¹, and DIETER KOELLE¹ — ¹Universität Tübingen, Physikalisches Institut - Experimentalphysik II, Auf der Morgenstelle 14, D-72076, Tübingen, Germany — ²Universität Karlsruhe, Institut für Mikro- und Nanoelektronische Systeme, Hertzstraße 16, 76187 Karlsruhe, Germany

We investigate experimentally a Josephson vortex ratchet — a fluxon in an asymmetric periodic potential driven by a deterministic force with zero time average. The highly asymmetric periodic potential is created in an underdamped annular long Josephson junction by means of a current injector providing an average velocity of the ac driven fluxon of up to 91% of the Swihart velocity. We measured the ratchet effect for driving forces with different spectral content. For monochromatic high-frequency drive the rectified voltage becomes quantized. At high driving frequencies we also observe chaos, sub-harmonic dynamics and voltage reversal due to the inertial mass of a fluxon.

[1] *Phys. Rev. Lett.* **95**, 090603 (2005).

DY 24.7 Tue 16:00 HÜL 186

Localization Transition of the 3D Lorentz Model and Continuum Percolation — •THOMAS FRANOSCH^{1,2}, FELIX HÖFLING¹, and ERWIN FREY² — ¹Hahn-Meitner-Institut, Abteilung Theorie, Glienicker St. 100, D-14109 Berlin — ²Arnold Sommerfeld Center and CeNS, Department of Physics, Ludwig-Maximilians-Universität München, Theresienstrasse 37, D-80333 München

The Lorentz model has served as a paradigm for transport in disordered media. It describes a structureless test particle moving in a random array of identical obstacles which interact with the test particle via a hard-sphere repulsion. At high densities, the model exhibits a localization transition, i. e., above a critical density, the test particle is always trapped by the obstacles.

It has been a longstanding open question whether the dynamics close to the critical density can be mapped to the transport properties of continuum percolation (“Swiss cheese model”). The fractal nature of the void space between the overlapping spheres in the Lorentz model suggested to use a description in terms of an equivalent random resistor network model.

We present extensive Molecular Dynamics simulations and provide the first unambiguous evidence for an intimate connection between the Lorentz model and continuum percolation [1]. In particular, we show the validity of a generalized dynamic scaling theory employing two divergent length scales, and discuss corrections to scaling. The non-Gaussian parameter is predicted to diverge close to the transition.

[1] F. Höfling, T. Franosch, and E. Frey, *cond-mat/0510442*.

DY 25 Granular Matter and Contact Dynamics I

Time: Tuesday 14:30–16:30

Room: SCH 251

DY 25.1 Tue 14:30 SCH 251

3D-Modelling of Powder Flow and Application to Gravity Die Filling — •CLAAS BIERWISCH, TORSTEN KRAFT, MICHAEL MOSELER, and HERMANN RIEDEL — Fraunhofer-Institut für Werkstoffmechanik, Wöhlerstraße 11, 79108 Freiburg, Germany

Gravity filling of a cavity (die) via filling shoe movement as used in powder technological molding is investigated by means of three-dimensional discrete element method (DEM) simulations. A homogeneous spatial density distribution of the powder after the filling stage is crucial for the quality of the produced part. Powder properties, filling shoe kinematics, and die geometry influence the density distribution.

The used powder model comprises granular friction and cohesion whereas particle morphology is taken into account by describing the grains as clusters of spherical subunits. This way powders with significant different rheological behavior can be simulated. Powder flow is characterized in terms of the dimensionless Beverloo coefficient C [1] and

validated by experimental flow meter data.

Realistic die filling processes including up to 10^7 particles are studied using a highly parallelized numerical code. Effects of cavity geometry and filling shoe movement on the final density distribution are presented for different powders. Comparisons with die filling experiments [2] will be given.

[1] W. A. Beverloo *et al.*, *Chem. Eng. Sci.* **15** (1961) 260-269

[2] L. C. R. Schneider *et al.*, *Powder Metallurgy* **48** (1) (2005) 77-84

DY 25.2 Tue 14:45 SCH 251

A discrete particle model for long time sintering — •STEFAN LUDING — Particle Technology, Nanostructured Materials, DelftChemTech, Julianalaan 136, 2628 BL Delft, Netherlands

A model for the sintering of polydisperse, inhomogeneous arrays of cylinders is presented with empirical contact force-laws, taking into account plastic deformations, cohesion, temperature dependence (melting),

and long-time effects. Samples are prepared under constant isotropic load, and are sintered for different sintering times. Increasing both external load and sintering time leads to a stronger, stiffer sample after cooling down. The material behavior is interpreted from both microscopic and macroscopic points of view.

Among the interesting results is the observation, that the coordination number, even though it has the tendency to increase, sometimes slightly decreases, whereas the density continuously increases during sintering – this is interpreted as an indicator of reorganization effects in the packing. Another result of this study is the finding, that strongly attractive contacts occur during cool-down of the sample and leave a sintered block of material with almost equally strong attractive and repulsive contact forces.

DY 25.3 Tue 15:00 SCH 251

A granular meltdown — ●ANDREAS GÖTZENDORFER¹, CHIH-HWANG TAI², CHRISTOF A. KRUELLE¹, and INGO REHBERG¹ — ¹Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth — ²Department of Mechanical Engineering, National Central University, Chung-Li 32054, Taiwan

The behaviour of vibrated granular matter is of paramount importance to many industrial processes, and is therefore studied extensively by engineers. But also in the physics community the fluidization of granular beds by vibration has evolved into a very active field of research during the last fifteen years. In our experiments we submitted a two-dimensional granular packing to vertical sinusoidal container oscillations. The initially close packed bed consists of six particle layers. With increasing shaking amplitude at first the particles close to the free surface start to become mobile. When a critical value of the forcing strength is reached the remaining crystalline structure suddenly breaks up and the bed fluidizes completely, causing the centre of mass height to increase by leaps and bounds. Further investigating into this discontinuous transition we examine the distribution of particles and their displacements as functions of the forcing strength.

DY 25.4 Tue 15:15 SCH 251

Axial segregation of granulate in a long horizontal rotating drum — ●TILO FINGER¹, ANDREAS VOIGT², and RALF STANNARIUS¹ — ¹Otto-von-Guericke-University Magdeburg — ²Max-Planck-Institute for Dynamics of Complex Technical Systems Magdeburg

The axial segregation of granular material in a long horizontal rotating drum is a well known phenomenon. We investigate experimentally the structures and the long time behaviour of this process. The drum is half filled with a mixture of glass beads of two different diameters and filled up with water. After starting a constant rotation, the material shows a radial segregation on a time scale of few seconds. On a time scale of few minutes, an additional axial segregation appears and a stripe pattern along the cylinder axis becomes visible. The initial width of stripes is more or less regular. When the rotation continues, the number of stripes decreases. The time scale of coarsening of the pattern is of the order of several hours up to days. We measure the coarsening at different rotation frequencies and determine the three dimensional distribution of the grains by magnetic resonance imaging. By preparation of initial stripe patterns with well defined geometry, we analyse details of the coarsening process and the relation between the 3D segregation structures and coarsening dynamics.

DY 25.5 Tue 15:30 SCH 251

The Horizontal Brazil-Nut Effect — ●KERSTIN MORBER, CHRISTOF KRUELLE, and INGO REHBERG — Universität Bayreuth, D-95440 Bayreuth, Germany

The behaviour of spheres rolling on a circularly vibrating table in a circular container is observed. In detail, transport effects in a monolayer

consisting of a binary mixture are studied. Depending on the ratio of the particles' material density and size, migration of the larger particles occurs either towards the boundary or to the center of the circular container. The precise crossing point between both migration effects is determined by varying the intruder's size and maintaining its material density.

DY 25.6 Tue 15:45 SCH 251

Behaviour of Granular Flow under Variable Gravitational Level — ●ANTJE BRUCKS¹, TIM ARNDT¹, and RICHARD M. LUEPTOW² — ¹Zentrum f. angew. Raumfahrttechnologie u. Mikrogravitation, Universität Bremen, Am Fallturm, 28357 Bremen — ²Department of Mechanical Engineering, Northwestern University, Evanston, IL 60208, USA

While gravity drives most granular shear flows including geologic situations (landslides and sandpiles on a beach) as well as in industrial applications (processing of food and pharmaceuticals), the effect of changing the gravitational acceleration is largely unexplored. Hence, our understanding of gravity-driven granular flows is based almost exclusively on experiments under Earth's gravity, with one exception (AIAA J. 28(10),1701-1702 (1988)). We explore the behaviour of the flowing shear layer flow in a tumbler of radius r rotating at ω and the underlying creeping motion subsurface flow over a range of g -levels from $1g$ to $25g$. We show that the dynamic angle of repose, or slope, of the flowing shear layer is properly characterized by the Froude number, $Fr = \omega^2 r/g$, when the gravitational acceleration g is varied over several orders of magnitudes of the Froude number in a large centrifuge. However, the flowing layer thickness is essentially independent of the g -level for identical Froude numbers, suggesting that the shear rate in the flowing layer must increase with increasing g -level.

DY 25.7 Tue 16:00 SCH 251

Discrete element model based simulation of the sintering of powders — ●ANDREAS WONISCH, TORSTEN KRAFT, MICHAEL MOSELER, and HERMANN RIEDEL — Fraunhofer-Institut für Werkstoffmechanik, Wöhlerstraße 11, 79108 Freiburg

Sintering is an important process step in powder technology in which the separate grains are bonded together by heating them at high temperature below the melting point. While this process has been successfully described by continuum-mechanics modeling there are still many open questions regarding the influence of grain rearrangement. By applying the discrete element method (DEM) we investigate how rearrangements on a microscopic scale change macroscopic properties like densification rate or viscosity. We simulate both free and pressure assisted sintering (sinter forging) by starting from a random aggregate of particles in a simulation box with periodic boundary conditions. We also observe crack formation when simulating constrained sintering with low density isotropic configuration of several hundred thousand particles. We further show how anisotropic starting configurations (e.g. from DEM powder compaction simulations) have a significant influence on the sintering behavior.

DY 25.8 Tue 16:15 SCH 251

Relaxation Times in Sheared Granular Matter — ●LOTHAR BRENDEL, DIRK KADAU, and DIETRICH E. WOLF — University Duisburg-Essen, Theoretical Physics

A significant feature of granular matter is the existence of memory effects, making a thermodynamic-like approach not generally applicable. In this context, monitoring of temporal correlations within the microstructure can provide crucial insights. We present auto correlation functions related to the local fabric, measured in discrete element simulation of non-cohesive as well as cohesive materials. We mainly focus on steady state flow which is an important concept for characterizing granular materials in the applied field of powder technology.

DY 26 Brownian Motion and Kinetic Theory II

Time: Tuesday 16:15–18:15

Room: HÜL 186

DY 26.1 Tue 16:15 HÜL 186

On reaction-subdiffusion equations — ●I.M. SOKOLOV¹, M.G.W. SCHMIDT², and F. SAGUÉS² — ¹Humboldt-Universität zu Berlin — ²Universitat de Barcelona

To analyze possible generalizations of reaction-diffusion schemes for

the case of subdiffusion we discuss a simple monomolecular conversion $A \rightarrow B$. We derive the corresponding kinetic equations for local A and B concentrations. Their form is rather unusual: The parameters of reaction influence the diffusion term in the equation for an educt A , a consequence of the nonmarkovian nature of subdiffusion. The equation for a product contains a term which depends on the educt concentration

at all previous times. Our discussion shows that reaction-subdiffusion equations may not resemble the corresponding reaction-diffusion ones.

Preprint: cond-mat/0510354

DY 26.2 Tue 16:30 HÜL 186

Stochastic resonance in a domain with two reflecting boundaries

— •ELISABETH PAULE¹, TH. PLETL¹, P. CHVOSTA², M. SCHULZ¹, and P. REINEKER¹ — ¹Department of Theoretical Physics, University of Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany — ²Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University, V Holesovickach 2, CZ-180 00 Praha, Czech Republic

We present our numerical results of a one-dimensional diffusion process of a particle in a linear time-dependent potential. The particle is moving in a domain with two reflecting boundaries. The corresponding external force consists of two parts, a time independent part pushing the particle to the right boundary and a harmonically oscillating part. We solve the Fokker-Planck equation (FPE) with the Finite-Element Method (FEM). From the numerical solution of the FPE we calculate the mean position of the particle for different diffusion coefficients and different strengths of the oscillating force. It is shown that the mean position is an oscillating function. In the stationary limit we regard the variation of the amplitude of the mean position with the diffusion coefficient for different strengths of the external time-dependent force. The response of the system shows resonance like behavior for a range of the strength of the external oscillating force. There is a force strength for which this resonance like behavior disappears.

DY 26.3 Tue 16:45 HÜL 186

Universal scaling in anomalous transport — •I. GOYCHUK¹, E. HEINSALU^{1,2}, M. PATRIARCA¹, G. SCHMID¹, and P. HÄNGGI¹ — ¹Institut für Physik, Universität Augsburg, Germany — ²Institute of Theoretical Physics, Tartu University, Estonia

Anomalous transport in tilted periodic potentials is investigated within the framework of the *fractional* Fokker-Planck dynamics and the underlying continuous time random walk (CTRW). The analytical solution for the stationary anomalous current is obtained in closed form. We also derive a scaling law relating the anomalous biased diffusion to the anomalous current which is universally valid for tilted periodic potentials. The agreement between analytical results and numerical simulations confirms our findings.

DY 26.4 Tue 17:00 HÜL 186

Hydrodynamic coupling of rotation and translation between two colloidal particles

— •T. GISLER, S. MARTIN, M. REICHERT, and H. STARK — Universität Konstanz, Fachbereich Physik, Fach M621, 78457 Konstanz

We use optical tweezers combined with fast video microscopy to measure the coupling between translation and rotation of two colloidal spheres with diameters of 3 – 4 μm . Imaging the birefringent particles under crossed polarizers allows us to determine the positions and orientations of both particles simultaneously. Cross-correlations between random displacements of one particle and orientational fluctuations of its neighbor allow us to quantify the translation-rotation coupling induced by hydrodynamic interactions. Our results are in good agreement with the theory in the creeping-flow limit (M. Reichert and H. Stark, Phys. Rev. E **69**, 031407 (2004)).

DY 26.5 Tue 17:15 HÜL 186

Anomalous diffusion in proteins — •THOMAS NEUSIUS and JEREMY C. SMITH — Computational Molecular Biophysics Group, Interdisziplinäres Zentrum für wissenschaftliches Rechnen, Im Neuenheimer Feld 368, 69120 Heidelberg

Diffusion processes which show long time memory effects are discussed in many fields of physics. The subdiffusive behavior of a single protein mode was described recently in the framework of generalised Langevin equations with fractional noise [1].

The underlying microscopic dynamics leading to this specific kind of noise are yet to be completely understood. The characterisation of the emergence of anomalous diffusion by looking at different types protein modes will be undertaken. We assume that there are different categories which can be defined by their contribution to quantities such as the mean square deviation or their degree of anharmonicity. As the anomalous diffusion is a property of the whole molecule, it is likely that only the modes involving a large number of atoms show strong deviations from the classical Brownian motion.

[1] S. C. KOU and X. SUNNEY XIE: Phys. Rev. Lett. **93** (2004) 18, p. 180603.

DY 26.6 Tue 17:30 HÜL 186

Random Walk Model with Waiting Times Depending on the Preceding Jump Length

— •VASILY ZABURDAEV — MPI for Dynamics and Self-Organization, Bunsenstr.10, 37073 Göttingen, Germany

In the present work the generalized continuous time random walk model with a coupled transition kernel is considered. The coupling occurs through the dependence of the waiting time probability distribution on the preceding jump length. The method, which involves the details of the microscopic distribution over the waiting times and arrival distances at a given point, is suggested for its description. In the particular case of coupling, when a waiting time is a simple function of a preceding jump length, a close analogy to the problem of a random walk with finite velocity is demonstrated. With its help an analytical solution for the generalized random walk model, including both effects (finite velocity and jump dependent waiting times) simultaneously, is found. Considered examples indicate a possibility to apply the developed approach to the biological problems where the random walk together with the recovery processes and the finite velocity are present, such as e.g. the foraging movements of animals or the motion of zooplankton.

DY 26.7 Tue 17:45 HÜL 186

On the Validity of the Peierls-Boltzmann Equation

— •MEHMET KADIROGLU — D-49069 Osnabrück

Thermodynamic behaviour of closed quantum chains and rings is investigated by using the "Hilbert Space Average-Method" (HAM). In the context of heat conduction we are especially interested in whether or not the "Stoßzahlansatz" which is crucial for the validity of the Boltzmann equation is justifiable for (small) quantum systems. To those ends we developed a modified "Peierls-Boltzmann-equation in which the "quasi-particles" are replaced by current-eigenstates. Our main aim is to decide whether this ansatz applies to heat transport in our finite quantum systems.

