International Symposium

Nonlinear Dynamics of Nanosystems

August 28-30, 2006
Chemnitz, Germany

Chemnitz 2006
Main Topics

Nonlinear Dynamics of Nanoscopic Systems: Scaling, Stochasticity, and Quantum Mechanics

Aims

The dynamics of nanometer-sized devices provides new challenges for science and engineering. In particular, nonlinear processes are fundamentally important for the function of nanosystems. Although a thorough comprehension is essential for the future development of technical applications, there is still a lack of understanding of these processes.

The goal of this symposium is therefore to work out the qualitative changes that occur when dynamical systems are scaled down to nanosize. The focus of the symposium will be especially on the effects on the nonlinear dynamical behaviour of scaling, stochasticity and quantum mechanics. The aim is to elaborate new guiding principles and nonlinear dynamics scenarios, which are valid for quite different types of nanoscopic systems. The symposium aims at bringing together researchers working in different fields of nanoscience and dynamical systems.
Organization

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Program

Sunday, August 27, 2006

18.00  Welcome Buffet

Monday, August 28, 2006

8.00 - 8.30  Registration
8.30 - 9.00  Welcome and Greeting Words
            Heinz Georg Schuster, University of Kiel
            Klaus-Jürgen Matthes, Head of Chemnitz University of Technology
            Franz Dettenwanger, VolkswagenStiftung

Plenary Talks

9.00 - 9.50  Nonlinearity: The Key to Creating and Detecting Mechanical Quanta
            Andrew Cleland, University of California, Santa Barbara

9.50 - 10.40  The Duffing Nonlinearity in Nanomechanical Systems
              Sequoyah Aldridge, California Institute of Technology, Pasadena

10.40 - 11.10  Coffee Break

11.10 - 12.00  Metastability and Structural Dynamics of Metal Nanowires
               Jérome Bürki, University of Arizona, Tucson

12.00 - 12.50  Nonlinear Response of Driven Nanoscale Conductors
               Sigmund Kohler, University of Augsburg

12.50 - 14.20  Lunch

14.20 - 15.10  Dynamics of Nonlinear Coupled Nanomechanical Resonators
               Ron Lifshitz, Tel Aviv University

15.10 - 16.00  Bonds that Strengthen under Force
               Viola Vogel, Eidgenössische Technische Hochschule Zürich

16.00 - 16.30  Coffee Break
Program

16.30 - 18.10  **Short Poster Announcements**

19.00  Dinner

**Tuesday, August 29, 2006**

**Plenary Talks**

9.00 - 9.50  **Excited-State Dynamics in Carbon Nanostructures**  
David Tománek, Michigan State University, East Lansing

9.50 - 10.40  **The Stochastic Dynamics of Arrays of Micro and Nanoscale Cantilevers in a Viscous Fluid - Fluctuations from Dissipation**  
Mark Paul, Virginia Tech, Blacksburg

10.40 - 11.10  Coffee Break

11.10 - 12.00  **The Fluctuation and NonEquilibrium Free Energy Theorems - Theory and Experiment**  
Denis Evans, The Australian National University, Canberra

12.00 - 12.50  **Nonequilibrium Nanosystems**  
Pierre Gaspard, Universite Libre de Bruxelles

12.50 - 14.20  Lunch

14.20 - 15.10  **Ultrasensitive Magnetic Resonance Detection with Micromechanical Cantilevers**  
Chris Hammel, Ohio State University, Columbus

15.10 - 16.00  **High-Frequency Dynamics and Phase Locking in Spin Transfer Nano-Oscillators**  
Steve Russek, National Institute of Standards and Technology, Boulder

16.00 - 16.30  Coffee Break

16.30 - 18.10  **Poster Session**

19.00  Conference Dinner
**Wednesday, August 30, 2006**

**Plenary Talks**

9.00 - 9.50  **Nanoscale Fluid Dynamics**  
David Erickson, Cornell University, Ithaca

9.50 - 10.40  **Nonlinear Dynamics of Electromigration-Driven Crystal Steps**  
Joachim Krug, University of Cologne

10.40 - 11.10  **Coffee Break**

11.10 - 12.00  **Casimir Forces and Geometry of Nanomechanical Systems**  
Thorsten Emig, Universite Paris Sud

12.00 - 12.50  **Pattern Formation and Control at the Nano-Scale**  
Eckehard Schöll, Technical University of Berlin

12.50 - 14.20  **Lunch**

14.20 - 15.10  **Nanoplasmonics: Generation and Control of Nanoscale Optical Fields**  
Mark I. Stockman, Georgia State University, Atlanta

15.10 - 16.00  **Biomolecules as Nonlinear Oscillators: Life-Enabling Dynamics**  
Igor Mezic, University of California, Santa Barbara

16.00 - 16.30  **Coffee Break**

16.30 - 18.10  **Round Table**

19.00  **Dinner**
Posters

Size and Microstructure Effects on Nonlinear Dielectric Properties of Nanoscaled Ferroelectrics
Kay Barz / Martin Diestelhorst / Horst Beige, Martin-Luther-Universität Halle-Wittenberg
Ludwig Geske / Marin Alexe / Dietrich Hesse, Max-Planck-Institut für Mikrostrukturphysik, Halle

Heat Conduction of Carbon Nanotubes in Fermi-Pasta-Ulam Approximation
Christian Brunhuber / Franz G. Mertens, Universität Bayreuth