DY 26.8 Tue 18:00 HÜL 186

On a Non-Markovian Fokker-Planck equation

— •KNUD ZABROCKI and STEFFEN TRIMPER — Martin-Luther-University Fachbereich Physik, 06099 Halle,

We consider a model for a probability distribution function $p(x,t)$ which is subjected to the distribution function at a former time via a feedback coupling. As a consequence the behaviour of $p(x,t)$ is changed drastically. Whereas for a long range feedback coupling, i.e. a coupling to the initial distribution function, the system offers non-trivial stationary solution, in case of a short time coupling this stationary distribution disappears. We demonstrate that this non-Markovian Fokker-Planck equation without a drift term is equivalent to a Fokker-Planck-equation with a drift term. Different initial distributions and their influence on the stationary solution in one dimension are analysed in detail. The investigation can be extended to higher dimensions. Depending on the initial condition and the dimension, the system reveals different drift terms and entirely different potentials. A further generalization is given by a kind of co-moving frame. In that case a particle, performing a random walk, is affected at a given time t by all processes taking place within a sphere of radius $R = vt$. For a non-zero velocity v the system exhibits three distinguished time regimes with complete different behaviour. The model could be applied for glasses and strongly inhomogeneous systems.

DY 27 Granular Matter and Contact Dynamics II

Time: Tuesday 16:30–18:00

Room: SCH 251

DY 27.1 Tue 16:30 SCH 251

Can one hear the shape of a ball? — ●C.A. KRÜLLE — Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth

The coefficient of restitution for the impact of a ball falling on a smooth horizontal surface can be measured by utilizing a very simple and practical method originally suggested by Alan D. Bernstein (Am. J. Phys. 45, 41 (1977)): The typical ticktack generated by multiple collisions between the bouncing object and the underlying plane is recorded by use of a microphone connected with the sound card of a PC. From this the restitution coefficient can be derived easily as the ratio of successive time intervals between sound signals. If the falling object is not precisely spherical the obtained values for the coefficient of restitution will scatter depending on - among other things - the degree of ellipticity. A careful analysis of this dependence shows that modern audio recording devices have been developed to such a high level that even deviations in the micron range can be detected and thus "heard" by a careful listener.

DY 27.2 Tue 16:45 SCH 251

Gas-grain simulations: the "Quicksand-Effect" — ●DIRK KADAU¹, EIRIK G. FLEKKØY², and DIETRICH E. WOLF¹ — ¹Department of Physics, Duisburg-Essen University, D-47048 Duisburg, Germany — ²Department of Physics, University of Oslo, Postbox 1048 Blindern, 0316 Oslo, Norway

When modeling granular matter often the influence of the surrounding gas or fluid is neglected for simplicity. A simple model to couple the discrete grain dynamics to the continuous dynamics of a compressible fluid or gas is presented. As an example we investigate the quicksand phenomenon using a model where the granular system is fluidized by an upward flow. Can one really drown in quicksand or will the buoyancy be even increased by the sand grains?

DY 27.3 Tue 17:00 SCH 251

Ripple generation under shear — ●ANDREAS WIERSCHEM¹, CHRISTOF KRÜLLE², INGO REHBERG², and NURI AKSEL¹ — ¹Technische Mechanik und Strömungsmechanik, Universität Bayreuth, D-95440 Bayreuth — ²Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth

The generation of ripples in deserts or at beaches by wind or tidal currents is a paradigm of instabilities in granular material under shear. Research has been focused mainly on the surface profile of the granular layer, describing the ripples and their instability in terms of global parameters. Here, we present an experimental study of the velocity field in the overlying fluid. We characterize the field at onset of ripple generation and show how the ripples exert a feedback on the fluid flow in an annular-ring geometry with driven upper lid.

DY 27.4 Tue 17:15 SCH 251

Sound propagation in granular matter — ●IOANNIS TZAVARAS and MICHAEL SCHULZ — Universität Ulm, Abteilung Theoretischer Physik, Albert-Einstein-Allee 11, 89069 Ulm

The aim of this contribution is to find a suitable mathematical description for the propagation of mechanical excitations as for example sound waves in granular matter. We determined numerically the frequency spectrum of a linear chain of particles (up to 5 particles under periodic boundary conditions). The calculations were based on equations of motion, that were derived from a potential that vanishes as long as

the particles are not in contact and that is that of a harmonic oscillator, when the particles press on each other, in other words when the distance of next neighbours is smaller than $2R$ (R : radius of the particles). The shape of the numerical solutions of the equations of motion for a linear chain of N particles suggested that a short time after the excitation solitons occur. We tried to approximate the equations of motion by fitting the parameters to the Toda lattice equation, which shows an exponential interaction between nearest neighbour particles and possesses analytical solutions especially soliton solutions. We could show that the soliton solution of the Toda lattice equations fulfils the equation of motion of granular matter too, if the soliton has a very small velocity, amplitude and a large width. At present time the concern of our work is to transfer the equation of motion of granular matter into the Korteweg de Vries (KdV) equation by performing the continuum limit and some transformations that connect also the Toda equation with the KdV equation.

DY 27.5 Tue 17:30 SCH 251

Velocity distributions of levitated granular gases — ●CORINNA MAASS, NATHAN ISERT, CHRISTOF AEGERTER, and GEORG MARET — Fachbereich Physik, Universität Konstanz, Universitätstrasse 10; 78457 Konstanz

Granular gases can show counterintuitive behaviour, such as clustering, non-Maxwellian velocity distributions and de-mixing. Theoretical studies have emphasised the role of inhomogeneous heating, collisions with boundaries and gravity on these effects, as well as the possibility of observing Maxwell-Boltzmann distributions also in granular materials. This is mainly due to the inelasticity of the collisions and different restitution coefficients of the bounding walls. In order to study the influence of the above effects, we diamagnetically levitate granular gases of different constituting particles, such as polystyrene and bismuth. A homogeneous heating of the granular gas is achieved by adjusting the magnetic field gradient, such that there is a simultaneous forcing of all of the granular particles. The resulting velocity distributions are recorded using video-microscopy and particle tracking. We also discuss the influence of particle number and restitution coefficient on the dynamics of the granular gas.

DY 27.6 Tue 17:45 SCH 251

Wet granular matter: A two component non-Abelian sandpile model — ●CHRISTOPH KOHLHAMMER and MICHAEL SCHULZ — Universität Ulm, Abteilung Theoretische Physik, Albert Einstein-Allee 11, 89069 Ulm

We consider a two component non-Abelian sandpile model reflecting several important properties of wet granular matter. By introducing appropriate threshold conditions and consistent toppling rules we obtain a model with SOC behaviour. On the basis of fluctuations of the dissipative work we define a temperature of the granular system and show its connection to the avalanche size. In particular, we find that our temperature, defined above, characterizes the tension of the sandpile. These tensions are influenced by resonances leading to very sharp extrema and phase transitions. Computer simulations show a broken renormalisation exponent which can be shown to be equivalent to that of the well known Abelian sandpile models. The particle density as a system size independent variable delivers also indications of a phase transition as a function of the relation between wet and dry particles.

DY 28 Glass I (joint session with DF)

Time: Tuesday 09:30–12:10

Room: MÜL Elch

Invited Talk

DY 28.1 Tue 09:30 MÜL Elch

Towards a Statistical Mechanics for Network Glasses — ●REIMER KÜHN¹, JORT M. VAN MOURIK², MARTIN WEIGT³, and ANNETTE ZIPPELIUS⁴ — ¹King's College London, UK — ²Aston University, Birmingham, UK — ³Institute for Scientific Interchange, Torino, Italy — ⁴Universität Göttingen, Germany

We introduce models of heterogeneous systems with finite connectivity defined on random graphs, to capture effects of finite coordination char-

acteristic of finite dimensional systems. Our models use a description in terms of small deviations from a set of reference positions, appropriate for the description of low-temperature phenomena. A Born-von-Karman type expansion with random coefficients is used to model glassy systems. Gel-phases can be described when anharmonicities are absent. The key quantity in the theoretical analysis is a distribution of effective single-site potentials. For gels, where anharmonicities are absent in the interactions, the single-site potentials are harmonic as well, and their distribution is equivalent to the distribution of localization lengths used

earlier for the description of such systems. With frustration in the interactions and anharmonicities present, the systems develop glassy phases at low temperature, characterized by an ensemble of single- and double-well potentials, the latter with a broad spectrum of barrier heights and asymmetries. The double well potentials are responsible for the universal glassy low-temperature anomalies, as previously described for fully connected systems

DY 28.2 Tue 10:10 MÜL Elch

Nanostructured Solid Electrolytes analyzed by Time-Domain Electrostatic Force Spectroscopy — ●AHMET TASKIRAN¹, ANDRE SCHIRMEISEN¹, HARALD FUCHS¹, BERNHARD ROLING², HARTMUT BRACHT³, FRANK NATRUP², and SEVI MURUGAVEL² — ¹Physikalisches Institut, Wilhelm-Klemm-Str.10, 48149 Münster, Germany — ²Institut für Physikalische Chemie, Corrensstr.30, 48149 Münster, Germany — ³Institut für Materialphysik, Wilhelm-Klemm-Str.10, 48149 Münster, Germany

Ion conducting solid materials are widely used as solid electrolytes in, e.g., batteries. An important prerequisite for further progress in this field is a better understanding of ion transport mechanisms on nanoscopic length scales. We are using an atomic force microscope (AFM) operated in the non-contact mode for electrostatic force spectroscopy to measure the ion conductivity in nanoscale volumes of homogeneous and heterogeneous solid electrolytes. The measurements are carried out at sample temperatures ranging from 200 K to 675 K and at different positions on the sample. The relaxation times at different temperatures follow the Arrhenius model, which yield the activation energy of the ion hopping processes [1]. Furthermore the local variation of the relaxation strength provides us with information on the different phases and interfaces in the sample. In our work we focus on nanostructured solid electrolytes. We find that the activation energies for the ions in the nanocrystallites and in the glass regions are different, in agreement with macroscopic results [2]. [1] Schirmeisen et al., Appl.Phys.Lett. 85,2053 [2] Roling et al., Phys.Chem.Chem.Phys. 7,1472

DY 28.3 Tue 10:30 MÜL Elch

Ionic Motion in Ion Beam Sputtered Borate Glasses — ●FRANK BERKEMEIER, REZA ABOUZARI, TOBIAS STOCKHOFF, and GUIDO SCHMITZ — Westfälische Wilhelms-Universität, Institut für Materialphysik, Wilhelm-Klemm Straße 10, 48149 Münster

Ion-conducting, amorphous thin films with a thickness of 20 – 500 nm are prepared by ion beam sputtering using glass targets of the compositions $0.2A_2O \cdot 0.8B_2O_3$, with $A = Li, Na, Rb$. The glass layers are deposited on a silicon substrate between two sputtered electrodes of Ag, Al, or Al-Li alloy. TEM cross-section investigations show a homogeneous thickness and a homogeneous, amorphous structure of the films. Chemical analysis, performed by EELS, gives alkali oxide concentrations comparable to those of the target material. Temperature-dependent impedance spectroscopy allows to differentiate between different electrical properties of the samples and to determine the specific dc-conductivities of the glass layers. Layers thicker than 100 nm show dc-conductivities which are about one order of magnitude higher than those of the target materials and activation enthalpies about 20 kJ mol^{-1} less compared to the targets. Additionally, layers thinner than 100 nm show a non-trivial increase in dc-conductivity with decreasing film thickness, which we attribute to the increasing influence of the glass-electrode interfaces.

DY 28.4 Tue 10:50 MÜL Elch

Theoretical model of the conductivity of alkali glasses — ●JOACHIM SOHNS and MICHAEL SCHULZ — Abteilung theoretische Physik, Albert-Einstein-Allee 11, 89069 Ulm

Our aim is to formulate a model of the conductivity of glasses which reproduces the mixed alkali effect. Therefore we analyze the conductivity of an ensemble of charged particles in a random environment. As in a former model this environment was static, the model proposed here includes the dynamics of the glass environment. The memory effects are described by the mode-coupling theory. A nonequilibrium Green function determines the properties of the alkali system. Finally the conductivity

of the system is calculated. Furthermore, we give some ideas how feedback mechanisms between the ions and the glass environment may be included in the theoretical description.

DY 28.5 Tue 11:10 MÜL Elch

Glasses, Clusters, and Philosophy — ●ANDREAS REISER, GERNOT KASPER, SIEGFRIED HUNKLINGER, and CHRISTIAN ENSS — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

Dielectric relaxation studies can reveal information on structural or chemical processes in liquids, soft matter, and partly crystalline or amorphous solids. Glass formers can belong to all of these groups, depending on the external control parameters temperature, pressure, and more generally on the thermodynamic present and history. We have measured the dielectric permittivity of several prototypical organic glass formers as a function of frequency, temperature, and pressure. Isobaric, isothermal and isochoric routes in the temperature-pressure plane were taken. We show basic scaling properties of the dielectric function. For data interpretation a cluster-based approach is discussed with respect to crystallization.

DY 28.6 Tue 11:30 MÜL Elch

Collective Single Particle Jumps Below The Glass Transition — ●KATHARINA VOLLMAYR-LEE — Institut für Theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

We study a binary Lennard-Jones mixture below the glass transition via molecular dynamics simulations. To investigate the dynamics of the system we define single particle jumps via their single particle trajectories. To study how the single particle jumps are correlated in time and space we investigate (I) clusters of simultaneously jumping particles and (II) temporally extended clusters, i.e. clusters of jump events for which the jumping particles are spatially nearby and the jumps occur at consecutive times. We find highly collective jump processes. The distribution of cluster sizes $P(s)$ is independent of temperature and follows a power law $P(s) \sim s^{-\tau}$ with $\tau \approx 2.7$ in case (I) and $\tau \approx 2.2$ in case (II). By studying the average coordination number within the clusters as a function of the cluster size, we find that the shape of the clusters is string-like.

We thank K. Binder, A. Zippelius, J. Horbach, and B. Vollmayr-Lee, and we gratefully acknowledge financial support from SFB 262 and DFG Grant No. Zi 209/6-1.

DY 28.7 Tue 11:50 MÜL Elch

Optical Properties of Colloidal Suspension of Silver Nanoparticles* — ●HELGE A. EGGERT¹, JIM R. ADLEMAN², DEMETRI PSALTIS², and KARSTEN BUSE¹ — ¹Institute of Physics, University of Bonn, Wegelerstr. 8, 53115 Bonn — ²Department of Electrical Engineering, California Institute of Technology, Pasadena, CA 91125

Colloidal suspensions of silver nanoparticles are an interesting optical material because of homogeneity, stability, and tailored absorption properties. To understand the thermal and nonlinear-optical response, holographic gratings are recorded in such colloidal suspensions of silver nanoparticles utilizing interfering nanosecond pulses (wavelength $\lambda=532 \text{ nm}$, pulse duration 6 ns, intensity 10 GW/m^2). The diffraction efficiency is measured with continuous-wave light ($\lambda=633 \text{ nm}$). An instantaneous response together with a longer lasting but also transient grating are observed: The nanoparticles absorb the pump light and heat up, which yields a response on the time scale of the laser pulse. Heat is transferred to the solvent, and a delayed thermal grating appears. The final decay time constant of this grating depends quadratically on the period length of the interference pattern and has a typical value of $1 \mu\text{s}$ for grating spacings of several micrometers.

*Financial support by the DFG (BU 913/17) and by the Deutsche Telekom AG is gratefully acknowledged.

Prize Talk

The prize talk (Max-Planck-Medaille) by Prof. Götzke takes place Tuesday, 13:15, HSZ 04. The title of the talk is "Glassy Relaxation: a Paradigm for Condensed-Matter Dynamic". See the plenary section for the abstract.

DY 29 Glass II (joint session with DF)

Time: Tuesday 14:30–16:10

Room: MÜL Elch

DY 29.1 Tue 14:30 MÜL Elch

Indications for a slow β -relaxation by mechanical spectroscopy of a strong and a fragile metallic glass — ●JÖRG HACHENBERG, ANNELEN KAHL, and KONRAD SAMWER — 1. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Mechanical spectroscopy is used to investigate the elastic properties of the strong metallic glass former $Zr_{65}Al_{7.5}Cu_{27.5}$ and the fragile $Pd_{77}Cu_6Si_{17}$. The dynamic mechanical analyser is used to measure the complex elastic modulus of melt spun bands in the low Hz regime while the double-paddle oscillator is applied for thin films at 5.4 kHz. In the vicinity of glass-transition, the α -relaxation is fitted using a Havriliak-Negami function in temperature domain. The measured data clearly deviate from the model for both metallic glasses. An explicit misfit on the low temperature flank, also termed excess wing, is interpreted as an underlying, merged slow β -relaxation. Our experimental results provide evidence that this secondary relaxation, existing in both strong and fragile amorphous metals, can be regarded as a universal property of glasses and is compared with recent MD-simulations by H. Teichler et al.

This work is supported by the Deutsche Forschungsgemeinschaft, Graduiertenkolleg 782 and SFB 602, TP B8.

DY 29.2 Tue 14:50 MÜL Elch

Sculpting the free energy landscape — ●TIMO ASPELMEIER¹, R. A. BLYTHE², A. J. BRAY³, and M. A. MOORE³ — ¹Institut für Theoretische Physik, Universität Göttingen — ²School of Physics, University of Edinburgh, UK — ³School of Physics and Astronomy, University of Manchester, UK

The free energy landscape of the Ising spin glass is analysed using the TAP equations. It is found that local minima of the free energy and saddles always occur in pairs, and that the saddles always have exactly one unstable direction. We show that local minima, which are usually very hard to find numerically, can be found in abundance using an iterative algorithm which operates “on the edge of chaos”. We compare these results with the free energy landscape generated by the naive mean field equations of the spin glass and show that despite identical groundstates the free energy landscape at finite temperatures is fundamentally different from the TAP landscape.

DY 29.3 Tue 15:10 MÜL Elch

Dynamic critical behaviour in Ising spin glasses — ●MICHEL PLEIMLING¹, MALTE HENKEL², and IAN CAMPBELL³ — ¹Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Germany — ²Laboratoire de Physique des Matériaux, Université Henri Poincaré Nancy I, France — ³Laboratoire des Colloïdes, Verres et Nanomatériaux, Université Montpellier II, France

The non-equilibrium ageing behaviour of critical Ising spin glasses with

Bimodal, Gaussian, and Laplacian interaction distributions is studied numerically in three and four dimensions. The same phenomenology of the time-dependent scaling as in non-disordered magnets is found. Our data strongly indicate that the values of the non-equilibrium exponents and of the critical limit fluctuation-dissipation ratio depend on the distribution of the coupling constants.

[1] M. Pleimling and M. Henkel, Europhys. Lett. 69, 524 (2005)

[2] M. Pleimling and I.A. Campbell, to appear in Phys. Rev. B (cond-mat/0506795)

DY 29.4 Tue 15:30 MÜL Elch

Dynamics of mobile particles in an immobile environment: Computer simulations of disparate-sized mixtures — ●JÜRGEN HORBACH and NORIO KIKUCHI — Institut für Physik, Johannes-Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz

Molecular dynamics computer simulations are used to study transport properties of mobile particles in an immobile environment. To this end, we consider simple binary mixtures. The first system consists of small and big soft spheres in two dimensions where the big spheres are a factor of 5 bigger than the small ones. We discuss whether the transport properties are similar to those obtained from mode coupling theory [1]. The second system contains also small and big particles with a size-ratio 1:5. But now a three-dimensional system is considered where the particles interact via a screened Coulomb (or Yukawa) potential (note, that this system can be realized experimentally [2]). Here, a transition is observed where the big particles crystallize while the small particles remain in a kind of fluid phase. We study the activated transport of the small particles in the crystalline matrix.

[1] J. Bosse and Y. Kaneko, Prog. Theoret. Phys. Suppl. 126, 13 (1997); Phys. Rev. Lett. 74, 4023 (1995).

[2] A. Imhof and J.K.G. Dhont, Coll. Surf. A 122, 53 (1997); Phys. Rev. E 52, 6344 (1995); Phys. Rev. Lett. 75, 1662 (1995).

DY 29.5 Tue 15:50 MÜL Elch

The m -component spin glass on the Bethe lattice — ●AXEL BRAUN and TIMO ASPELMEIER — Institut für theoretische Physik, Universität Göttingen

We investigate the m -component vector spin glass on the Bethe lattice in the limit $m \rightarrow \infty$. This is done analytically via the cavity method on a replica symmetric level. We exhibit a phase transition and calculate the critical temperature. Furthermore we confirm numerically the condensation of the lattice spins into a subspace in the groundstate (generalized Bose-Einstein condensation). The dimension n_0 of this subspace is proportional to N^μ , where N is the number of spins and μ is an exponent less than $2/5$. This result is compared to the fully connected, the 2-d and the 3-d m -component spin glass.

DY 34 Nonlinear Dynamics, Synchronization and Chaos I

Time: Wednesday 14:30–16:15

Room: HÜL 186

DY 34.1 Wed 14:30 HÜL 186

Multifractal distribution of spike intervals for two neurons with unreliable synapses — ●WOLFGANG KINZEL and JOHANNES KESTLER — Theoretical Physics, University Würzburg

Two neurons coupled by unreliable synapses are modeled by leaky integrate-and-fire neurons and stochastic on-off synapses. The dynamics is mapped to an iterated function system. Numerical calculations yield a multifractal distribution of interspike intervals. The Hausdorff, entropy and correlation dimensions are calculated as a function of synaptic strength and transmission probability.

Preprint: <http://theorie.physik.uni-wuerzburg.de/TP3>

DY 34.2 Wed 14:45 HÜL 186

Nonperturbative Calculation of a Limit Cycle in a Two-Neuron System with Delayed Feedback — ●AXEL PELSTER¹, SEBASTIAN BRANDT², MICHAEL SCHANZ³, and RALF WESSEL² — ¹Fachbereich Physik, Universität Duisburg-Essen, Universitätsstraße 5, 45117 Essen, Germany — ²Physics Department, CB 1105 Washington University, 1 Brookings Drive, St. Louis, USA — ³IPVS, Universität Stuttgart, Universitätsstraße 38, 70569 Stuttgart, Germany

Neural circuits composed of a small number of neurons form the basic feedback mechanisms involved in the regulation of neural activity. We use a bifurcation analysis and numerical simulations in order to investigate a model system which consists of two Hopfield-like neurons with a time delayed feedback. It is described by the system of delay differential equations $du_{1/2}(t)/dt = -u_{1/2}(t) + a_{1/2} \tanh[u_{2/1}(t - \tau)]$, where $u_{1/2}(t)$ denote the voltages of the Hopfield neurons at time t . If the delay τ exceeds a certain critical value τ_c , the trivial fix point at the origin

loses its stability and a stable limit cycle emerges. Using the Poincaré-Lindstedt method, we calculate both period and amplitude of the limit cycle perturbatively. Then we perform a resummation of the respective perturbation series by applying variational perturbation theory and compare our nonperturbative analytic results with numerical simulations.

DY 34.3 Wed 15:00 HÜL 186

2-tori and bursting oscillations close to a generalized Hopf bifurcation in the fast subsystem — ●RONNY STRAUBE^{1,2}, DIETRICH FLOCKERZI³, MARCUS J. B. HAUSER², and STEFAN C. MÜLLER² — ¹Abteilung Theoretische Physik, Hahn-Meitner-Institut Berlin, Glienicke Str. 100, 14109 Berlin — ²Abteilung Biophysik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg — ³Max-Planck-Institut für Dynamik komplexer technischer Systeme, Sandtorstr. 1, 39106 Magdeburg

Many chemical and biological systems exhibit bursting behavior which may be conveniently classified by the type bifurcations occurring in the fast subsystem [1]. Using two examples, we demonstrate that, depending on the dynamics of the slow subsystem, the existence of a generalized Hopf bifurcation in the fast subsystem may likewise account for the emergence of bursting oscillations (which are then of subHopf/fold-cycle type) or the emergence of a 2-torus exhibiting a typical phase flow on it. This investigation reveals a common origin of both types of dynamics.

[1] E. M. Izhikevich, *Int. J. Bifurcat. Chaos* **10** (2000) 1171.

DY 34.4 Wed 15:15 HÜL 186

Breathing 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 possible destabilization mechanisms of stationary solutions in a three-component reaction-diffusion system with one activator and two inhibitors due to change of the inhibitor's time constants. The case we are interested in is that the breathing mode becomes unstable first and the dissipative soliton undergoes a bifurcation from a stationary to a "breathing" state. In this case, both self- and hard-excitations can be observed. This situation is analyzed performing a two-time-scale expansion in the vicinity of the bifurcation point resulting in the corresponding amplitude equation is obtained. Numerical simulations are also carried out showing good agreement with the analytical predictions.

DY 34.5 Wed 15:30 HÜL 186

Chaotic properties of systems of many hard particles. — ●ASTRID S. DE WIJN — Max-Planck-Institut fuer Physik Komplexer Systeme, Noethnitzer Strasse 38, 01187 Dresden, Germany

The dynamics of a system consisting of many spherical hard particles can be described as a single point particle moving in a high-dimensional space with fixed hypercylindrical scatterers with specific orientations and positions. The similarities in the Lyapunov exponents between systems of many particles and high-dimensional billiards are investigated. Comparisons are made between billiards with randomly oriented cylinders and numerical results for systems of many hard particles as well as the analytical results for the high-dimensional Lorentz gas. The similarity shows that the hard-disk systems may be approximated by a spatially

homogeneous and isotropic system of scatterers for a calculation of the smaller Lyapunov exponents, apart from the exponent associated with localization. The method of the partial stretching factor is used to calculate these exponents analytically, with results that compare well with simulation results of hard disks and hard spheres.

[1] A. S. de Wijn, *Phys. Rev. E* **72**, 026216 (2005)

[2] A. S. de Wijn and Henk van Beijeren, *Phys. Rev. E* **70**, 036209 (2004)

[3] A. S. de Wijn, *Phys. Rev. E* **71**, 046211 (2005)

DY 34.6 Wed 15:45 HÜL 186

Instability of a Limit Cycle in the Van-der-Pol Oscillator with Time Delay — ●KAI SCHNEIDER¹, VIKTOR AVRUTIN¹, MICHAEL SCHANZ¹, and AXEL PELSTER² — ¹IPVS, Universität Stuttgart, Universitätsstraße 38, 70569 Stuttgart, Germany — ²Fachbereich Physik, Universität Duisburg-Essen, Universitätsstraße 5, 45117 Essen, Germany

The classical Van-der-Pol oscillator represents a paradigmatic model for electronic circuits with intrinsic negative resistance as, for instance, a tunnel diode. The Van-der-Pol oscillator with time delay represents an extension of this model which takes into account the finite propagation time of signals. We analyze both analytically and numerically the stability of an emerging limit cycle. To this end, we use the Poincaré-Lindstedt method and set up perturbation series for the frequency and the amplitude of the limit cycle. Then we use the Floquet theory for delay differential equations [1] to systematically perform a linear stability analysis for this time periodic reference state. Finally, we compare our analytic results for the instability point of the limit cycle with numerical simulations carried out with the software package AnT 4.669 [2].

[1] C. Simmendinger, A. Pelster, and A. Wunderlin, *Phys. Rev. E* **59**, 5344 (1999)

[2] <http://www.AnT4669.de>

DY 34.7 Wed 16:00 HÜL 186

Coherence resonances in semiconductor lasers — ●OLEG V. USHAKOV, H.-J. WÜNSCHE, F. HENNEBERGER, I. A. KHOVANOVA, L. SCHIMANSKY-GEIER, and M.A. ZAKS — Humboldt Universität zu Berlin, Inst. für Physik, Newtonstr. 15, 12489 Berlin, Germany

Semiconductor laser with ultrashort optical feedback are excellent candidates to study novel scenarios of self-organization in optical systems. We have investigated the influence of external Gaussian noise close to the onset of sub- and super-critical Hopf bifurcations. Noise-induced oscillations appear as a Lorentzian-shaped peak in the power spectrum. The coherence factor defined by the product of height and quality factor (width divided by frequency) exhibits non-monotonous behavior with a distinct maximum at a certain noise intensity for both types of Hopf bifurcations, demonstrating coherence resonance. However, the spectral width of the peak behaves qualitatively different. Whereas it increases monotonically for the supercritical bifurcation, a pronounced minimum is observed for the subcritical case. These experimental findings are examined in terms of general potential models for the noise driven motion close to bifurcations [V.S. Anishchenko, et al., *Nonlinear Dynamics of Chaotic and Stochastic Systems* (Springer, Berlin, Heidelberg 2002)]. We conclude that our observations reveal a generic mode for the occurrence of coherence resonance in non-linear systems.

DY 35 Ferro Fluids / Liquid Chrystals

Time: Wednesday 14:30–16:30

Room: SCH 251

DY 35.1 Wed 14:30 SCH 251

Growth behaviour of solitary spikes on the surface of magnetic fluids — ●HOLGER KNIELING, REINHARD RICHTER, and INGO REHBERG — University of Bayreuth, Institute for experimental physics V, 95440 Bayreuth, Germany

The Rosensweig or normal-field instability on the surface of a ferrofluid is well known. A hexagonal pattern of liquid spikes emerges in a normal magnetic field when a certain threshold of the magnetic induction is surpassed. Recently a stable solitary spike was found in the hysteretic regime of this instability [1]. It can easily be generated by a local perturbation of the surface or the magnetic induction. We now have performed time resolved measurements of its amplitude by recording it with a high-speed camera. The analysis of the pictures results in information about the shape of the structure and the growth behaviour of the amplitude

and the volume. The final static shape is compared with numerical calculations.

[1] R. Richter and I.V. Barashenkov, *Phys. Rev. Lett.* **94**, 184503 (2005)

DY 35.2 Wed 14:45 SCH 251

More precise simulations of ferrofluids' reology — ●ERIC COQUELLE¹, PATRICK ILG^{1,2}, and SIEGFRIED HESS¹ — ¹Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany — ²LPMCN, Université Lyon I, F-69662 Villeurbanne France

Ferrofluids have attracted considerable attention in the recent years, as their field-controlled physical properties has led to numerous application, as well as in material science as in medical field [1,2]. However, acutal simulations study "perfect" magnetic suspensions, and may neglect some experimental important parameters, such as the wide size dispersion of

magnetite particles. Moreover, the hydrodynamic interactions (HI) between moving particles are neglected.

Present study first investigates the influence of these HI; the difficulty arises from the need to uncorrelate the random motion of the particles. A method inspired from the polymers simulations has been employed, reducing the computational effort to $O(N^2.25)$. For comparison, another method based on the mobility matrix is used. The results are then compared to experimental SAXS and XPCS data.

As a second step, we model real polydisperse ferrofluid, through a system containing small and large particles. It reveals a sharp modification of the state of the simulated fluid. To go further, predictions on the magnetoviscous effect of a simulation involving both bidispersity and many-body hydrodynamic interaction will be confronted to experimental results.

[1] G. BOSSIS, E. COQUELLE, *Ann. Ch. Sci. Mat.* **29** (2004) 43 [2] Z. WANG, C. HOLM, *Phys. Rev. E* **68** (2003) 041401

DY 35.3 Wed 15:00 SCH 251

Pattern formation in the Faraday instability on a ferrofluid in a vertical magnetic field — •VLADISLAV MEKHONOSHIN — Institut für Theoretische Physik, Universität des Saarlandes, PF 151150, Saarbrücken

The parametrical generation of standing waves on a surface of a liquid is well known as Faraday instability since its discovery in 1831. Ferrofluids are colloidal dispersions of single-domain particles in an ordinary (non-magnetic) carrier liquid. Thus, ferrofluids combine the ability to flow with strong interaction with magnetic field. This allows one to use magnetic field to control the motion of a ferrofluid, and in particular, the pattern formation in the Faraday instability.

In this work, an amplitude equation for the Faraday instability is derived following the standard procedure, described in [1]. The amplitude equation is used to investigate the pattern formation in the system and to explain the experimental observations.

DY 35.4 Wed 15:15 SCH 251

Rheology of a bidisperse inverse ferrofluid — •ROBERT KRAUSS, REINHARD RICHTER, and INGO REHBERG — Experimentalphysik 5, Universität Bayreuth, D-95440 Bayreuth, Germany

By dispersing non-permeable particles in a common ferrofluid we obtain a so called inverse ferrofluid [1]. In our case fairly large polystyrene particles create magnetic holes which have magnetic moments opposite to the ferrofluid they are displacing. In previous studies we investigated the viscoelastic properties of a mono- vs a polydisperse inverse ferrofluid [2]. In order to quantify the influence of polydispersity we prepare samples of a bidisperse size distribution of spherical particles. The ratio of small to large particles is varied systematically. On the one hand rheological measurements are carried out to describe the viscoelastic properties of the magneto-rheological fluid. On the other hand we investigate optically the chain formation of the system in an external field by a long-range microscope. We compare the results with the ones obtained for monodisperse samples.

[1] A. T. Skjeltorp, *Phys. Rev. Lett.* **51**, 2306 (1983).

[2] Ruben Saldivar-Guerrero, Reinhard Richter, Ingo Rehberg, Nuri Aksel, Lutz Heymann and Oliverio S. Rodriguez-Fernández, *Viscoelasticity of mono- and polydisperse inverse ferrofluids*, subm. to *J. Chem. Phys.* (2005).