Complex Surface Patterning by Dynamic Molecular Self-Organization
Xiaodong Chen / Michael Hirtz / Harald Fuchs / Lifeng Chi, Westfälische Wilhelms-Universität Münster

Nonlinear Stochastic Models of Electrochemical Etching: Scale-Invariant and Scale-Variant Dynamics and Fluctuations from Macroscale to Nanoscale
Jens Christian Claussen, Christian Albrecht University Kiel

Formation of Longitudinal Patterns of Nonlinear Spin Waves in Ferromagnetic Stripes
Andrei N. Slavin, Oakland University, Rochester

Nonlinear Growth Dynamics of Magnetic Nanoclusters
Mario Einax / Stefan Heinrichs / Wolfgang Dieterich, Universität Konstanz
Philipp Maass, Technische Universität Ilmenau

On Anomalous Transport and Localisation Mechanisms in Classical Dynamical Systems
Andreas Fichtner / Günter Radons, Chemnitz University of Technology

Gradient Induced Movement of Solitary Structures in an LCLV Single Feedback Experiment
Björn Güttlich / Holger Zimmermann / Carsten Cleff / Cornelia Denz, Westfälische Wilhelms-Universität Münster

Simulation of Liesegang Pattern Formation by Nano-Particles in Glass
Jan W. Kantelhardt / Lukas Jahnke, Martin-Luther University Halle

Coherent Destruction of the Current through Molecular Wires Using Short LASER Pulses
Ulrich Kleinekathöfer / Guang Qi Li / Sven Welack / Michael Schreiber, Chemnitz University of Technology
Synchronization and Structure Formation in Coupled Nonlinear Optic Systems
Guido Krüger / Rudolf Friedrich, University of Münster

Negative Conductivity in Superlattices under High Frequency Radiation
Grzegorz Litak, Technical University of Lublin

Dynamics of Sheared Polymer Solutions
Vladimir Lobaskin, Technische Universität München

Transport across Carbon Nanotube Quantum Dots
Leonhard Mayrhofer / Milena Grifoni, Universität Regensburg

Quantum Resonances and Rectification of Driven Cold Atoms in Optical Lattice
Luis Morales Molina / Sergey Denisov / Sergej Flach, Max-Planck-Institute for Physics of Complex Systems, Dresden

Charge Transport Statistics through Quantum Shuttles
Thomas Novotny / Andrea Donarini / Christian Flindt / Antti-Pekka Jauho, University of Copenhagen

Thin Film Dynamics Influenced by Thermal Fluctuations
Markus Rauscher, Max Planck Institut für Metallforschung, Stuttgart

Simple Dynamical Systems with Preisach Nonlinearity
Sven Schubert / Roland Lange / Günter Radons, Chemnitz University of Technology

Fluctuation-Dissipation Relations for Nonequilibrium Steady States
Thomas Speck / Udo Seifert, Universität Stuttgart

Small-Scale Transport Phenomena and Mixing: Continuum Description and beyond
Arthur Straube / Arkady Pikovsky, University of Potsdam

Nonlinear Wave Propagation and Photonic Lattices in Anisotropic Photorefractive Media
Bernd Terhalle / Denis Traeger / Christoph Bersch / Jörg Imbrock / Cornelia Denz, Westfälische Wilhelms-Universität Münster
Anton.S. Desyatnikov / Yuri S. Kivshar, The Australian National University, Canberra

Mobility of Discrete Solitons in a Two-Dimensional Array with Saturable Nonlinearity
Rodrigo Vicencio / Magnus Johansson, Max Planck Institute for the Physics of Complex Systems, Dresden
Abstracts of Lectures

Monday, August 28, 2006

9.00 - 9.50

Nonlinearity: The Key to Creating and Detecting Mechanical Quanta
Andrew Cleland, University of California, Santa Barbara

We are engaged in a project to investigate mechanical resonators in the single-phonon quantum regime. The key to achieving quantum control of a mechanical system is to use an extremely strong nonlinearity in either the resonator or in its measurement system; we have chosen to use the latter. We are coupling the highly nonlinear inductance of a Josephson phase qubit with a microwave frequency mechanical resonator, which we hope will enable us to demonstrate the coherent creation and manipulation of single phonons in the resonating element. The mechanical system is a novel type of high quality factor, GHz frequency piezoelectric resonator, which can have unprecedented quality factor in this frequency band. The quantum mechanical properties of the resonators, especially in the single-phonon regime, will be probed by the Josephson qubit, and we plan to measure the single phonon T1 decay and T2 coherence times. I will describe our progress to date in developing this unique system.
Nanomechanical oscillators can easily be driven into the nonlinear regime. I will discuss experiments probing the energy required for nonlinear transitions between basins of attraction for such an oscillator.
Metastability and Structural Dynamics of Metal Nanowires
Jérome Bürki, University of Arizona, Tucson

I will present the nanoscale free-electron model, which provides a continuum description of metal nanostructures. I will argue that surface and quantum-size effects are the two dominant factors in the energetics of metal nanowires, and that much of the phenomenology of nanowire stability and structural dynamics can be understood based on the interplay of these two competing factors. In particular, I will discuss the exceptional linear stability of wires with certain magic conductance values, their dynamics under thermal fluctuations, as well as their escape dynamics.
Nonlinear Response of Driven Nanoscale Conductors
Sigmund Kohler, University of Augsburg

Electromagnetic ac fields can alter significantly the transport properties of mesoscopic systems like molecular wires and coherently coupled quantum dots. Resonant excitations of electrons e.g. enhance drastically the time-averaged currents. These systems may also be used to study the so-called ratchet or pump effect: in asymmetric molecules, an ac field induces a dc current even in the absence of any bias voltage. Of particular interest is the fact that the ratchet current as a function of the wire length converges to a non-zero value [1]. The opposite phenomenon also exists: a proper off-resonant driving field reduces the coherent transport resulting in a strong current suppression. Most of these effects require a treatment beyond linear response theory.