DY 35.5 Wed 15:30 SCH 251

Pattern reorientation at the tilted field instability — •CHRISTOPHER GROH, REINHARD RICHTER, and INGO REHBERG — Experimentalphysik 5, Univ. Bayreuth, D-95440 Bayreuth, Germany

We investigate the surface instability of a horizontal layer of magnetic liquid in a magnetic field experimentally. By means of two pairs of orthogonal Helmholtz coils we are able to apply a vertical and a tangential magnetic field. Whereas the vertical component destabilizes the flat layer, the tangential one preserves its stability. In this way different surface patterns can be observed, comprising regular hexagons, stretched hexagons and ridges [1,2]. We measure transitions between these patterns under variation of the field components. The surface reliefs are quantitatively characterized via help of a radiosopic technique [3]. This enables us to present the proper bifurcation diagrams and phase diagrams for the tilted field instability. Moreover, we report a new effect: the rotation of

the hexagonal pattern under a increasing tangential field component.

[1] Rene Friedrichs, *Phys. Rev. E* **66**, 066215 (2002).

[2] Bert Reimann, Reinhard Richter, Holger Knieling, Rene Friedrichs, and Ingo Rehberg, *Phys. Rev. E* **71** 1(R) (2005).

[3] Reinhard Richter, and Jürgen Bläsing, *Rev. Sci. Instrum.* **72**, 1729 (2001).

DY 35.6 Wed 15:45 SCH 251

The effect of rough surfaces on nematic liquid crystals.

— •FRIEDERIKE SCHMID¹, DAVID CHEUNG^{1,2}, and JENS ELGETI^{1,3} — ¹Universität Bielefeld — ²University of Warwick UK — ³Forschungszentrum Jülich

We investigate the effect of rough surfaces on nematic liquid crystals with continuum theories and computer simulations. First we reconsider the phenomenon of Berreman anchoring, where highly ordered nematic liquid are oriented by surfaces with anisotropic roughness. Then we study liquid crystals close to the nematic-isotropic transition. Surface roughness reduces the order and the anchoring strength at the surface. As a result, the transition between the isotropic and the nematic phase is shifted in confined systems. Under certain circumstances, one can even enforce a wetting-induced anchoring transition.

DY 35.7 Wed 16:00 SCH 251

The influence of shear rate fluctuations on the orientational dynamics — •SEBASTIAN HEIDENREICH¹, PATRICK ILG^{1,2}, and SIEGFRIED HESS¹ — ¹Institut für Theoretische Physik, Technische Universität Berlin, D-10623, Germany — ²Department de Physique des Materiaux, UCB Lyon1, F-69622 Villeurbanne, France

The flow behavior of liquid crystals is strongly affected by the coupling between the flow and the molecular orientation. Nematic liquid crystals which respond with a time-dependent orientational behavior can be rather complex. A relatively simple model based on a nonlinear equation for the second rank alignment tensor which can be derived from irreversible thermodynamics [1-3]. Here we investigate the influence of fluctuating shear rates on the orientational dynamics in the case of spatially homogeneous and spatially inhomogeneous alignment. We found that uncorrelated fluctuations of the shear rate in general have little effect on the orientational dynamics of nematics, whereas the effect of correlated fluctuation is more significant. Further we present a new amended potential modeling the isotropic-to-nematic transition. In contrary to the Landau-de Gennes potential our potential has the advantage to restrict the order parameter to physically admissible values.

[1] S. Hess, *Z. Naturforsch.* **30a**, 728 (1975), **31a** 1507 (1976). [2] P. D. Olmsted and P. Goldbart, *Phys. Rev. A* **41**, 4578 (1990); *Phys. Rev. A* **46**, 4966 (1992). [3] C. Pereira Borgmeyer and S. Hess, *J. Non-Equilib. Thermodyn.* **20**, 359 (1995).

DY 35.8 Wed 16:15 SCH 251

The surface relief of the Rosensweig instability – experimental and numerical results compared quantitatively — •CHRISTIAN GOLLWITZER¹, GUNAR MATTHIES², REINHARD RICHTER¹, INGO REHBERG¹, and LUTZ TOBISKA³ — ¹Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany — ²Ruhr-Universität Bochum, Universitätsstraße 150, — ³Institut für Analysis und Numerik, Otto-von-Guericke-Universität Magdeburg, PF 4120, D-39106 Magdeburg

The surface of a magnetic fluid exposed to a normal magnetic field above a threshold B_c forms a pattern of hexagonal crests [1]. We record the full three-dimensional surface profile recently made possible by the attenuation of an X-ray beam [2]. This enables us to compare the amplitude and shape of the peak pattern in an extended container with those obtained from numerical simulations [3]. We have measured 540 surface reliefs under adiabatic increase and decrease of the magnetic induction. The measured nonlinear magnetization law and material parameters have been taken into account in the simulations. Very good qualitative agreement with the experiment is found for both the pattern amplitude and the shape of the peaks. Very good quantitative agreement within the statistical errors is achieved with almost no adjustable parameter. “Almost” will be explained in the talk. Fourier decomposition of the shape exposes, that most ($\approx 90\%$) of the energy is in the first Fourier mode.

[1] M. D. Cowley and R. E. Rosensweig, *J. Fluid Mech.* **30**, 671 (1967).

[2] R. Richter and J. Bläsing, *Rev. Sci. Instrum.* **72**, 1729 (2001).

[3] G. Matthies and L. Tobiska, *JMMM* **289**, 346 (2005).

DY 36 Nonlinear Dynamics, Synchronization and Chaos II

Time: Wednesday 16:15–18:00

Room: HÜL 186

DY 36.1 Wed 16:15 HÜL 186

Oscillatory Zoning: Nonlinear Dynamics and Self-Organization Governing Crystal Growth from Solution — ●FELIX KALISCHESKI¹, IHOR LUBASHEVSKY², and ANDREAS HEUER¹ — ¹Institut für Physikalische Chemie, Westfälische Wilhelms-Universität, 48149 Münster — ²Theory Department, General Physics Institute, Russian Academy of Sciences, Moscow, 119991 Russia

A large number of solid solutions grown from aqueous media exhibit fluctuating end-member concentrations along the core-rim profile. This phenomenon, called "oscillatory zoning", can be attributed to complex self-organizing effects resulting from competition between thermodynamics and kinetics.

In contrast to existing phenomenological models, we developed a model based on epitaxial growth driven by bulk-diffusion, ad/desorption, surface-diffusion, and finally adatom-incorporation. The critical nonlinearity enters through the dependence of the adatom-crystal interactions on the crystal-composition.

First, we present a linear stability analysis of our "Boundary Reaction Diffusion Model", as well as its 1D evolution in time obtained by numerical analysis. Second, we expand the numerical scheme to 2D to explore the synchronization behavior observed in experiments.

DY 36.2 Wed 16:30 HÜL 186

Step meandering in epitaxial growth — ●FRANK HAUSSER and AXEL VOIGT — caesar, Ludwig-Erhard-Allee 2, 53175 Bonn

Asymmetric attachment kinetics at the atomic steps on a crystalline surface leads to a morphological instability: slightly perturbed straight steps begin to meander. The small amplitude (linear) regime of this instability is well understood [1]. We present results on the nonlinear regime, which are based on numerical simulations of the corresponding moving boundary problem [2]. Three types of nonlinear evolution are found: (a) endless growth of the meander amplitude; (b) stationary profile with fixed amplitude; (c) mushroom formation and pinch-off. Moreover, the influence of anisotropic edge energies as well as edge diffusion is investigated.

[1] G.S. Bales, A. Zangwill, Phys. Rev. B 41 (1990) 5500

[2] E. Bänsch, F. Hauffer, O. Lakkis, B. Li, A. Voigt, J. Comp. Phys. 194 (2004) 409

DY 36.3 Wed 16:45 HÜL 186

Robust control of torsionfree unstable periodic orbits — ●KLAUS HÖHNE¹, CHOL-UNG CHOE^{1,2}, HIROYUKI SHIRAHAMA^{1,3}, HARTMUT BENNER¹, and KESTUTIS PYRAGAS⁴ — ¹Institut für Festkörperphysik, TU Darmstadt, Germany — ²Department of Physics, University of Science, Pyongyang, DPR Korea — ³Ehime University, Matsuyama, Japan — ⁴Semiconductor Physics Institute, Vilnius, Lithuania

Torsionfree unstable periodic orbits cannot be stabilized by conventional time-delayed feedback control. The most simple example of such an orbit occurs at a subcritical Hopf bifurcation. Analytical and numerical investigations showed successful control of a torsionfree unstable periodic orbit in an unstable van der Pol oscillator by applying the idea of a nonlinear unstable time-delayed feedback controller [1].

We succeeded to stabilize a torsionfree unstable periodic orbit in experiment by an electronic circuit realization of this model. The experiment pointed out that the basin of attraction of the controlled orbit is very small, so that the practical application of this method might be difficult. In order to achieve robust control of such an orbit we modified the nonlinear coupling of the unstable time-delayed feedback control. We discuss the advantages of this method in comparison with the original idea.

[1] K. Pyragas et al., Phys. Rev. E 70, 026412

DY 36.4 Wed 17:00 HÜL 186

Stationary Hamiltonian transport with dc bias — ●DENISOV SERGEY — MPIPES, Dresden

We obtain stationary transport in a Hamiltonian system with ac driving in the presence of a dc bias. A particle in a periodic potential under the influence of a time-periodic field possesses a mixed phase space with regular and chaotic components. An additional external dc bias allows to

separate effectively these structures. We show the existence of a stationary current which originates from the persisting invariant manifolds (regular islands, periodic orbits, and cantori). The transient dynamics of the accelerated chaotic domain separates fast chaotic motion from ballistic type trajectories which stick to the vicinity of the invariant submanifold. Experimental studies with cold atoms in laser-induced optical lattices are ideal candidates for the observation of these unexpected findings.

DY 36.5 Wed 17:15 HÜL 186

Synchronization of an aeroacoustical system — ●MARKUS ABEL, KARSTEN AHNERT, and STEFFEN BERGWELER — Universität Potsdam, 14469 Potsdam

A classical example of synchronisation concerns the simultaneous sound emission of two organ pipes. We have measured the response of an organ pipe to an external source as well as the synchronisation properties of two organ pipes positioned side by side. We investigate two different questions. First, the mutual influence of two pipes with different pitch. In analogy to the coupling of two nonlinear oscillators with feedback, one observes a frequency locking, which can be explained by synchronization theory. Second, we measure the dependence of the frequency of the signals emitted by two mutually detuned pipes with varying distance between the pipes. The spectrum shows a broad "hump" structure, not found for coupled oscillators. This indicates a complicated aeroacoustical coupling of the two jets creating the acoustic field when exiting from the pipe mouth. We interpret the measurements in terms of a simplified model.

DY 36.6 Wed 17:30 HÜL 186

Time-delayed feedback control with variable phase-dependent coupling — ●PHILIPP HÖVEL¹, ECKEHARD SCHÖLL¹, and HANS-JÜRGEN WÜNSCHE² — ¹Technische Universität Berlin, 10623 Berlin, Germany — ²Humboldt-Universität zu Berlin, 12489 Berlin, Germany

During the last decade time-delayed feedback methods have been successfully used to control unstable periodic orbits as well as unstable steady states[1]. In most of the theoretical analysis, this control method is considered in the realization of diagonal coupling, i.e., the control force applied to the i -th component of the system is a function of exclusively the same component. Although diagonal coupling is suitable for a theoretical investigation, it is often not feasible for an experiment. Therefore we consider the more general case where control is effected by a non-diagonal coupling matrix. Specifically, we investigate the time-delayed feedback scheme for a rotational coupling matrix parametrized by a variable phase. We present an analysis of the domain of control and show the application to optical systems [2] where the optical phase is an additional degree of freedom.

[1] P. Hövel and E. Schöll, Phys. Rev. E 72, 046203 (2005)

[2] V. Z. Tronciu, H.-J. Wünsche, M. Wolfrum, and M. Radziunas, submitted to Phys. Rev. E (2005)

DY 36.7 Wed 17:45 HÜL 186

Universal features of hydrodynamic Lyapunov modes in extended systems with continuous symmetries — ●HONG-LIU YANG and GÜNTER RADONS — Institute of Physics, Chemnitz University of Technology, D-09107 Chemnitz

We study the Lyapunov instability of spatially extended systems with continuous symmetries. Numerical and analytical evidence is presented to show that hydrodynamic Lyapunov modes (HLMs) do exist in lattices of coupled Hamiltonian and dissipative maps. More importantly, we find that HLMs in these two class of systems are different with respect to their spatial structure and their dynamical behavior. To be concrete, the corresponding dispersion relations of Lyapunov exponent versus wave-number are characterized by $\lambda \sim k$ and $\lambda \sim k^2$, respectively. Moreover, the HLMs in Hamiltonian systems are propagating, whereas those of dissipative systems show only diffusive motion. Extensive numerical simulations of various systems, including coupled map lattices (CMLs), the dynamical XY model, and the Kuramoto-Sivashinsky equation confirm that the existence of HLMs is a very general feature of extended dynamical systems with continuous symmetries and that the above-mentioned differences between the two classes of systems are universal.

DY 38 Fluid Dynamics

Time: Wednesday 16:45–18:00

Room: SCH 251

DY 38.1 Wed 16:45 SCH 251

Asymptotic theory for a moving droplet driven by a wettability gradient — ●UWE THIELE¹ and LEN M. PISMEN² — ¹Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany — ²Department of Chemical Engineering and Minerva Center for Nonlinear Physics of Complex Systems, Technion – Israel Institute of Technology, Haifa 32000, Israel

An asymptotic theory is developed for a moving drop driven by a wettability gradient [1]. We distinguish the mesoscale where an exact solution is known for the properly simplified problem [2]. This solution is matched at both – the advancing and the receding side – to respective solutions of the problem on the microscale. On the microscale the velocity of movement is used as the small parameter of an asymptotic expansion in analogy to [3]. Matching gives the droplet shape, velocity of movement as a function of the imposed wettability gradient and droplet volume.

[1] L. M. Pismen and U. Thiele, preprint at <http://arXiv.org/abs/physics/0509260>.

[2] B. R. Duffy and S. K. Wilson, *Appl. Math. Lett.* **10**, 63-68 (1997).

[3] J. Eggers, *Phys. Rev. Lett.* **93**, 094502 (2004).

DY 38.2 Wed 17:00 SCH 251

Complex Singularities of the Euler Equation — ●WALTER PAULS — Observatoire de la Cote d'Azur, BP 4229, 06304 Nice Cedex 4, France — Fakultät für Physik, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld

A detailed study of complex-space singularities of the two-dimensional incompressible Euler equation is performed in the short-time asymptotic regime when such singularities are very far from the real domain; this allows an exact recursive determination of arbitrarily many spatial Fourier coefficients. Using 35 to 100-digit high-precision arithmetic we find that the Fourier coefficients of the stream function are given over more than two decades of wavenumbers by $\hat{F}(\mathbf{k}) = C(\theta)k^{-\alpha}e^{-\delta(\theta)k}$, where $\mathbf{k} = k(\cos\theta, \sin\theta)$. The prefactor exponent α , typically between $5/2$ and $8/3$, is determined with an accuracy better than 0.01. It depends on the initial condition but not on θ . The vorticity diverges as $s^{-\beta}$, where $\alpha + \beta = 7/2$ and s is the distance to the (complex) singular manifold. This new type of non-universal singularity is permitted by the strong reduction of nonlinearity (depletion) which is associated to incompressibility. Spectral calculations show that the scaling reported above persists well beyond the time of validity of the short-time asymptotics. A simple model in which the vorticity is treated as a passive scalar is shown analytically to have universal singularities with exponent $\alpha = 5/2$.

DY 38.3 Wed 17:15 SCH 251

Propagating fronts in spiral Poiseuille flow — ●MATTI HEISE, JAN ABSHAGEN, and GERD PFISTER — Institute of Experimental and Applied Physics, University of Kiel, Germany

One of the classical hydrodynamic systems for the study of Hopf bifurcation with $O(2)$ -symmetry is counter rotating Taylor Couette flow. This is the flow of a viscous liquid in the gap between two concentric rotating cylinders. We present the results of an experimental study on the transition between two different types of spiral vortices in counter ro-

tating spiral Poiseuille flow, the Taylor Couette flow between two counter rotating cylinders in the presence of an axial through flow. As a result of an applied axial through flow the 'classical' Hopf bifurcation to spiral vortices splits up and a primary and secondary branch of down- and upward propagating spirals, respectively, as well as a transient quasiperiodic flow appear. The bifurcation structure observed in this open flow experiment is in qualitative agreement with predictions from theory of Hopf bifurcation with broken reflection symmetry and also in quantitative agreement with results from recent numerical calculations. We also observed the transition from upward to downward propagating spirals in form of a propagating front in spiral Poiseuille flow.

DY 38.4 Wed 17:30 SCH 251

Shear flow in freely suspended liquid crystal films induced by elastic stress — ●ALEXEY EREMIN, CHRISTIAN BOHLEY, and RALF STANNARIUS — Otto-von-Guericke-Universität Magdeburg, Institut für Experimentalphysik

Hydrodynamic phenomena observed in liquid crystalline materials are far more complex than those in conventional Newtonian fluids. The reasons lies in the coupling of macroscopic translational motions to inner degrees of freedom, created by broken symmetries. We present an experimental and theoretical study of vortex flow in freely suspended smectic films that is induced entirely by elastic distortions of the orientational director field. By means of an external electric field, a periodically deformed director field is prepared, which, after the field is switched off, relaxed into a homogeneous state. Macroscopic flow is induced by this director reorientation. It is visualized by tracer particles imposed on the film surface. We discuss experimental results and theoretical models developed for different configurations of the director field. It is shown that the presence or absence of a central topological defect has essential influence on the relaxation dynamics of flow and director fields. From a quantitative analysis, shear viscosities of the material can be accessed.

DY 38.5 Wed 17:45 SCH 251

Statistics of temperature fluctuations measured by a new microscopic temperature sensor — ●FLORIAN HEIDEMANN, MARCO MUNZEL, and ACHIM KITTEL — University of Oldenburg, D-26111 Oldenburg

The basic principals of turbulence are still not well understood. On the basis of the measurements in a homogeneous isotropic free jet it is possible to characterize its invariant parameters and investigate the nature of turbulence. We have analyzed a heated free jet of water in a water tank with a new developed fast thermosensor with a high spatial and temperature resolution at different positions and for different flow velocities. The used nozzle has a diameter of 2mm, which provides a laminar flow with a rectangular velocity profile at the outlet. The sensor is based on a miniaturized thermocouple and has an active area of approx. $0.05\mu\text{m}^2$ and a response time of approx. $10\mu\text{s}$ in water with a temperature resolution of 50mK (measured with a bandwidth of 100kHz). Our aim is to characterize the temperature fluctuations perpendicular and parallel to the symmetry axis of the free jet with power spectra and increment distributions depending on the position with respect to the nozzle. Furthermore the measured fluctuations are analyzed with the markov analysis.

DY 40 Critical Phenomena and Phase Transitions I

Time: Thursday 09:30–11:00

Room: HÜL 186

Invited Talk

DY 40.1 Thu 09:30 HÜL 186

Random polymers and depinning transitions — ●CECILE MONTHUS and THOMAS GAREL — SPHT Saclay, France

According to recent progresses in the finite size scaling theory of disordered systems, thermodynamic observables are not self-averaging at critical points whenever disorder is relevant. This lack of self-averageness at criticality is directly related to the scaling properties of the probability distribution of pseudo-critical temperatures $T_c(i, L)$ over the ensemble of samples i of size L . This framework is very useful to characterize various depinning transitions involving random polymers:

(i) wetting transition in dimension $1 + 1$,

(ii) Poland-Scheraga model of DNA denaturation
(iii) the selective interface model.

DY 40.2 Thu 10:00 HÜL 186

On the breakdown of finite-size scaling in high dimensional systems — ●ALFRED HUCHT and SVEN LÜBECK — Theoretische Physik, Universität Duisburg-Essen, D-47048 Duisburg

Finite-size scaling functions of continuous phase transitions exhibit a scaling anomaly above the upper critical dimension d_c . This so-called breakdown of finite-size scaling is well-established on the basis of field theoretical and numerical approaches for system with periodic bound-

ary conditions, both in equilibrium (e.g. the Ising model, see [1] for an overview) and non-equilibrium (e.g. directed percolation [2]). Less work was done for geometric phase transitions and for Dirichlet boundary conditions. Therefore, we numerically investigate the bond percolation transition in $2 \leq d \leq 10$ dimensions with various boundary conditions. For $d < d_c = 6$ the spatial correlation length is limited by the systems size at criticality, whereas it exceeds the systems size above d_c , the hallmark of the breakdown of finite-size scaling.

We present, to our knowledge for the first time, a phenomenological and descriptive interpretation of this breakdown of finite-size scaling. Furthermore, we show that the high-dimensional behavior depends strongly on the boundary conditions.

[1] X. S. Chen and V. Dohm, Phys. Rev. E 63, 016113 (2000)

[2] S. Lübeck and H.-K. Janssen, Phys. Rev. E 72, 016119 (2005)

DY 40.3 Thu 10:15 HÜL 186

Finite-size behaviour of the microcanonical specific heat — ●HANS BEHRINGER¹ and MICHEL PLEIMLING² — ¹Fakultät für Physik, Universität Bielefeld, D-33615 Bielefeld — ²Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, D-91058 Erlangen

The basic quantity in the microcanonical approach to statistical properties of physical systems is the entropy $S(E) = \ln \Omega(E)$ where $\Omega(E)$ is the density of states as a function of the energy. The specific heat of the system is related to the inverse of the curvature of the entropy. The behaviour of the microcanonical specific heat of systems that undergo a continuous phase transition in the thermodynamic limit is investigated for finite systems. The numerical study of small Ising and Potts systems reveals a non-monotonic behaviour of the microcanonical specific heat as a function of the system size in contrast to a canonical treatment where the maximum of the specific heat increases monotonically with the system size. A general phenomenological theory is developed which permits a description of this peculiar behaviour of the microcanonical specific heat and allows in principle the determination of the microcanonical critical exponents from asymptotically large systems. In the case of the Baxter-Wu model the microcanonical analysis reveals a behaviour of the specific heat that suggests at first sight the appearance of a discontinuous phase transition in the infinite volume limit contrary to the known continuous character. However, the proposed phenomenological theory shows that this peculiar behaviour stems from a finite-size effect which disappears in the thermodynamic limit and therefore the observations are consistent with the continuous phase transition of in the Baxter-Wu model.

DY 40.4 Thu 10:30 HÜL 186

Critical Binder cumulant in two-dimensional Ising and Potts models — ●WALTER SELKE¹, LEV N. SHCHUR², and MARTIN HOLTSCHNEIDER¹ — ¹Institut fuer Theoretische Physik, RWTH Aachen — ²L.D. Landau Institute for Theoretical Physics, Chernogolovka, Russia

The Binder cumulant is known to be a very interesting quantity to characterize phase transitions. We report new results, using Monte Carlo techniques, on the value of that cumulant at the critical point, in particular in square lattice Ising (see W. Selke and L.N. Shchur, J. Phys. A 38, L739-L744 (2005)) and Potts models. The role of anisotropy, boundary condition, aspect ratio, and of the order of the phase transition is emphasized. Universal and nonuniversal features as analyzed recently by X. S. Chen and V. Dohm (Phys. Rev. E 70, 0566136 (2004)) are discussed.

DY 40.5 Thu 10:45 HÜL 186

Neutron optics of confined liquids near the critical point — ●ALEXANDER CHALYI¹, LEONID BULAVIN², and KYRYLO CHALYI³ — ¹Department of Physics, National Medical University, 13, Shevchenko Blvd., 01601 Kiev, Ukraine — ²Department of Molecular Physics, Kiev Taras Shevchenko National University, 6, Acad. Glushkov Boulevard, 03022 Kiev, Ukraine — ³Department of Medical Informatics, Kiev Medical Academy, 9, Dorogozhytska Str., 04112 Kiev, Ukraine

The neutron optics methods are applied to theoretical studies of the critical properties of confined liquids. In frame of this approach, analytical calculations are carried out for the density profile together with the neutron refractive index profile for non-uniform liquids at restricted geometry. Special attention is paid to gravity effects on properties of liquid systems. New results are obtained for the shifts of the critical temperature on the phase coexistence curve and positions of inflection points on the critical isotherm in confined liquids. The problem of propagation of the neutron beam in a non-uniform liquid at restricted geometry is solved. Special attention is paid to peculiarities of the refraction of neutrons due to the spatial limitation of a liquid system (namely, the corresponding formula for refractive angle of neutrons in finite-size individual and binary liquids are obtained and analyzed). The form of refractive index ellipsoid is studied and possible experimental consequences of neutron refraction in confined liquids are discussed. Dependence of the neutron propagation and elastic scattering in finite-size liquids on temperature (field) variables and geometrical factors is studied with confinement effects taken into account.

DY 41 Dynamical Physics in Biological Systems

Time: Thursday 10:00–11:30

Room: SCH 251

DY 41.1 Thu 10:00 SCH 251

DNA as a rigid-body chain — ●NILS BECKER and RALF EVERAERS — MPI Physik Komplexer Systeme, Dresden

The functioning of the DNA molecule in many biological situations depends on its sequence-dependent elastic behavior on a scale of a few base pairs to a few helical turns. Examples include winding onto nucleosomes and transcription regulation.

We investigate the elastic properties of DNA at this scale. We study a chain model in which the monomers are the base pairs, considered as rigid bodies. We take into account the full detail of their sequence dependent nearest neighbor interaction, including coupling of rotational and translational degrees of freedom, within a harmonic approximation.

This model fits in as a natural step in a coarse-graining hierarchy of DNA models. On the microscopic side, it can be parametrized by existing inter-base pair harmonic potentials. This allows a calculation of the sequence-dependent elastic response to forces and moments that are applied to short stretches of DNA. Towards larger scales, by taking an appropriate continuum limit, we can relate it to classic chain models for semiflexible polymers.

DY 41.2 Thu 10:15 SCH 251

A Bayesian Approach to the Evaluation of Dynamic Force Spectroscopy Experiments — ●SEBASTIAN GETFERT, PETER REIMANN, and MARTIN RAIBLE — Condensed Matter Theory, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld

The components of a biomolecular complex can be connected via suit-

able linkers to the tip of an atomic force microscope and a moving surface. When this surface is pulled apart at constant velocity the force f that acts on the bond increases (approximately) linearly in time until the chemical bond ruptures. This process is of stochastic nature. The distribution of the rupture forces and in particular the maximum depends in a characteristic way on the loading rate \dot{f} and on binding parameters like dissociation length and (force-free) dissociation rate [1]. Thus the evaluation of rupture force data from dynamic force spectroscopy experiments allows to draw conclusions about the energy landscape of the bond. We present a Bayesian approach to this evaluation in which experimental uncertainties can be included in a natural way. Further we discuss from a statistical point of view to which degree of accuracy the parameters of the distribution can be determined.

[1] E. Evans and K. Ritchie, Biophys. J. 72, 1541 (1997)

DY 41.3 Thu 10:30 SCH 251

Neuronal Growth: A Bistable Stochastic Process — ●TIMO BETZ, DARYL LIM, and JOSEF KÄS — Institut für Soft Matter Physics, University of Leipzig, Linnestr. 5, 04103 Leipzig, Germany

During the past decade, modeling biological systems as stochastic processes has given tremendous insight into nature's working principles at the level of networks, single cells, and molecules. However, the stochastic nature of neuronal growth has hardly been investigated. The basic step in the correct neuronal wiring of a developing organism is the controlled advancement of a highly motile structure, called the growth cone, which is directed by gradients of chemical guidance cues. We report on the first statistical analysis of the stochastic fluctuation of a neuronal growth

cone's leading edge movement. Describing the edge movement with a stochastic process allows inferring a bistable potential from the edge velocity distribution. Using Kramers' approach to calculate decay rates, an isotropic noise parameter can be determined, which we used to consistently connect the measured edge velocity distribution and the residence time distribution. An according analysis of the growth cone's motility confirms the model, and predicts that linear changes of the bistable potential might result in the directed growth cone translocation. These results help to understand how the growth cone can detect chemical gradients that are on the order of one molecule across its diameter, even in the highly noisy environment of a developing organism.

DY 41.4 Thu 10:45 SCH 251

The emergence of Ca^{2+} puffs as intracellular escape process — ●RÜDIGER THUL and MARTIN FALCKE — Hahn-Meitner Institut, Abteilung Theorie, Glienickestrasse 100, 14109 Berlin

Recent experiments and theoretical investigations have demonstrated that intracellular Ca^{2+} is a stochastic nonlinear medium. Local and global patterns are exclusively driven by fluctuations. These patterns form a hierarchy. Global events are built from a series of local incidents, which are termed Ca^{2+} puffs. A detailed study of Ca^{2+} puffs reveals that their emergence can be mapped to an escape process. That permits an analytic calculation of the mean stochastic fraction of the puff period. A quantification of the leading time scales provides further insights into this escape process. Moreover, we show that the spatial restriction of Ca^{2+} puffs enforces a discrete modeling of the Ca^{2+} dynamics.

DY 41.5 Thu 11:00 SCH 251

Discrete Model for Pattern Formation in Bacterial Colonies — ●PAWEŁ ROMANCZUK¹, UDO ERDMANN², HARALD ENGEL¹, and LUTZ SCHIMANSKY-GEIER² — ¹Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — ²Institute für Physik, Humboldt Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Bacterial colonies of *Escherichia coli* and *Salmonella typhimurium* show complex patterns of high density cell aggregates when exposed to certain nutrients. Decisive for this pattern formation is the production of a potent chemoattractor by the bacteria as a reaction to the nutrient [1]. The observed bacterial patterns range from temporary spots formed in liquid medium to “sunflower like” spot arrangements of strik-

ing complexity in a semi-solid medium. Motivated by this observations we suggest a simple model for the description of bacterial colonies based on the concept of Active Brownian motion [2]. Our model represents an interesting alternative to the usually employed “pure” reaction-diffusion equations as it allows us to study the macroscopic pattern formation of the colony, the mesoscopic dynamics of bacterial ensembles (swarming), as well as the microscopic dynamics of single cells. Here we will present the obtained qualitative and quantitative numerical results of our model and compare them with the experimentally observed bacterial dynamics.

[1] Budrene, E. O. und H. C. Berg: *Dynamics of formation of symmetrical patterns by chemotactic bacteria*. Nature, 376:49-53, 1995.

[2] Erdmann, U., *Kollektive Bewegung*, Logos Verlag, Berlin, 2004.

DY 41.6 Thu 11:15 SCH 251

Dynamics of epidemic outbreaks in heterogeneous populations — ●ALEJANDRO MORALES GALLARDO, DIRK BROCKMANN, LARS HUFNAGEL, and THEO GEISEL — MPI for Dynamics and Self-Organization, Göttingen, Germany

The dynamics of epidemic outbreaks have been investigated in recent years within two alternative theoretical paradigms. Among the most successful models is the deterministic susceptible-infected-recovered (SIR) model which approximately describes the dynamics for a large number of individuals and in which homogeneous contact rates are assumed. The central parameter of the SIR model is the basic reproduction number, the average number of secondary infections caused by one infected individual. Recently, scale free network models have received much attention as they account for the high variability in the number of social contacts involved. These models predict an infinite basic reproduction number in some cases. We investigate the impact of heterogeneities of contact rates in a generic model for epidemic outbreaks. In contrast to common static network models we investigate a system in which both the time periods of being infectious and the time periods between transmissions are Poissonian processes. The heterogeneities are introduced by means of strongly variable contact rates which yield power laws in the number of overall contacts. In contrast to scale free network models we observe a finite basic reproduction number and, counterintuitively a smaller overall epidemic outbreak as compared to the homogeneous system. Our study thus reveals that heterogeneities in contact rates does not facilitate the spread to infectious disease but rather attenuates it.

DY 42 Critical Phenomena and Phase Transitions II

Time: Thursday 11:00–13:00

Room: HÜL 186

DY 42.1 Thu 11:00 HÜL 186

Fortuin-Kasteleyn versus geometrical cluster — ●WOLFHARD JANKE¹ and ADRIAAN M.J. SCHAKEL² — ¹Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11, 04109 Leipzig — ²Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

We discuss how suitably defined geometrical objects encode in their fractal structure thermal critical behaviour [1]. Emphasis will be placed on the two-dimensional Potts model for which two types of spin clusters can be defined. Whereas the Fortuin-Kasteleyn clusters describe the standard critical behaviour of the pure model, the geometrical clusters describe the tricritical behaviour that arises when including vacant sites in the pure Potts model. The close connection between the two models respectively the two cluster types can be explained by a “dual map” that conserves the central charge, so that both model/cluster types are in the same universality class. The geometrical picture is supported by Monte Carlo simulations.

[1] W. Janke and A.M.J. Schakel, Nucl. Phys. **B700**, 385 (2004); Phys. Rev. **E71**, 036703 (2005); Phys. Rev. Lett. **95**, 135702 (2005); and e-print cond-mat/0508734.