The corresponding transport mechanisms leave their fingerprints also in the noise whose relative strength is measured by the so-called Fano factor. In general, we find that resonant excitations reduce the noise level while current suppressions are accompanied by a noise reduction [2,3].

In our studies, we model the external field by a periodic time-dependence of the wire Hamiltonian. This requires a generalization of established transport theories like, e.g., the Landauer formula. Such a generalization, that is based on the Floquet theorem and includes the full nonlinear response to the driving, will be presented and the main differences to the static situation will be discussed.

Dynamics of Nonlinear Coupled Nanomechanical Resonators
Ron Lifshitz, Tel Aviv University

We are studying the dynamics of nonlinear coupled oscillators, motivated by recent experiments with arrays of micromechanical and nanomechanical resonators at Caltech and Cornell. Our studies to date have focused on the weakly nonlinear regime where we have looked at (1) The response of 1-dimensional arrays of coupled oscillators to parametric excitation; and (2) The synchronization of coupled mechanical resonators with a distribution of frequencies. We have obtained exact results for the parametric excitation of small arrays using secular perturbation theory [1], as well as an amplitude equation to describe the slow dynamics of the parametric excitation of large arrays [2], with many features in common with Faraday waves. We have investigated a model of synchronization, based on reactive coupling and nonlinear frequency pulling [3,4] (rather than the more common linear dissipative models), obtaining a phase diagram for the onset of synchronization, exhibiting interesting hysteretic behavior.

While the adhesive strength of most receptor-ligand interactions is exponentially reduced if strained, some receptor-ligand complexes exist that strengthen under force which is the hallmark of catch bonds. Although the existence of catch bonds was theoretically predicted, the first experimental demonstrations of their existence were given only recently, i.e. for the bacterial adhesin FimH that is located at the tip of type I fimbriae of E. coli and for p-selectin. In a major collaborative effort, we studied the structural origin by which the FimH-mannose bond is switched by force to a high binding state. Mutational studies were thereby combined with steered molecular dynamic simulations to decipher how force might affect protein conformation. Force-activation of FimH leads to a complex ‘stick-and-roll’ bacterial adhesion behavior in which E. coli preferentially rolls over mannosylated surfaces at low shear but increasingly sticks firmly as the shear is increased. The possibilities by which force can switch protein functions will be broadly discussed.

Tuesday, August 29, 2006

9.00 - 9.50

**Excited-State Dynamics in Carbon Nanostructures**
David Tománek, Michigan State University, East Lansing

The quantum nature of phenomena, dominating the behavior of nanostructures such as nanotubes, raises new challenges when trying to predict and understand their response to electronic excitations. Addressing this challenge is imperative in view of the continuous reduction of device sizes, which is rapidly approaching the atomic level. Due to fundamental limitations imposed on observations by the quantum nature of these systems, ab initio computer simulations, involving a combination of time-dependent density functional theory for electrons and molecular dynamics for the ions, emerge as a powerful tool to understand and predict the behavior of nanotubes following electronic excitations [1]. Addressing possible limitations in the frequency response of carbon nanotube-based electronic components, I will discuss the microscopic decay mechanism of photoexcitations, including the cross-over from purely electronic to phonon decay channels, and show its temperature dependence. Depending on the energy scale, electronic excitations may play a decisive role in determining the outcome of sputtering events by ions, which could induce selective structural modifications. Nanotubes, one of the most promising building blocks of Nanotechnology, display an unexpected defect tolerance, owing to an efficient self-healing mechanism, which may be triggered by electronic excitations [2]. Due to the long lifetime of electronic excitations in nanotubes, which is comparable to phonon periods, irradiation by monochromatic light emerges also as a selective and powerful technique to purify nanotubes from chemical impurities [3].


The Stochastic Dynamics of Arrays of Micro and Nanoscale Cantilevers in a Viscous Fluid - Fluctuations from Dissipation
Mark Paul, Virginia Tech, Blacksburg

The hydrodynamic correlations of the stochastic motion of an array of closely spaced micro and nanoscale elastic cantilevers in a viscous fluid are explored. A thermodynamic approach using the fluctuation-dissipation theorem is discussed and it is shown that the stochastic cantilever dynamics can be determined from straightforward deterministic calculations. Using this approach the stochastic dynamics for two cantilever configurations of possible experimental interest are quantified. Absolute predictions of the auto and cross-correlations of the equilibrium fluctuations in cantilever displacement are used to yield limits on the force and time scales of operation for a correlation detection method. The cross correlations in cantilever displacement reveal interesting dynamics that are explained using the thermodynamic approach as the interplay between the viscous and potential fluid dynamics around an oscillating object at low Reynolds number.
We give a brief summary of the derivations of the Evans-Searles Fluctuation Theorems (FTs) and the NonEquilibrium Free Energy Theorems (Crooks and Jarzynski). The discussion is given for time reversible Newtonian dynamics. We emphasize the role played by thermostatting. We also highlight the common themes inherent in the Fluctuation and Free Energy Theorems. We discuss a number of simple consequences of the Fluctuation Theorems including the Second Law Inequality, the Kawasaki Identity and the fact that the dissipation function which is the subject of the FT, is a nonlinear generalization of the spontaneous entropy production, that is so central to linear irreversible thermodynamics. Lastly we give a brief update on the latest experimental tests of the FTs (both steady state and transient) and the NonEquilibrium Free Energy Theorem, using optical tweezer apparatus.
**Nonequilibrium Nanosystems**