DY 42.2 Thu 11:15 HÜL 186

Casimir effect in the presence of van-der-Waals-type interactions: exact results for the spherical model with periodic boundary conditions — ●DANIEL GRÜNEBERG¹, DANIEL DANTCHEV^{1,2}, and H. W. DIEHL¹ — ¹Fachbereich Physik, Universität Duisburg-Essen, D-45117 Essen, Germany — ²Institute of Mechanics—BAS, Acad. G. Bonchev St. bl. 4, 1113 Sofia, Bulgaria

It is studied how the Casimir effect in d -dimensional slabs with $2 < d < 4$ and periodic boundary conditions is affected at and near the bulk critical temperature $T_{c,\infty}$ by long-range pair interactions whose potential decays as $bx^{-(d+\sigma)}$ as $x \rightarrow \infty$, with $2 < \sigma < 4$ and $2 < d + \sigma \leq 6$. While such interactions decay sufficiently fast to leave bulk critical exponents and other universal bulk quantities unchanged, they entail important modifications of the standard scaling behavior of the excess free energy and the Casimir force, and give algebraically decaying contributions that dominate the behavior of these quantities for $T \neq T_{c,\infty}$ as a function of the slab's thickness. An appropriate mean spherical model in a slab geometry with periodic boundary conditions is solved exactly. The scaling functions of the excess free energy and the Casimir force are determined, including the contributions to first order in the usual leading irrelevant scaling field g_ω and the scaling field g_σ to which the long-range interactions give rise. In the case $d + \sigma = 6$, which includes that of nonretarded van-der-Waals interactions in $d = 3$ dimensions, the power laws of the corrections to scaling $\propto b$ of the spherical model get modified by logarithms. The origin of these anomalies is clarified.

DY 42.3 Thu 11:30 HÜL 186

When topology triggers a phase transition — ●MICHAEL KASTNER — Physikalisches Institut, Lehrstuhl für Theoretische Physik, Universität Bayreuth, 95440 Bayreuth

Two mathematical mechanisms, responsible for the generation of a thermodynamic singularity, are individuated. For a class of short-range, confining potentials, a topology change in some family of configuration space submanifolds is the only possible such mechanism. Two examples of systems in which the phase transition is *not* accompanied by such a topology change are discussed. The first one is a model with long-range interactions, namely the mean-field φ^4 -model, the second example is a one-dimensional system with a non-confining potential energy function. For both these systems, the thermodynamic singularity is generated by a maximization over one variable (or one discrete index) of a smooth function, although the context in which the maximization occurs is very different.

DY 42.4 Thu 11:45 HÜL 186

Free-Energy Barriers in a Mean-Field Spin Glass — ●ELMAR BITTNER and WOLFHARD JANKE — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

The mean-field Sherrington-Kirkpatrick spin-glass model is investigated by means of Monte Carlo simulations employing multioverlap and parallel tempering methods. We investigate the finite-size scaling behaviour of the free-energy barriers which are visible in the probability density of the Parisi overlap parameter. Assuming that the mean barrier height diverges with the number of spins N as N^α , our data show good agreement with the theoretical value $\alpha = 1/3$. We also found that the free-energy barriers of the Sherrington-Kirkpatrick spin-glass model are non-self-averaging and distributed according to the Fréchet extremal value distribution.

DY 42.5 Thu 12:00 HÜL 186

Observation of the critical regime near Anderson localization of light — ●MARTIN STÖRZER, PETER GROSS, CHRISTOF AEGERTER, and GEORG MARET — Fachbereich Physik Universität Konstanz; Universitätsstrasse 10; 78457 Konstanz

Diffusive transport is among the most common phenomena in nature. However, as predicted by Anderson, diffusion may break down due to interference. The transition from diffusive transport to localization of waves should occur for any type of classical or quantum wave in any media as long as the wavelength becomes comparable to the transport mean free path ℓ^* . The signatures of localization and those of absorption, or bound states, can however be similar, such that an unequivocal proof of the existence of wave localization in disordered bulk materials is still lacking. Here we present time resolved measurements of light transport through strongly scattering samples with $k\ell^*$ values as low as

2.5. In transmission, we observe deviations from diffusion which cannot be explained by absorption, sample geometry or reduction in transport velocity. Furthermore, the deviations from classical diffusion increase strongly with decreasing ℓ^* as expected for a phase transition. This constitutes an experimental realization of the critical regime in the approach to Anderson localization.

DY 42.6 Thu 12:15 HÜL 186

Numerical Results for the 3D Edwards-Anderson-Ising Model — ●ANDREAS NUSSBAUMER, ELMAR BITTNER, and WOLFHARD JANKE — Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11, 04109 Leipzig

We investigate the three-dimensional Edwards-Anderson-Ising model using a combination of the multicanonical method for the overlap parameter q (multi-overlap) with parallel tempering in temperature. To obtain the barrier heights in the overlap parameter q an effective one-dimensional Markov chain is constructed reproducing the distribution of q . From the eigenvalue spectrum of the resulting transition matrix the autocorrelation time can be calculated, leading to the sought barrier height [1].

The results for different temperatures well below the freezing point are compared to theoretical predictions (“replica” theory and “droplet” theory).

[1] B.A. Berg, A. Billoire, W. Janke, *Spin Glass Overlap Barriers in Three and Four Dimensions*, Phys. Rev. B **61** (2000) 12143.

Invited Talk

DY 42.7 Thu 12:30 HÜL 186

Universal scaling behavior of non-equilibrium phase transitions — ●SVEN LÜBECK — Theoretische Physik, Universität Duisburg-Essen, 47048 Duisburg

In contrast to equilibrium, a complete classification of the universal scaling behavior of non-equilibrium critical phenomena is still lacking. Thus the rich and often surprising variety of non-equilibrium phase transition has to be studied for each system individually. Here, we discuss the critical behavior of several systems exhibiting continuous phase transitions into absorbing states. By measuring certain universal scaling functions the systems can be grouped into universality classes, similar to equilibrium. It is the aim of this work to demonstrate the usefulness of universal scaling functions for the analysis non-equilibrium phase transitions. Determining the universal behavior it is often a more accurate test to consider scaling functions rather than the values of the critical exponents. While for the latter ones the variations between different universality classes are often tiny the scaling functions usually differ significantly. Additionally to the manifestation of universality classes, universal scaling functions are useful in order to check renormalization group results quantitatively.

DY 43 Signals and neuronal Networks

Time: Thursday 11:30–12:45

Room: SCH 251

DY 43.1 Thu 11:30 SCH 251

Precise Timing in Strongly Heterogeneous Neural Networks with Delay — ●RAOUL-MARTIN MEMMESHEIMER^{1,2} and MARC TIMME^{1,2,3} — ¹Max-Planck-Institut für Dynamik und Selbstorganisation (MPIDS) Göttingen — ²Bernstein Center for Computational Neuroscience BCCN Göttingen — ³Center for Applied Mathematics, Cornell University, Ithaca, USA

Precise timing of spikes is discussed to be a key element of neural computation [1], but it is still an open question how patterns of precisely timed spikes emerge in the dynamics of neural networks [2]. Here we demonstrate that and how deterministic neural networks which simultaneously exhibit delayed interactions [3], complex topology [4] and strong heterogeneities can yet display periodic patterns of spikes that are precisely timed. We develop an analytical method to design networks that display a given non-degenerate pattern with realistic temporal extent and complicated temporal structure. We point out that the same pattern can exist in very different networks; its stability depends on the particular coupling architecture. Using a nonlinear stability analysis, we show that networks with purely inhibitory (or purely excitatory) coupling can either store only stable or only unstable patterns.

[1] M. Abeles, *Science* **304**:523 (2004).

[2] I.J. Matus Bloch, C. Romero Z., *Phys. Rev. E* **66**:036127 (2002); D.Z. Jin, *Phys. Rev. Lett.* **89**:208102 (2002); M. Denker et al., *Phys. Rev. Lett.* **92**:074103 (2004).

[3] U. Ernst, K. Pawelzik, T. Geisel, *Phys. Rev. Lett.* **74**:1570 (1995).

[4] M. Timme, F. Wolf, T. Geisel, *Phys. Rev. Lett.* **89**:258701 (2002).

DY 43.2 Thu 11:45 SCH 251

Delay induced instability in a small neural network model — ●BERNHARD HEISLBETZ¹ and ARNE WUNDERLIN² — ¹DLR Lampoldshausen, Institut für Raumfahrtantriebe, D-74239 Hardthausen — ²Universität Stuttgart, 1. Institut für Theoretische Physik, D-70550 Stuttgart

We present the linear stability analysis of a small neural network model consisting of two neurons with time-delayed coupling and feedback. Numerical simulations illustrate the analytical results and show the dynamical behavior of the neural network model after destabilisation.

DY 43.3 Thu 12:00 SCH 251

Phase-Rectified Signal Averaging Detects Quasi-Periodicities in Non-Stationary Data — ●J. W. KANTELHARDT¹, A. BAUER², A. BUNDE³, P. BARTHEL², R. SCHNEIDER², M. MALIK⁴, and G. SCHMIDT² — ¹Fachber. Physik u. Zentr. f. Computational Nanoscience, Martin-Luther-Universität, Halle (Saale), Germany — ²Med. Klinik u. Dt. Herzzentrum der Technischen Universität München, Germany — ³Inst. f. Theoretische Physik III, Justus-Liebig-Universität, Giessen, Germany — ⁴Dept. of Cardiac and Vascular Sciences, St. George's, University of London, UK

We present an efficient technique for the study of quasi-periodic oscillations in noisy, non-stationary signals, which allows the assessment of system dynamics despite phase resetting and noise. It is based on the definition of anchor points in the signal (in the simplest case increases or decreases of the signal) which are used to align (i. e., phase-rectify) the oscillatory fluctuations followed by an averaging of the surroundings of the anchor-points. We give theoretical arguments for the advantage of the technique, termed phase-rectified signal averaging (PRSA), over conventional spectral analysis and show in a numerical test using surrogate heartbeat data that the threshold intensity for the detection of additional quasi-periodic components is approximately 75% lower with PRSA. With the use of different anchor point criteria PRSA is capable of separately analysing quasi-periodicities that occur during increasing or decreasing parts of the signal.

DY 43.4 Thu 12:15 SCH 251

Influence of negative feedback on the dynamics of a stochastic signalling module — ●PETER BOROWSKI, MANOJ GOPALAKRISHNAN, FRANK JÜLICHER, and MARTIN ZAPOTOCKY — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden

DY 44 Critical Phenomena and Phase Transitions III

Time: Thursday 14:30–16:00

Room: HÜL 186

Invited Talk

DY 44.1 Thu 14:30 HÜL 186

Spin liquids: from frustrated magnets to quantum dimer models — ●FREDERIC MILA — Institute of Theoretical Physics, Ecole Polytechnique Federale de Lausanne, BSP Unil, CH-1015 Lausanne (Switzerland)

The search for Resonating Valence Bond (RVB) spin liquids has been extremely active since the discovery of high temperature superconductivity in a family of cuprates and the proposal by Anderson that doping RVB spin liquids might lead to superconductivity. Very significant progress has been made recently on two fronts: 1) Experimentally, with the synthesis of compounds which seem to resist any kind of ordering down to the lowest accessible temperatures; 2) Theoretically, with the numerical proof that the Quantum Dimer Model on the triangular lattice has an RVB phase. In this talk, I will review both aspects of the field, and I will discuss the possible relationships between Quantum Dimer Models and realistic effective models of Mott insulators.

DY 44.2 Thu 15:00 HÜL 186

Anomalous superferromagnetic relaxation behavior in ordered magnetic structures — ●STEFANIE RUSS and ARMIN BUNDE — Institut für Theoretische Physik III, Universität Giessen, D-35392 Giessen

We perform Monte-Carlo simulations to study the anomalous magnetic relaxation behavior of single-domain ferromagnetic nanoparticles under the combined forces of dipolar interaction and anisotropy effects, located at the sites of a simple cubic lattice. The anisotropy axes are orientated along the z -axes. We study how the system relaxes from two ordered states where all dipoles are orientated (a) along the antiferromagnetic ground-state and (b) along the z -direction of the lattice. We introduce appropriate order parameters O_{\parallel} and O_{\perp} along the z -direction and in the xy -plane, respectively, to describe both, relaxation and final structure.

We find that below a critical temperature T_c , different structures are reached in both cases, which are described by the same value of O_{\parallel} but by different values of O_{\perp} . We discuss the possibility of obtaining a superferromagnetic state and compare the results with experiments on ultrafine magnetic particles.

We study the stochastic kinetics of a two-state signalling module. In the active state, the module produces a chemical species which enhances the rate of deactivation, giving rise to negative feedback. Examples are an ion channel whose closing rate depends on the ion concentration that it conducts, or a gene whose protein product acts as a repressor. We develop a path-integral formulation of the two-state process, based on the temporal statistics of its state-flips. In the limit of weak feedback, analytic results are obtained for the mean values and correlation functions as well as response functions. Monte Carlo simulations are performed which support these analytical predictions and provide results beyond linear perturbation theory.

DY 43.5 Thu 12:30 SCH 251

One dimensional driven lattice gas of dimers coupled to on-off bulk kinetics — ●PAOLO PIEROBON^{1,2}, THOMAS FRANOSCH^{1,2}, MAURO MOBILIA¹, and ERWIN FREY¹ — ¹Arnold Sommerfeld Center, Theresienstr.37, D-80333 Muenchen — ²Hahn-Meitner Institut, Glienickerstr.100, D-14109 Berlin

We investigate the properties of a system that couples the Totally Asymmetric Simple Exclusion Process (TASEP) to the on/off kinetics in the bulk. We consider extended particles showing the robustness of the picture found in the case of monomers. We highlight analogies and differences between monomers and dimers using a refined mean field analysis (consistent with both the TASEP part and the on/off bulk kinetics) to rationalize the Monte Carlo data and derive the phase diagram. Furthermore we investigate the effect of the presence of a bottleneck in this kind of systems.

DY 44.3 Thu 15:15 HÜL 186

Critical Dynamics of Magnets with Random Anisotropy — ●REINHARD FOLK¹, MAXIM DUDKA², YURIJ HOLOVATCH², and GÜNTER MOSER³ — ¹Institute for Theoretical Physics University Linz Austria — ²Institute for Condensed Matter Physics National Academy of Sciences of Ukraine Lviv Ukraine — ³Molecular Biology University of Salzburg Salzburg Austria

We investigate the relaxational critical dynamics with non-conserved order parameter coupled to the energy density (model C critical dynamics) for three-dimensional magnets with disorder in a form of a random anisotropy axis. For a random distribution of cubic symmetry, the static asymptotic critical behaviour coincides with that of random site Ising systems. Therefore the asymptotic critical dynamics is governed by the dynamical exponent of the random Ising model. However, the disorder influences considerably the dynamical behaviour in the non-asymptotic regime. We perform a field-theoretical renormalization group analysis within the minimal subtraction scheme in two-loop order to investigate the asymptotic and effective critical dynamics of random anisotropy systems. The results demonstrate a rich non-monotonic behaviour of the dynamical effective critical exponent z_{eff} . The limiting case of a purely relaxational dynamics [1] is also considered. (Work supported by the Fonds zur Foerderung der wissenschaftlichen Forschung Project No. P16574) [1] M. Dudka, R. Folk, Yu. Holovatch, and G. Moser, submitted to Condensed Matter Physics (Ukraine) 2005 (cond-mat/0506325)

DY 44.4 Thu 15:30 HÜL 186

Integral equation study of an ideal Ising mixture — ●WOLFGANG FENZ¹, IGOR OMELYAN^{1,2}, and REINHARD FOLK¹ — ¹Institute for Theoretical Physics, Linz University, Altenberger Str. 69, A-4040 Linz, Austria — ²Institute for Condensed Matter Physics, 1 Svientsitskii Street, UA-79011 Lviv, Ukraine

We construct an integral equation scheme for magnetic binary mixtures of an ideal soft-core Ising fluid and a soft-sphere fluid by mapping the system onto an equivalent nonmagnetic ternary mixture. We apply the multi-component Ornstein-Zernike equation together with a closure relation based on the soft mean spherical approximation and a field constraint for the Ising fluid component. Phase coexistence curves at constant pressure or temperature are calculated both by directly eval-

uating the chemical potentials via the bridge function [1], and by using a Maxwell-like construction. Our results are compared to Monte Carlo data obtained earlier [2], and we find that the second method yields much better agreement with the simulations.