Pierre Gaspard, Universite Libre de Bruxelles

Many nanosystems are important because they are driven out of equilibrium. Examples of nonequilibrium nanosystems are:

1. Sliding carbon nanotubes where friction already manifests itself;
2. F1-ATPase molecular rotary motor;
3. Nonequilibrium chemical clocks.

Because of their small sizes, their thermodynamic properties are affected by the molecular fluctuations. It is shown how a fluctuation theorem for currents can take into account the molecular fluctuations in the thermodynamics of nanosystems.

14.20 - 15.10

Ultrasensitive Magnetic Resonance Detection with Micromechanical Cantilevers
Chris Hammel, Ohio State University, Columbus

The magnetic resonance force microscope (MRFM) is a novel scanned probe instrument which combines the three-dimensional imaging capabilities of magnetic resonance imaging with the high sensitivity and resolution of atomic force microscopy. Mechanical detection, in which the spin magnetization is coupled to a micromechanical cantilever offers exceptional sensitivity (detection of a single electronic spin was recently demonstrated) and high spatial resolution in this scanned probe magnetic resonance technique. MRFM offers very high spatial resolution in non-destructive, microscopic studies and imaging of subsurface properties of a broad range of materials. We will present the principles of the MRFM and discuss applications of the MRFM to the detection of NMR, ESR and Ferromagnetic Resonance (FMR).
15.10 - 16.00

High-Frequency Dynamics and Phase Locking in Spin Transfer Nano-Oscillators
Steve Russek, National Institute of Standards and Technology, Boulder

Understanding and controlling high-frequency magnetization dynamics in magnetic nanostructures has become important in data storage and biomedical imaging applications. Magnetic hard disk bits and read sensors will soon have dimensions of 20 nm and operating speeds above 1 GHz. At these sizes and speeds both the intrinsic dynamical response and the stochastic thermal effects determine system performance. Magnetic nanostructures are currently being used for magnetic resonance imaging (MRI) contrast agents. The stochastic magnetic fluctuations determine the effectiveness of the contrast agent and the ability to turn on and off contrast will lead to new types of molecular imaging in which MRI contrast is turned on when the contrast agents binds to a target molecule or cell. Finally, there are new types of devices that are enabled by physical effects that are only present at the nanoscale. One such nano-enabled effect is spin transfer induced dynamics where the transport of the electron's spin momentum can induce sustained microwave oscillations in magnetic nanostructures. Spin transfer devices can be used to fabricate nanoscale microwave oscillators that can be tuned by adjusting the applied current or magnetic field and can be phase locked to external microwave signals or other nanoscale oscillators. Spin transfer nano-oscillators (STNOs) are highly non-linear devices that can exhibit mode hopping, chaos, and hysteresis. In this talk I will give an introduction to dynamics in magnetic nanostructures; discuss our experimental measurements of dispersion relations, line widths, and phase locking of STNOs; and present numerical simulations of the dynamics of single and multiple STNOs.
Integrated microfluidic devices have proven themselves a particularly useful technology for a broad swath of applications ranging from now commercially viable Labs-on-Chip to still emerging devices like microscale fuel cells and other energy conversion devices. With the success of these devices and the broader availability of nanofabrication tools a significant amount of academic interest has shifted towards the development of nanofluidic devices. This downsizing of fluidic systems provides revolutionary opportunities for a number of application areas ranging from single-molecule biophysics to ultra precise sensing. Significant challenges are introduced however as we attempt to translate our extensive knowledge of traditional transport mechanisms, such as pressure driven flow and electrokinetics, to this new regime. In this talk a detailed review of the physics describing fluid dynamics and transport mechanics in nanofluidic devices will be provided, with a focus on the how some of these challenges can be addressed. Emphasis will be placed on the limitations of continuum modeling and other widely accepted assumptions along with the importance of non-linear effects in these systems. New and emerging transport mechanisms such as optofluidics will also be reviewed.
Nonlinear Dynamics of Electromigration-Driven Crystal Steps
Joachim Krug, University of Cologne

Nanoscale step morphologies on crystal surfaces can be manipulated by the directed migration of adatoms under the influence of an electric current in the bulk. Theoretical and experimental studies of this process are motivated both by the importance of electromigration as a reliability concern in integrated circuit technology, and by a general interest in nonlinear surface dynamics far from equilibrium. In the talk I will discuss recent results obtained for two model problems: The oscillatory motion of electromigrating islands on metal surfaces [1], and a novel type of dynamic phase transition discovered in a model of electromigration-induced step bunching on Si(111) [2]. The talk is based on joint work with Philipp Kuhn, Frank Hausser, Marko Rusanen and Vladislav Popkov.

According to quantum mechanics, all space is filled with electromagnetic vibrations, even at ultracold temperatures. Two parallel uncharged metal plates limit the number of vibrations between them, creating an effective inward pressure that pushes the plates together - known as Casimir effect. But the most challenging aspect of this effect is its dependence on geometry. Due to its topological nature, Casimir forces can be controlled by tailoring the shapes of the interacting bodies. However, due to the diffraction of vibrations and the non-additivity of fluctuation induced interactions, there is no intuitive way to tell how the force will change with the object’s shape. Recently, there was a resurgence of experiments on Casimir forces, showing also their profound effect on micro- and nanostructures.

In this talk, I shall present a brief introduction to Casimir forces, and a new approach to study the geometry dependence of this interaction. A novel trace formula is presented which yields the relevant information of the spectrum of the Helmholtz wave equation in arbitrary geometries. Perturbative and numerical implementations of this formula yield new and unexpected forms for the Casimir interaction in rather simple geometries. Implications on the non-linear dynamics of nanomechanical systems and actuation schemes will be presented. Our results may lead to the engineering of nano machines in which the geometry dependence of the Casimir force is used to tailor their function.
Pattern Formation and Control at the Nano-Scale
Eckehard Schöll, Technical University of Berlin

Self-organized pattern formation due to nonlinear charge transport arises in various semiconductor nanostructures [1]. Our focus is on control of those patterns by time-delayed feedback methods. On one hand, deterministic chaos can be suppressed, and unstable periodic space-time patterns can be stabilized. On the other hand, purely noise-induced patterns can be considered, and their temporal coherence and time-scales can be controlled. Our findings are applied to two important classes of nanostructures: (i) Nonlinear spatio-temporal dynamics of double-barrier resonant-tunneling (DBRT) diodes; (ii) Charge carrier fronts and field domains in superlattices.

**Nanoplasmonics: Generation and Control of Nanoscale Optical Fields**  
Mark I. Stockman, Georgia State University, Atlanta

This talk introduces and reviews recent new ideas and progress in coherent, nonlinear and ultrafast nanoplasmonics. Nanoplasmonic phenomena are based on resonant excitation of surface plasmons causing highly enhanced and localized optical fields on nanoscale. These nanoscale fields induce a multitude of enhanced optical effects, in particular, surface enhanced Raman scattering (SERS) including single-molecule SERS, enhanced second- and third-harmonic generations, enhanced two-photon electron emission from nanostructured surfaces, and others. Special emphasis of the talk is on ultrafast and nonlinear nanoplasmonics. There are many existing and prospective applications of nanoplasmonics in nanoprobing, ultrasensitive detection, biomedical monitoring, etc. The talk will include a broad Introduction to the topic and also certain forefront, focus areas based partially on original contributions [1-6], including ultrafast, nonlinear, and stimulated phenomena.


We present a study of complex biomolecules from the perspective of nonlinear dynamical systems theory. The basic - so-called minimalist - models used in molecular dynamics consist of a Hamiltonian part that captures the internal interactions among the atoms the molecule consists of, and viscous and stochastic interactions with the surrounding solvent. The question of particular interest is that of switching from one conformed configuration of a biomolecule to another. In fact, understanding the mechanism of fast transitions between conformed states of large biomolecules is central to reconciling the dichotomy between the relatively high speed of metabolic processes and slow (random-walk based) estimates on the speed of biomolecular processes. Here we utilize the dynamical systems approach to suggest that the reduced time of transition between different conformations is due to features of the dynamics of molecules that are a consequence of their structural features. Long-range and local effects both play a role. Long-range molecular forces account for the robustness of final states and nonlinear resonant processes that channel localized, bounded disturbances into collective, modal motions. Local interconnections provide fast transition dynamics. We also present some experimental evidence of effect of resonance in conformational transitions.
Abstracts of Posters

Size and Microstructure Effects on Nonlinear Dielectric Properties of Nanoscaled Ferroelectrics
Kay Barz / Martin Diestelhorst / Horst Beige, Martin-Luther-Universität Halle-Wittenberg
Ludwig Geske / Marin Alexe / Dietrich Hesse, Max-Planck-Institut für Mikrostrukturphysik, Halle

The influence of size effects and of the microstructure of interfaces and thin films on the linear properties of ferroelectrics is presently a widely studied topic worldwide. However, their influence on nonlinear properties of nanoscaled ferroelectrics is entirely unknown. The project is devoted to the well-defined preparation of nanoscaled ferroelectrics and to investigations into the influence of size and microstructure effects on their nonlinear properties.
Heat Conduction of Carbon Nanotubes in Fermi-Pasta-Ulam Approximation
Christian Brunhuber / Franz G. Mertens, Universität Bayreuth

The heat conduction in 1-dimensional anharmonic systems is anomalous in the sense that the conductivity scales with a positive power of the system size. In two dimensions, previous studies gave a logarithmic divergence. Recently, this feature which seems to be generic for models with momentum conserving potentials was also observed for carbon nanotubes, a promising candidate for future technical applications. Our simulations with deterministic thermostats at the boundaries of the 2-dimensional Fermi-Pasta-Ulam plane agree well with molecular dynamics simulation for carbon nanotubes. We discuss the role of dimensionality in the underlying system and the crossover from the 1-dimensional to the 2-dimensional behaviour.
Complex Surface Patterning by Dynamic Molecular Self-Organization
Xiaodong Chen / Michael Hirtz / Harald Fuchs / Lifeng Chi, Westfälische Wilhelms-Universität Münster