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

[1] L. L. Lee, J. Chem. Phys. 97, 8606 (1992)

[2] W. Fenz and R. Folk, Phys. Rev. E 71, 046104 (2005)

[3] W. Fenz, I. Omelyan, and R. Folk, to be published in Phys. Rev. E

DY 44.5 Thu 15:45 HÜL 186

Critical exponents of 3D Ising model from theory and Monte Carlo simulations of very large lattices — ●JĒVGENIJS KAUPUŽS — Institute of Mathematics and Computer Science, University of Latvia, LV-1459 Riga, Latvia

We report the results of extended Monte Carlo simulations of 3D Ising model near criticality for linear lattice sizes up to $L = 640$. Our aim is to verify the essentially different predictions for the values of the critical

exponents made by the perturbative RG theory [1] and our method of grouping of Feynman diagrams [2]. Our basic method of analysis is to look how the effective critical exponents evaluated either at the critical or at a suitable pseudocritical coupling change with the lattice size. It allows us to control visually the systematic deviations in the results depending on the lattice sizes used in simulations and to evaluate the asymptotic values of the critical exponents by a suitable fit (extrapolation). The usually reported values of the critical exponents appear to be effective rather than asymptotic. Although the currently simulated effective values come closer to the RG ones, the plots of the effective exponents show a tendency to deviate from the RG values towards those found in [2]. We compare this behaviour with that of the effective exponent ν evaluated in [3] from the known experimental data for the superfluid fraction in liquid helium very close to the λ -transition point.

[1] J. Zinn-Justin, Quantum Field Theory and Critical Phenomena, Clarendon Press, Oxford, 1996

[2] J. Kaupužs, Ann. Phys. (Leipzig) 10, 299 (2001)

[3] J. Kaupužs, Eur. Phys. J. B 45, 459 (2005)

DY 45 Soft Matter

Time: Thursday 14:30–16:00

Room: SCH 251

DY 45.1 Thu 14:30 SCH 251

Coil-globule and globule-globule transition of a three-dimensional, flexible homopolymer — ●THOMAS STRAUCH, FEDERICA RAMPF, KURT BINDER, and WOLFGANG PAUL — Institute for Physics, Johannes Gutenberg University, 55099 Mainz Germany

We present simulation results for the phase behavior of a flexible homopolymer using the Wang-Landau sampling algorithm. The chain is modeled with the bond-fluctuation model with an attractive square well interaction between the monomers. For finite chain length the model shows a two stage collapse, from the coil state to the globular state followed by a crystallization at temperatures beneath the θ -temperature. In a recently published investigation by F. Rampf, W. Paul and K. Binder on this model, it was shown that for interaction range $\sqrt{6}$ the coil-globule phase transition and the crystallization phase transition coincide in the thermodynamic limit.

In order to check the general validity of this phase behavior we investigated a system with longer interaction range, which should stabilize the liquid phase because of entropic effects. We show that in our model with interaction range of $\sqrt{10}$ the liquid phase will exist also in the thermodynamic limit. The transition temperatures do not coincide.

The crystal structure in the ground state displays a mixture of hexagonal and cubic packing.

DY 45.2 Thu 14:45 SCH 251

Surface segregation of conformationally asymmetric polymer blends — ●SEMION STEPANOW and ANDREI FEDORENKO — Martin-Luther-Universität Halle, Fachbereich Physik, D-06099 Halle

We have generalized the Edwards' method of collective description of dense polymer systems in terms of effective potentials to polymer blends in the presence of a surface. With this method we have studied conformationally asymmetric athermal polymer blends in the presence of a hard wall to the first order in effective potentials. For polymers with the same gyration radius R_g but different statistical segment lengths l_A and l_B the excess concentration of stiffer polymers at the surface is derived as $\delta\rho_A(z=0) \sim (l_B^{-2} - l_A^{-2}) \ln(R_g^2/l_c^2)$, where l_c is a local length below of which the incompressibility of the polymer blend is violated. For polymer blends differing only in degrees of polymerization shorter polymers enrich the wall.

DY 45.3 Thu 15:00 SCH 251

Structures and elastic properties for 2-d model colloidal crystals in confined geometry — ●ANDREA RICCI — Institut fuer Physik, J Gutenberg Universitaet Mainz

A model for colloidal particles confined between two parallel boundaries separated a distance D is simulated by Monte Carlo, for the two-dimensional (2-d) case at densities where the bulk 2-d is well in crystalline phase. While the positional order is enhanced for a suitably corrugated boundary potential, for a planar boundary potential, positional ordering normal to the walls is enhanced ("layering") but destroyed parallel to the walls: the behavior of the system is more 1-d like. Due to the layering the orientational order is always present. It is also discussed how, for

different T above the bulk melting point, the ordering induced by the walls decays towards the bulk values when we move to the inner part of the system.

If D does not fit the lattice parameter we observe, in both cases of walls considered, formation of misfits.

DY 45.4 Thu 15:15 SCH 251

Magneto-optics with capped colloids — ●LARYSA BARABAN, FLORIAN MERKT, BJÖRN BIEHLER, PAUL LEIDERER, and ARTUR ERBE — Universität Konstanz, Fachbereich Physik, 78457 Konstanz, Deutschland

Colloidal suspensions are fascinating examples of soft matter, but also model systems for studying the behavior of atoms and molecules. In most cases, the colloidal particles used for these investigations have spherical symmetry. Here we present the fabrication and characterization of magnetically *anisotropic* particles.

Metallic bi-layers (Ni, Au) are evaporated on top of silica colloids, thus generating hemispheric magnetic "caps". In order to detect the magnetization of particles we use the magneto-optic (m-o) Faraday effect. Capped particles are placed on a reflecting surface (usually aluminum or silver), evaporated on a m-o active garnet film (YIG). Their magnetic moments induce a distribution of the magnetic field in the m-o film; therefore the Faraday rotation changes from point to point. Reflected by the mirror, polarized light carries information about the local magnetization in the YIG.

As expected, the magnetization of capped colloids displays hysteresis-like behavior. From these data we evaluate the initial magnetic moment and magnetic moment in the saturation regime. The remanent magnetization and coercivity of magnetic particles are estimated as well.

As a possible application, this technique can be used to check the magnetic monodispersity of big particles arrays by a single magneto-optic measurement.

DY 45.5 Thu 15:30 SCH 251

Optimal cell approach to osmotic properties of finite stiff-chain polyelectrolytes — ●CHRISTIAN HOLM^{1,2} and DMYTRO ANTYPPOV³ — ¹Frankfurt Institute for Advanced Studies (FIAS), Johann Wolfgang Goethe University, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany — ²Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128, Mainz, Germany — ³Department of Materials Science and Metallurgy, Pembroke St., Cambridge, CB2 3QZ, UK

We propose a self-consistent geometry optimized cell model approach to study osmotic properties of stiff-chain polyelectrolyte solutions. In contrast to the usual monotonic Poisson-Boltzmann prediction, the osmotic coefficient is a non-monotonic function of concentration with a pronounced minimum. In the dilute regime, a lower degree of polymerization

is found to reduce significantly the counterion condensation. Despite its simplicity, the single-chain cell model yields the same osmotic behavior as a corresponding many-body bulk system up to a dense semi-dilute regime.

[1] D. Antypov, C. Holm, manuscript submitted

DY 45.6 Thu 15:45 SCH 251

Surface dynamics of capillary waves close to the glass transition - Experiments with static and dynamic x-ray scattering — ●CHRISTIAN GUTT^{1,2}, HENNING STERNEMANN², MICHAEL PAULUS², SIMONE STREIT², ANDERS MADSEN³, MICHAEL SPRUNG⁴, and METIN TOLAN² — ¹HASYLAB at DESY, Notkestrasse 85, 22607 Hamburg — ²Experimentelle Physik I, Universität Dortmund — ³ESRF, Grenoble, France — ⁴Advanced Photon Source, ANL, Argonne, IL

Liquid surfaces are subject to thermally excited capillary waves which produce a surface roughness of a few Angstrom. Our surface scattering experiments with synchrotron radiation address the question of how these hydrodynamic surface modes become arrested close to the bulk glass transition. For this purpose x-ray reflectivity, grazing incidence diffraction and x-ray photon correlation spectroscopy experiments have been performed. The experiments cover a broad temperature range from room temperature down to temperatures close to the bulk glass transition at 180K. We were able to measure the temperature dependent surface roughness [1], the static height-height correlation function on a length-scale of nanometers and the dynamic structure factor of the capillary wave fluctuations. The results are compared with theoretical predictions on the freezing behavior of capillary waves at the glass transition [2].

[1] M. Sprung et al. Phys.Rev. E 70, 051809 (2004) [2] J. Jäckle and K. Kawasaki, J.Phys.:Condens.Matter 7, 4351 (1998)

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 than 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 BLEIL¹, DAVID MARR², and CLEMENS BECHINGER¹ — ^{1,2} Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — ²Chemical 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 BAUMGARTL¹, JOSE-LUIS ARAUZ-LARA², and CLEMENS BECHINGER¹ — ^{1,2} Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — ²Instituto 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 BLICKLE¹, THOMAS SPECK², LAURENT HELDEN¹, UDO SEIFERT², and CLEMENS BECHINGER¹ — ¹2. Physikalisches Institut, Universität Stuttgart, Germany — ²II. 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: $\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}$. 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 HERTLEIN¹, LAURENT HELDEN¹, ELENA EREMINA², THOMAS WRIEDT², and CLEMENS BECHINGER¹ — ¹2. Phys. Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart — ²Institut 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 exponential 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 Magdeburg, 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 representation of the data are updated either 'offline' 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 first results.

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 probability 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 CLAUSSEN¹, ARNE TRAUlsen², and CHRISTOPH HAUERT² — ¹Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany — ²Center 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 explicitly 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 effect in ferrofluids with mean-field interactions — ●VOLKER BECKER and ANDREAS ENGEL — Carl-von-Ossietzky-Universität, 26111 Oldenburg

Ferrofluids are suspensions of magnetic particles in a 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. — ●MALGORZATA 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-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 Committee 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-UGLU, 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 -dependence 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 RUSS¹, ARMIN BUNDE¹, and JÖRG KÄRGER² — ¹Institut für Theoretische Physik III, JLU Giessen — ²Institut 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 neglected.

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 weighted 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 processes 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 KAHL¹, MARY LAURA LIND², STEFAN BUSCHHORN¹, JÖRG HACHENBERG¹, WILLIAM L. JOHNSON², and KONRAD SAMWER¹ — ¹1. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — ²138-78 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 functions 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 synchronization 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 order to understand the relationship between underlying dynamics and biophysics.

We use an extended Hindmarsh-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 comparison 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 synchronization. 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 DEREVYANKO¹ and JAROSLAW PRILEPSKIY² — ¹Photonics Research Group, Aston University, Aston Triangle, Birmingham, UK — ²B.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 deterministic 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 observation 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 attractor 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 obtained 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 HINKEL¹, REINHARD MAHNKE¹, and REINHART KUEHNE² — ¹Institute of Physics, Rostock University, D-18051, Rostock — ²German 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 STEGEMANN¹, ALEXANDER BALANOV^{1,2}, and ECKEHARD SCHÖLL¹ — ¹Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin — ²School 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:

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

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 rotational motion [1]. The other utilizes the irreversible Langevin equation.

Priority is given to the comparison 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 POMPLUN¹, ECKEHARD SCHÖLL¹, and ALEXANDER BALANOV^{1,2} — ¹Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, 10623 Berlin — ²School 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 chaotic 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. Höbberger-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 ZYKOV¹, VASILIJ DAVYDOV², and HARALD ENGEL¹ — ¹Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — ²Moscow 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-MOLINA¹, NIURKA QUINTERO², ANGEL SANCHEZ³, and FRANZ MERTENS⁴ — ¹Max-Planck Institut für Physik Komplexer Systeme, 01187 Dresden, Germany — ²Departamento de Física Aplicada I, E.U.P., *Universidad de Sevilla, 41011 Sevilla, Spain — ³Departamento de Matemáticas, Universidad Carlos III de Madrid, 28911 Leganes, Madrid, Spain — ⁴Physikalisches 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 necessary 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 $10 \mu\text{m}$, 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 ZELLER¹, MARTIN FALCKE², STEN RÜDIGER², and HARALD ENGEL¹ — ¹Institut für Theoretische Physik, TU-Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — ²Abteilung 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 Ca^{2+} 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 through 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 CHO^{1,2}, HIROYUKI SHIRAHAMA^{1,3}, KLAUS HÖHNE¹, and HARTMUT BENNER¹ — ¹Institut für Festkörperphysik, TU Darmstadt, Germany — ²Department of Physics, University of Science, Pyongyang, DPR Korea — ³Ehime 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, *Bunsenstr. 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 TEUFEL 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.

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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 analytically 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 non-equilibrium steady state on a numerically (or might be also physically) accessible time-scale.

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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 WEDEKIND¹, DAVID REGUERA², and REINHARD STREY¹ — ¹Institut für Physikalische Chemie, Universität zu Köln, Luxemburger Str. 116, D-50939 Köln, Germany — ²Departament 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 mimicking 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 nonconserved 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-GEIER¹ — ¹Humboldt Universität zu Berlin — ²Universität 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.

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DY 46.63 Thu 16:00 P1

Modern Methods in Protein Simulations — ●CHRISTOPH JUNGHANS^{1,2} and ULRICH H.E. HANSMANN² — ¹Institut für Theoretische Physik, Universität Leipzig — ²Computational 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 multi-canonical 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.

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DY 46.64 Thu 16:00 P1

Fractional calculus applied to the ion dynamics in porous matter — ●DEAN KOROŠAK¹, BRUNO CVIKL^{1,2}, RENATA JECL¹, JANJA KRAMER¹, and ANITA PRAPOTNIK BRDNIK¹ — ¹University of Maribor, Faculty of Civil Engineering, Chair for Applied Physics, Smetanova 17, 2000 Maribor Slovenia — ²J. 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 anomalous 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.

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DY 46.65 Thu 16:00 P1

Dynamics of glass-forming liquids in soft confinement — ●MARIA MAYOROVA¹, REINER ZORN¹, DIETER RICHTER¹, and BERNHARD FRICK² — ¹IFF, FZJ, Germany — ²ILL, 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 interpreted 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].

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DY 46.67 Thu 16:00 P1

Adsorption of random correlated copolymer: the Morita approximation — ●ALEXEY POLOTSKY^{1,2}, ANDREAS DEGENHARD¹, and FRIEDERIKE SCHMID¹ — ¹Fakultät für Physik, Universität Bielefeld, Universitätsstraße 25, D-33615 Bielefeld, Germany — ²Sérvíce 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).

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DY 46.68 Thu 16:00 P1

Shear-driven gelation in two dimensions — ●DANIEL RINGS¹, KAJETAN BENTELE², and KLAUS KROY¹ — ¹Institut für Theoretische Physik, Universität Leipzig, Vor dem Hospitalore 1, D-04103 Leipzig — ²Abteilung Theoretische Physik (SF5), Hahn-Meitner-Institut Berlin, Glienicke 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.

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DY 46.70 Thu 16:00 P1

Like-charged rods at zero temperature — ●AXEL ARNOLD¹ and CHRISTIAN HOLM² — ¹FOM Institute for Atomic and Molecular Physics, Kruislaan 407, 1098 SJ Amsterdam, The Netherlands — ²Frankfurt 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 BLOCHOWISZ, 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 water droplets 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°C and 10⁻²Hz to 10⁶Hz 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.

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DY 46.72 Thu 16:00 P1

Colloidal 2d-transport in restricted geometry — ●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 from 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 HEYDT¹, HENNING LÖWE², PETER MÜLLER^{1,3}, and ANNETTE ZIPPELIUS¹ — ¹Institut f. Theoretische Physik, Universität Göttingen, Germany — ²Eidgen. Institut f. Schnee- und Lawinenforschung SLF, Davos, Switzerland — ³Fakultät 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_{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 $\text{Re} \chi_c(\omega)$ 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].

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DY 46.74 Thu 16:00 P1

Computer Simulation of Stochastic Dynamics in Hard-Sphere Systems — •THOMAS VOIGTMANN¹, CRISTIANO DE MICHELE², and ANTONIO SCALA² — ¹University of Edinburgh, U.K. — ²Universita 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 occurrence 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.

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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 dy-

namics 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.

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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 SCHUMANN¹, JAN W. KANTELHARDT¹, and THOMAS PENZEL² — ¹Fachbereich Physik und Zentrum für Computational Nanoscience, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — ²Klinikum 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 healthy subjects during sleep. Sleep minimizes physical and mental disturbances which camouflage the intrinsic autonomous variabilities of interest. 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. AMECKE¹, R. RADÜNZ¹, M. DÖRING¹, and M. SCHREIBER¹ — ¹Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — ²Max-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. Luczka 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 mathematical 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 systems.