We demonstrate a bottom-up approach to form complex surface patterns by transferring Langmuir monolayers of phospholipid from air/water interface onto solid substrate. Linear stripe patterns – parallel and perpendicular orientated to the dipping direction – as well as rectangular patterns with different lateral sizes can be achieved by adjusting the experimental conditions such as surface density (surface pressure), transfer speed, temperature, humidity and molecular compositions. Substrate induced molecular condensation and dynamic contact angle (or density) oscillation is considered as the mechanism for the formation of stripe patterns perpendicular to the dipping direction. Further works together with theoretic group are necessary to understand the mechanism quantitatively.
Nonlinear Stochastic Models of Electrochemical Etching: Scale-Invariant and Scale-Variant Dynamics and Fluctuations from Macroscale to Nanoscale
Jens Christian Claussen, Christian Albrecht University Kiel

Electrochemical etching defines a class of systems exhibiting rich varieties of nonlinear spatiotemporal behaviour, and show inherent stochasticity of the chemical reactions. An accessibility of the full system, including nanohydrodynamics and double-layer formation in addition to the bulk/surface and reaction kinetics description by ab initio methods is computationally quite prohibitive for the immediate next decades. Nonlinear models of reaction kinetics at larger scale are successful, but in future have to be pursued down to atomic scale, where fluctuations and nonlinearities both become relevant. Fluctuations at the nanoscale result in, eventually nontrivial, spectra characterizing the fluctuation in the reaction rate. The atomistic nature of the reactants (discrete Lotka-Volterra processes, largely equivalently to finite-populations coevolutionary dynamics) has to be taken into account, and nontrivial finite-size-effects can occur. For etching, much less systematically developed theory is available. Fractal etching of metal surfaces by a limited reactant resource has been modeled by directed percolation. But the general case of corrosion still gives enough riddles of technical relevance. Electrochemical etching of semiconductors offers an enormously complex variety of structures that can emerge, from nanoporous silicon, over branching and periodic structures, photonic crystals, to regular pores on different scales. Theoretic paradigmas have been established, like the Current-Burst model of Foell and Carstensen, and step by step quantitatively support the understanding of experiments. Compared to the various applications, however, much more theoretical efforts have to be pursued here.
Formation of Longitudinal Patterns of Nonlinear Spin Waves in Ferromagnetic Stripes
Vladislav E. Demidov / Ulf-Hendrik Hansen / Oleksandr Dzyapko / Nikolay Koulev / Sergej O. Demokritov, Westfälische Wilhelms-Universität Münster
Andrei N. Slavin, Oakland University, Rochester

Formation of stationary longitudinal amplitude patterns by propagating nonlinear spin waves has been discovered and studied experimentally by means of space-resolved Brillouin light scattering spectroscopy. The pattern formation is observed for the spin waves propagating in narrow, longitudinally magnetized yttrium iron garnet stripes, characterized by the attractive nonlinearity in both longitudinal and transverse directions.
Nonlinear Growth Dynamics of Magnetic Nanoclusters
Mario Einax / Stefan Heinrichs / Wolfgang Dieterich, Universität Konstanz
Philipp Maass, Technische Universität 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 CoPt$_3$ 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 L1$_2$-ordering [3].

On Anomalous Transport and Localisation Mechanisms in Classical Dynamical Systems
Andreas Fichtner / Günter Radons, Chemnitz University of Technology

Anomalous transport is not only a phenomenon of systems with stochastic environmental forces, which act e.g. on a heavy particle, and require for description the action of many degrees of freedom. It is also observable in low dimensional systems with static randomness in the equations of motion such as random walks in random environments. Closely connected to these anomalous transport properties are dynamical localisation mechanisms, which generalise previous results by Golosov and Sinai [1, 2]. Sinai disorder denotes a class of random walks with restriction to nearest neighbour transitions for which analytical results can be obtained to describe anomalous transport. Thereby the quantities under concern are the time evolution of the disorder averaged mean square displacement and the system size dependent quantities density of states of the propagator and escape rate. The latter is directly connected with the mean first passage time. For each of them one can define a characteristic exponent. In our work we extend the Sinai model to systems whose transitions are not restricted to next-nearest neighbours [3, 4]. We could show numerically that the characteristic exponents also exist for our extended model. But the absence of detailed balance causes problems in analytical treatment and in numerics. At least for relative small systems the characteristic exponents show a non-trivial dependence on system size and coincide. Perturbation theory, which is exact in the Sinai case, enables us to calculate escape rates for significant larger systems. For our extended model we find as function of system size a transition from a large preasymptotic regime to the asymptotic behaviour in dependence on the system parameters.

Gradient Induced Movement of Solitary Structures in an LCLV Single Feedback Experiment
Björn Gütlich / Holger Zimmermann / Carsten Cleff / Cornelia Denz, Westfälische Wilhelms-Universität Münster

We present experimental results on invasive control of solitary structures in a single feedback experiment using a liquid crystal light valve (LCLV) as nonlinearity. Due to their formation based on a self organisation processes solitary structures are robust against perturbations and show binary features. These features make them attractive for applications in context of all-optical information processing. For potential applications, the control of their positions and dynamics is crucial. To control solitary structures, we apply an invasive forcing technique, which uses an incoherent white light intensity distribution. Via the nonlinearity, the forcing induces a phase gradient landscape, in which the solitary structures move. Depending on its strength, the forcing can either be used to favour addressing positions or to address (ignite and erase) solitary structures. Also dynamical positioning of arrays and individual solitary structures is demonstrated. In detail, we study the movement of solitary structures in a conoidal phase gradient. The structures move towards the maximum of the intensity gradient and their velocity linearly depends on the absolute value of the conus gradient. In addition to the control of solitary structures, the forcing is also useful in compensating spatial inhomogeneities of the nonlinearity.
Simulation of Liesegang Pattern Formation by Nano-Particles in Glass
Jan W. Kantelhardt / Lukas Jahnke, Martin-Luther University Halle