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. KANTELHARDT¹, RICHARD BERKOVITS², and SHLOMO HAVLIN² — ¹Fachbereich Physik und Zentrum für Computational Nanoscience, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — ²Minerva 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 diagrams. 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 KLEMM¹ and STEFAN BORNHOLDT² — ¹Dept. of Bioinformatics, University of Leipzig, Germany — ²Institute 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, $P(J) \sim 1/|J|^{(4+\alpha)}$ 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 equilibrium shape 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 20th 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 KITKY³, CHRISTIAN WAGNER¹, and PATRICK HUBER² — ¹Experimentalphysik, Universität des Saarlandes, D-66041 Saarbrücken — ²Technische Physik, Universität des Saarlandes, D-66041 Saarbrücken — ³Institute 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 ECHEHARD SCHÖLL — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

Various growth phenomena 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 WEBER¹, MICHAEL BIEHL², THORSTEN VOLKMANN¹, and MIROSLAV KOTRLA³ — ¹Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg — ²Institute for Mathematics and Computing Science, University of Groningen, P.O. Box 800, NL-9700 AV Groningen — ³Institute 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 WALTHER¹, MICHAEL BIEHL², FLORIAN MUCH¹, and CHRISTIAN VEY¹ — ¹Institut für Theoretische Physik und Astrophysik, Sonderforschungsbereich 410, Universität Würzburg, Am Hubland, D-97074 Würzburg — ²Institute 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 $\propto R^{4\pm 0.2}$. 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 $\approx 80^\circ$. 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. KRÜLLE¹, A. WIERSCHEM², N. AKSEL², and I. REHBERG¹ — ¹Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth — ²Technische 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 HERMANN¹, and DIETRICH STOYAN² — ¹Institute for Solid State and Materials research, IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — ²Institute 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 SOHALI 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 loses 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, Germany

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 MARTHALER¹ and MARK DYKMAN² — ¹Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe, Germany — ²Michigan 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 $T \rightarrow 0$; 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 FRÜHNER 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 4th order were used. Here an alternative potential with terms up to 6th 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 occurrence 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 \mathbf{H} stabilizes a flat surface of a ferrofluid by suppressing surface modulations when the magnetic field is parallel

to the wave vector \mathbf{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 Bidisperse Ferrofluid with Chain Aggregates: Theory and Computer Simulations — •CHRISTIAN HOLM^{1,2}, SOFIA KANTOROVICH³, ALEXEI O. IVANOV³, and E.S. PYANZINA³ — ¹Frankfurt Institute for Advanced Studies (FIAS) Johann Wolfgang Goethe University, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany — ²Max-Planck-Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz, Germany — ³Urals 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 simulation 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 ferrocoldoids. 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 PLEIMLING¹ — ¹Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Germany — ²Laboratoire 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

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

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 ($T \rightarrow 0$) 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 HELLMUND¹ and WOLFHARD JANKE² — ¹Mathematisches Institut, Universität Leipzig — ²Institut 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 ($q \rightarrow 1$) and tree percolation ($q \rightarrow 0$) and obtain critical exponents in various dimensions.

DY 46.120 Thu 16:00 P1

Molecular dynamics simulations of argon nucleation — ●JAN WEDEKIND¹, DAVID REGUERA², and REINHARD STREY¹ — ¹Institut für Physikalische Chemie, Universität zu Köln, Luxemburger Str. 116, D-50939 Köln, Germany — ²Departament 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 SCHEHR¹ and RAJA PAUL² — ¹Theoretische Physik, Universität Saarbrücken — ²BIOMS, 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. RÖSSLER², and R.L. STAMPS¹ — ¹School of Physics, University of Western Australia, Perth, Australia — ²IFW 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. Kloppe 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, VLADIMIR 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. Feodosyev, 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 SUBSTITUTIONAL 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 $\bar{E}(^2E)$ 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 VICENCIO¹ and MAGNUS JOHANSSON^{1,2,3} — ¹Max-Planck-Institut für Physik Komplexer Systeme — ²Department of Physics, Chemistry and Biology (IFM), Linköping — ³University 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 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 H₂O/D₂O, and THF-d8-H₂O/D₂O-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.

DY 50 Lattice Dynamics and Non-Linear Excitations

Time: Friday 10:15–11:30

Room: HÜL 186

DY 50.1 Fri 10:15 HÜL 186

Continuous time quantum Monte-Carlo simulations of polarons and bipolarons — ●J.P. HAGUE¹, P.E. KORNILOVITCH², A.S. ALEXANDROV¹, and J.H. SAMSON¹ — ¹Dept. of Physics, Loughborough University, LE11 3TU, UK — ²Hewlett-Packard Company, 1000 NE Circle Blvd, Corvallis, Oregon 97330, USA

We present the results of a continuous-time quantum Monte-Carlo algorithm for simulating polarons and bipolarons. An exact integration over phonon degrees of freedom leads to an efficient algorithm, which may be used for arbitrary interaction range. We consider the effects of lattice geometry and dimensionality on polaron properties including the effective mass, energy, number of phonons involved in the polaron, mass isotope coefficient, polaron spectrum and polaron density of states. In particular, we find that the coordination number has a greater effect on the polaron dynamics than the dimensionality, and that long-range Fröhlich interactions wash-out the effects of the lattice geometry (condmat/0509590). Finally, we discuss extensions of the algorithm to simulate bipolarons on various lattice configurations (e.g. the staggered ladder).

DY 50.2 Fri 10:30 HÜL 186

Phonons at the β -tin \rightarrow Imma \rightarrow sh phase transitions in Si: An *ab-initio* study — ●KATALIN GAAL-NAGY — Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, 20133 Milano (Italy)

We present an *ab-initio* study of the lattice statics and dynamics of Si near the β -tin \rightarrow Imma \rightarrow sh phase transitions. Our results allow a new interpretation of measured Raman phonon frequencies of what was thought to be the β -tin phase. A comparison of our data with the experimental ones shows that the phase transitions β -tin \rightarrow Imma \rightarrow sh have been already indicated in the Raman spectra even though not realized because of marginal changes. Furthermore, we find a soft-mode behavior for the phase transition sh \rightarrow Imma. The transition pressure for the β -tin \rightarrow Imma phase transition can be determined precisely from the phonon frequencies rather than from the lattice parameters. This work has been performed using the plane-wave pseudopotential approach to the density-functional theory and the density-functional perturbation theory within the local density approximation.

DY 50.3 Fri 10:45 HÜL 186

Soft local phonon modes in thermoelectric materials — ●WERNER SCHWEIKA¹ and RAPHAEL HERMANN² — ¹Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, 52425 Jülich — ²Department of Physics, B5, University of Liege, Belgium

We have studied powders of three different thermoelectric materials, Tl-filled skutterudites[1], Ba- and Sr-filled germanium clathrates[2], and Zn₄Sb₃ alloys, by inelastic neutron scattering. For all materials, a common feature of a prominent soft local phonon mode with an energy of

about 5 meV has been observed consistently with Einstein modes of rattling atoms in these relatively open cage-like structures. While approaches to thermoelectric properties often focus on the electronic structure our results indicate that local phonon modes play a key role in providing an effective scattering mechanism for the heat transporting acoustic phonons.

[1] Phys. Rev. Lett. 90, 135505-1 (2003).

[2] Phys. Rev. B 72, 174301 (2005).

DY 50.4 Fri 11:00 HÜL 186

Raman spectroscopy studies on THF clathrate hydrates — ●BEATA WALASEK, SASCHA ESCHBORN, and RUDOLF FEILE — Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt

Clathrate hydrates consist of an ice-like tetrahedral network of hydrogen bonded water molecules, forming polyhedral cages in which various guest molecules can be enclosed. The host lattice is stabilised by van der Waals interaction between guest and water molecules.

We investigate the interaction of tetrahydrofurane (THF) molecules with the host water cage comparing THF molecular vibrations in pure THF with those of THF molecules in the neighbourhood of either water molecules in liquid water or water molecules forming the clathrate cages. Raman spectra of aqueous and deuterated water solutions of THF were recorded from 500 cm⁻¹ to 3500 cm⁻¹. The strongest influence of the THF-water interaction is observed for the ring breathing mode (C-C-C stretches) and C-O-C stretch mode around 920 cm⁻¹. In pure THF both vibrational modes have almost the same frequency. The interaction (hydrogen bonding) with H₂O/D₂O shifts the C-O-C mode in liquid water. On formation of the clathrate both vibrations have almost the same frequency again, showing that the hydrogen bonds of the THF molecule to neighboring H₂O/D₂O molecules are strongly weakened in the clathrate.

Below 120 K a splitting of the two modes set in. This may reflect either structural changes in the host lattice or the freezing of the THF molecule into inequivalent orientations within the cage.

DY 50.5 Fri 11:15 HÜL 186

Stability limits for CuAu phase of CuInS₂ — ●JAN ŁAŻEWSKI and KRZYSZTOF PARLINSKI — Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 32-342 Kraków, Poland

The ternary chalcopyrite compounds CuInX₂ (X=S,Se) and its alloys are promising semiconductor materials with practical application as stable and radiation resistant polycrystalline thin film photovoltaic solar cells with power conversion efficiencies increasing steadily over the years. One of the interesting features of these materials is high contamination of chalcopyrite structure with nearly isenthalpic CuAu-structure.

We present the results of a comparative first-principles calculation of the structure parameters and the lattice dynamical properties for the CuAu-ordered and chalcopyrite phases of CuInS_2 . The frequencies and symmetries of five optical phonon modes are determined for CuInS_2 with CuAu-ordered structure. We have found very small difference between the total energies of both structure types at elevated temperatures according to our calculations. The frequency range covered by the zone-center vibrational modes, the phonon dispersion, and the phonon density

of states are very similar for both structure types. Furthermore, the frequencies of the infrared modes of the CuAu-ordered phase deviate only slightly from mode frequencies observed for the chalcopyrite phase. The only exception is the fully symmetric A1 mode having a distinctly higher frequency in CuAu-ordered CuInS_2 .

This work was partially supported by the State Committee of Scientific Research (KBN), grant no 1P03B10426.

DY 51 Non-Linear Stochastic Systems

Time: Friday 11:30–13:30

Room: HÜL 186

DY 51.1 Fri 11:30 HÜL 186

The power spectrum of a driven nonlinear stochastic system — ●BENJAMIN LINDNER — MPI fuer Physik komplexer Systeme, Noethnitzer Str.38, 01187 Dresden

We study the effect of an external broad band driving on the power spectrum of a nonlinear stochastic system. A heuristic formula used frequently in the literature is shown to be valid at large internal noise of the system, i.e. when the system is effectively close to a linear dynamics. In the opposite limit of small internal noise, however, this formula may fail. We show that an external broadband perturbation can have effects not described by a purely linear theory: (1) power is reduced or added at frequencies which are outside the frequency band of the driving; (2) sharp peaks of the unperturbed system become much broader under the influence of random noise; (3) side bands appear in certain cases. We present two simple systems for which the power spectrum can be analytically calculated or at least approximated and discuss the implications of our findings for more general situations.

Ref. Lindner, Chacron, Longtin Phys. Rev. E 72, 021911 (2005)

DY 51.2 Fri 11:45 HÜL 186

A stochastic model for noise-free stochastic resonance near a merging crisis — ●THOMAS STEMLER¹, WOLFRAM JUST², and HARTMUT BENNER¹ — ¹Institut für Festkörperphysik, TU Darmstadt — ²Department of Mathematics, Queen Mary/University of London, UK

We provide a stochastic model for stochastic multiresonance which is found in dynamical systems exhibiting crisis induced intermittency. The role played by the external noise in conventional stochastic resonance (SR) is replaced by the fast chaotic dynamics of the system. The latter causes a slow jump dynamics between the two intermittent states. The stochastic model is derived following the spirit of the Kramers-Moyal expansion. It can be used to map the deterministic chaotic dynamics to the standard model of SR, i.e. the overdamped motion of a particle in a double-well potential subjected to noise. We applied the method successfully to an electronic Chua-type circuit. The deterministic and stochastic terms of the corresponding Langevin equation were obtained by analysing the time series of the circuit. The dependence of both terms on the control parameter of the intermittent system explains the complexity of the observed resonance phenomenon and introduces a new mechanism for stochastic multiresonance.

DY 51.3 Fri 12:00 HÜL 186

Precursors of Extreme Increments — ●SARAH HALLERBERG, EDUARDO G. ALTMANN, DETLEF HOLSTEIN, and HOLGER KANTZ — Max Planck Institute for the Physics of Complex Systems Noethnitzer Str. 38,

We investigate precursors and predictability of extreme events in time series, which consist in large increments within successive time steps. We determine analytically the marginal and the joint probability density function (PDF) for large increments in uncorrelated random numbers and AR(1)-correlated data. These PDFs provide us with different possibilities to choose convenient precursors for the events we are looking for. The performance of these precursors is then tested via creating receiver operator characteristics (ROC). Surprisingly we obtain better predictions for completely uncorrelated Gaussian random numbers than for AR(1)-correlated data. This apparent paradox can be qualitatively explained by clustering of the AR(1)-correlated data, which inhibits large increments. Additionally we present a quantitative discussion of this effect by using a not common summary index for smooth ROC-curves. Furthermore this index can be used to estimate the quality of smooth ROC-curves for any given event size and correlation strength.

DY 51.4 Fri 12:15 HÜL 186

Statistics of a noise-driven Manakov soliton — ●STANISLAV DEREVYANKO¹, JAROSLAW PRILEPSKIY², and DENNIS YAKUSHEV³ — ¹Photonics Research Group, Aston University, Birmingham, UK — ²B.I. Verkin Institute for Low Temperature Physics and Technology, Kharkov, Ukraine — ³Institute for Radiophysics and Electronics, Kharkov, Ukraine

We investigate the statistics of a vector Manakov soliton in the presence of additive Gaussian white noise. The adiabatic perturbation theory for Manakov soliton yields a stochastic Langevin system which we analyze via the corresponding Fokker-Planck equation for the probability density function (PDF) for the soliton parameters. We obtain marginal PDFs for the soliton frequency and amplitude as well as soliton amplitude and polarization angle. We provide the expressions for the Stokes parameters of soliton polarization and determine the depolarization length. We also derive formulae for the variances of all soliton parameters and analyze their dependence on the initial values of polarization angle and phase.

DY 51.5 Fri 12:30 HÜL 186

Controlling noise-induced oscillations by time-delayed feedback — ●CLEMENS V. LOEWENICH and HARTMUT BENNER — Institut für Festkörperphysik, Technische Universität Darmstadt

Noise-induced oscillations may be observed in a van der Pol oscillator in the regime just below the Hopf bifurcation, where the noise-free system still has a stable fixed point. It was shown analytically and numerically that these oscillations can be controlled by time-delayed feedback, which allows to maximize their correlation time on variation of delay time and feedback strength [1,2].

In order to check the validity of these theoretical findings we made experimental investigations on a van der Pol type electronic circuit. In fact, we observed the occurrence of noise-induced oscillations and studied the dependence between correlation time, noise and feedback strength. Discrepancies between experimental and theoretical data could be attributed to the limited bandwidth of our experimental noise source in contrast to the white noise assumption of the model.

[1] N. B. Janson et al., Phys. Rev. Lett. **93**, 010601 (2004)

[2] J. Pomplun et al., Europhys. Lett. **71**, 366 (2005)

DY 51.6 Fri 12:45 HÜL 186

Formation of shocks in forced Burgers Equation — ●STEPHAN EULE and RUDOLF FRIEDRICH — Institute of Theoretical Physics Wilhelm-Klemm-Straße 9 48149 Münster

We analyze the formation of shocks in the Burgers-equation with linear forcing on a bounded interval. We numerically determine the probability distribution for velocity increments. We show that shock formation can be considered in close analogy to the behaviour of an excitable system under external perturbations.

DY 51.7 Fri 13:00 HÜL 186

Phase transitions and “negative heat capacity” of active Brownian particles — ●HENDRIK U. BÖDEKER¹, ANDREAS W. LIEHR², and HANS-GEORG PURWINS¹ — ¹Westfälische Wilhelms-Universität Münster, Institut für Angewandte Physik, Corrensstr. 2/4, 48149 Münster — ²Freiburger Materialforschungszentrum, Stefan-Meier-Str. 21, 79104 Freiburg i. Br.

Active Brownian particles as a generalization of classical Newtonian particles exhibit a large variety of dynamical properties that have no classical counterpart. In this talk, we focus on the interaction of many

active Brownian particles by investigating the clustering behavior under short-ranged interaction. Numerical simulations show that a number of phenomena like phase transitions from a solid to a liquid phase can be found that qualitatively resemble the behavior of classical many-body systems. In addition, new phenomena like “negative heat capacity”, i.e. the decrease of the mean-squared velocity of the particles with increasing fluctuation strength, can be found. We show that these findings essentially depend on the nature of the interaction and that “negative heat capacity” can be looked upon as a stochastic resonance effect.

DY 51.8 Fri 13:15 HÜL 186

Foraging Active Brownian Agents - Do they diffuse normal or not? — •UDO ERDMANN and SEBASTIAN GÖLLER — Institut für Physik, Humboldt-Universität zu Berlin

First results on the (anomalous) diffusive behavior of foraging active agents are presented. As could have been observed in nature the individuals are able to take up energy and convert it into free degrees of freedom. The uptaken energy is located in randomly distributed food depots. A whole population of Active Brownian agents is investigated. Hereby our main interest is to distinguish between regimes of normal and anomalous diffusion depending on the system parameters.