By numerical simulations we study chemical diffusion-reaction processes in glass that lead to the self-organized formation of Liesegang patterns on the nanometer scale. Such patterns formed by silver particles have been observed experimentally with electron microscopy in silicate glass. Based on Monte Carlo simulations with cellular automata models and kinetic Monte Carlo simulations we focus upon the stability of the pattern formation process on the nano scale and investigate the possibility to control the created patterns. In addition to the arrangement of the metal nano particles, their size distribution and their shapes are essential for the optical properties of the material. Both can be controlled by tempering and by short polarized laser pulses, which locally heat the particles. The aim of the simulation of these processes is to distinguish different particle formation and growth modes (diffusion controlled shaping, Ostwald ripening, and possibly also coagulation growth).
Coherent Destruction of the Current through Molecular Wires Using Short LASER Pulses
Ulrich Kleinekathöfer / Guang Qi Li / Sven Welack / Michael Schreiber,
Technische Universität Chemnitz

The influence of Gaussian laser pulses on the transport through molecular wires is investigated within a tight-binding model for electrons without and with spin including electron-electron interaction [1]. Motivated by the phenomenon of coherent destruction of tunneling for monochromatic laser fields, situations are studied in which the maximum amplitude of the electric field fulfills the conditions for the destructive quantum effect. It is shown that, as for monochromatic laser pulses, the average current through the wire can be suppressed [2]. For parameters of the model, which do not show a net current without any optical field, a Gaussian laser pulse can establish a temporary current. In addition, the effect of electron correlation on the current is investigated.

Synchronization and Structure Formation in Coupled Nonlinear Optic Systems
Guido Krüger / Rudolf Friedrich, University of Münster

Synchronization in coupled nonlinear systems is a challenging task for signal and data transmission. In this poster we will present numerical and analytical studies to structure formation in coupled nonlinear optical systems under the aspect of synchronizing the structures. One part is the synchronization and transmission of solitary structures in an unidirectional coupled system, another with a bidirectional coupled system.
Negative Conductivity in Superlattices under High Frequency Radiation
Grzegorz Litak, Technical University of Lublin

In this note nonlinear responses of semiconductor super-lattices in the field and current in presence of terahertz laser radiation [1-3] are studied. Especially we are interested in terahertz field induced nonlinear dynamics of electrons in a semiconductor super-lattice leading to a negative conductance observed experimentally [4] and studied theoretically [1-2]. We reexamine this effect decoupling the dynamics into the fast and slow components [5]. In this way we were able to get the effective dynamics electrons showing negative conductance for interesting ranges of system parameters.

Dynamics of Sheared Polymer Solutions
Vladimir Lobaskin, Technische Universität München

We perform a computer simulation study of dynamic behaviour of a confined polymer solution under shear. The solution forms a thin interlayer between two solid surfaces and poor solvent conditions (collapsing chains) are considered. We observe an intriguing behaviour of chain conformation and effective viscosity of the solution when the layer thickness becomes comparable to the chain length.
Transport across Carbon Nanotube Quantum Dots
Leonhard Mayrhofer / Milena Grifoni, Universität Regensburg

We present a low-energy theory for non-linear transport in single walled carbon nanotube quantum dots. Finite size effects and electron-electron interactions play a decisive role for such a setup. Due to the multiple degeneracy of the energy spectrum, off-diagonal elements of the density matrix can not be ignored. Current calculations for low and high bias voltages are shown.
Quantum Resonances and Rectification of Driven Cold Atoms in Optical Lattice
Luis Morales Molina / Sergey Denisov / Sergej Flach, Max-Planck-Institute for Physics of Complex Systems, Dresden

Classical Hamiltonian ratchets have been recently successfully realized using cold atoms in driven optical lattices. Here we study the current rectification of the motion of a quantum particle in a periodic potential exposed to an external ac field. The dc current appears due to the desymmetrization of Floquet eigenstates, which become transporting. Quantum dynamics enhances the dependence of the current on the initial phase of the driving field. By changing the laser field parameters which control the degree of space-time asymmetry, Floquet eigenstates are tuned through avoided crossings. These quantum resonances induce resonant changes of the resulting current. The width, strength and position of these quantum resonances are tunable using control parameters of the experimental realization with cold atoms.
Charge Transport Statistics through Quantum Shuttles
Thomas Novotny / Andrea Donarini / Christian Flindt / Antti-Pekka Jauho, University of Copenhagen

We study charge transport statistics of a quantum shuttle using generalized master equation description of the shuttle dynamics. We identify several dynamical regimes of transport through the shuttle with distinctive features in the current fluctuations characterizing the particular dynamical regimes. Simple analytical models describing respective regimes are presented and their predictions for the current fluctuations are compared with the full numerical solutions with excellent agreement.
Thermal noise becomes more and more important the smaller a system is. Recent studies of thin film evolution indicate that thermal noise might influence characteristic time-scales of film dewetting. Up to now, thin film flow was only studied with deterministic equations. We develop a stochastic version of the thin film equation. In the thin film approximation, the stochastic incompressible hydrodynamic equations [Landau and Lifshitz, Vol. IV] reduce to the deterministic thin film equation plus a conserved noise term. We show that the noise term is consistent with the thermodynamical equilibrium distribution of the film thickness. With numerical solutions of the stochastic thin film equation we show, that thermal fluctuations significantly influence the time scales of dewetting. We also find clear indications for thermal fluctuations in the early linear regime of spinodal dewetting.
Simple Dynamical Systems with Preisach Nonlinearity
Sven Schubert / Roland Lange / Günter Radons, Chemnitz University of Technology

Many physical and technical systems such as shape memory alloys [1] or nanowires [2] 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.

Fluctuation-Dissipation Relations for Nonequilibrium Steady States
Thomas Speck / Udo Seifert, Universität Stuttgart

In non-equilibrium, the fluctuation-dissipation theorem (FDT) relating the response function of an observable with its auto-correlation is violated. This violation has been studied intensely, especially in the context of aging systems and glasses. In the case of colloidal systems, the heat permanently dissipated in order to maintain the violation of detailed balance has been identified as “housekeeping“ heat, providing a new insight into the FDT violation. As the crucial ingredient, the housekeeping heat involves two aspects of the velocity, namely the actual velocity and the local mean velocity. Studying a paradigmatic single colloidal particle moving in a periodic potential, we discuss the close connection between the violation of the velocity FDT and the violation of detailed balance. We derive an explicit expression for this violation and illustrate our result with numerical simulations.
Small-Scale Transport Phenomena and Mixing: Continuum Description and beyond
Arthur Straube / Arkady Pikovsky, University of Potsdam

We focus theoretically on three directions: (i) new instabilities in reaction-advection-diffusion systems; (ii) particle manipulation and collective effects in microchannels; (iii) mesoscopic modelling of microfluidic systems and bridging the length scales. In the first direction, we address problems of mixing in reaction-diffusion systems in open and closed flows: new instabilities due to competition of spatial mixing and chaotic in time reaction, competition of absolute (global mode) and convective instabilities in open flows, a chemical instability induced by a mixing flow. In the second group of problems we control the dynamics of disperse media with small amplitude high-frequency vibrations and with travelling wave dielectrophoresis (particle capture). In the last direction, we apply a recently developed mesoscopic technique (Stochastic Rotation Dynamics) to model the dynamics of colloids in microflows and find out the role of interparticle interactions and boundaries.
Nonlinear Wave Propagation and Photonic Lattices in Anisotropic Photorefractive Media
Bernd Terhalle / Denis Traeger / Christoph Bersch / Jörg Imbrock / Cornelia Denz, Westfälische Wilhelms-Universität Münster
Anton. S. Desyatnikov / Yuri S. Kivshar, The Australian National University, Canberra

Wave propagation in periodic nonlinear systems is associated with exciting phenomena that do not have a counterpart in bulk media. A very common example are discrete self-localized states known as discrete solitons. In optics, the periodic structure is provided by a periodically varying refractive index which can be optically induced in a photorefractive material, and soliton formation in these structures is due to a balance of nonlinearity and discrete diffraction. When modulational instabilities are controlled, two-dimensional photonic lattices can be generated, using ordinarily as well as extraordinarily polarized light. We show that the extraordinarily polarized lattice wave induces a much stronger modulated refractive index assuming otherwise the same parameters. We also exploit the photorefractive anisotropy to generate a quasi-one-dimensional refractive index pattern for the formation of two-dimensional solitons and corroborate these experiments by numerical simulations.
Mobility of Discrete Solitons in a Two-Dimensional Array with Saturable Nonlinearity
Rodrigo Vicencio / Magnus Johansson, Max Planck Institute for the Physics of Complex Systems, Dresden

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, focusing 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.
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Notes
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<th>Time</th>
<th>Monday</th>
<th>Tuesday</th>
<th>Wednesday</th>
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<td>8.00 - 8.30</td>
<td>Registration</td>
<td>David Tománek</td>
<td>David Erickson</td>
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<tr>
<td>8.30 - 9.00</td>
<td>Welcome</td>
<td>Andrew Cleland</td>
<td>Joachim Krug</td>
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<td>9.00 - 9.50</td>
<td>Andrew Cleland</td>
<td>Sequoyah Aldridge</td>
<td>Coffee Break</td>
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Monday:
- Welcome Dinner
- Registration
- Welcome
- Andrew Cleland
- Sequoyah Aldridge
- Andrew Cleland
- Sequoyah Aldridge
- Coffee Break
- Jérome Bürgi
- Coffee Break
- Lunch Break
- Ron Lifshitz
- Coffee Break
- Round Table
- Conference Dinner
- Dinner

Tuesday:
- Welcome Dinner
- Registration
- Welcome
- Andrew Cleland
- Sequoyah Aldridge
- Coffee Break
- Thorsten Emig
- Pierre Gaspard
- Eckehard Schöll
- Lunch Break
- Sigmund Kohler
- Coffee Break
- Round Table
- Short Posters
- Announcements
- Conference Dinner
- Dinner

Wednesday:
- Welcome Dinner
- Registration
- Welcome
- David Erickson
- Joachim Krug
- Coffee Break
- Thorsten Emig
- Eckehard Schöll
- Lunch Break
- Mark I. Stockman
- Igor Mezic
- Coffee Break
- Dinner