TUT 1: Tutorial: From spin models to macroeconomics (SOE with DY/AGjDPG)

Formulated as a minimal model of ferromagnets, the Lenz-Ising model received a recent renaissance serving as paradigmatic basis for the formulation and analysis of models of social and economic behaviour. Prominent examples are microscopic market and price formation models incorporating herding behaviour of the economic agents and leading to nonlinear and nonequilibrium macroeconomic dynamics. The Sznajd-Weron opinion formation model introduced spin models with outflow kinetics into quantitative social modeling. Finally, the macroscopic (replicator) equations of evolutionary game theory again can be based on microscopic (Glauber-like) reaction kinetics for discretized behavioral states, whereby the payoffs from the neighborhood resemble a local meanfield. This series of tutorial lectures shows that methods adapted from statistical phyics can serve as concepts in quantitative social and economic theories and are worth the effort of bridging the disciplines, which includes properly connecting to economic frameworks. (Session compiled by Jens Christian Claussen.)

Time: Sunday 16:00–18:30 Location: H 0104

Tutorial TUT 1.1 Sun 16:00 H 0104

Economics in a nutshell, for physicists — •Sylvie Geisendorf — ESCP Europe Berlin

The talk explains why and how the economic mainstream, the theory of neoclassical economics, is based on the idea of Newtonian physics. It also discusses why a real Newtonism would probably have been a good idea and where economists deviate from it.

Although modern economists rarely refer to physics, economic theory is based on Newtons idea of universal gravity. Following Newtons discovery, physics became an exact science with rigorous mathematical descriptions. In physics, Newton marked the beginning of the era of rational mechanics. Society was fascinated by Newtons insights and economists based their theory on classical mechanics with the explicit aim to make economics a rational science as well. But instead of adopting Newtons laws of motion they employed the simplified principle of general maximization. Whereas the laws of motion name the forces acting in a system, optimization calculus only deduces the final outcome. Even in physics, the realization of global minima or maxima is only possible under specific conditions. In economics, where actions of bounded rational agents have to be considered, these conditions are even rarer. The talk argues that a real Newtonian approach could have moderated the current lack of contact with reality, economic theory displays, and could have facilitated the necessary transition to an evolutionary theory of the economy.

Tutorial TUT 1.2 Sun 16:50 H 0104

Connecting microscopic behavioral economics to macroscopic financial market models — •Sebastian M. Krause — Rudjer Boskovic Institute, Zagreb, Croatia

Time series of prices show the stylized facts of broadly distributed price jumps which occur clustered. This has serious implications for the accumulation of risk. Macroscopic price evolution models for estimating risk are commonly used. They extend the random walk by including auxiliary volatility variables to model time dependent volatility. On the other hand, agent based models that include behavioral insights are used to enlighten the mechanisms behind stylized facts. This could help to predict crashes and to improve market regulation.

After briefly illustrating this background, I discuss a way of interconnecting these two strands of research. Using an agent based model with herding, I exemplify a general recipe for finding macroscopic models numerically: A macroscopic variable which might control volatility is identified; The stochastic process ruling this volatility variable is measured, using the numeric evolution of the microscopic model. This procedure is suitable for models with puzzling emergent behavior, as well as for complicated models with many parameters. The resulting macroscopic price evolution model can be much simpler, allowing for proceeding investigations. Therefore, the field of agent based modeling profits from a macroscopic description. Another advantage is the microfoundation of macroscopic financial market models which are so far pure phenomenological. The auxiliary volatility variable can inherit a clear behavioral meaning from the microscopic model.

Tutorial TUT 1.3 Sun 17:40 H 0104

You are a young and aspiring physicist. Is working at the interface with economics a good idea? — •Tobias Galla — Theoretical Physics, School of Physics and Astronomy, The University of Manchester, Manchester M13 9PL, UK

The terms econophysics and sociophysics describe research in which physicists apply their ideas and methods to problems in economics and the social sciences. What do you have to know about the field to find your own answer to the question in the title? Well, one way is to talk to as many 'older' physicists as possible who have worked in this area, and then to form your own opinion. In this tutorial I will give you my personal assessment of what physicists can contribute to the field of economics, and comment on why they cannot contribute as easily as it may seem. We will discuss the main achievements of physicists, for example the detection of non-Gaussian features and long-range correlations in financial data, theories of market impact, non-equilibrium ideas and bottom-up models of game theory, decision making and market microstructure. At the same time you will hear about the things physicists have not achieved (despite occasional claims to the contrary). I will then present some of our own work on chaotic dynamics in the learning of complicated games and discuss the potential consequences this has for agent-based market models, and the limitations of our work. In the final part of the tutorial I will comment on the potential hurdles young physicists moving into this area might want to be aware of, and I will highlight the potentials and benefits of working in this field.

TUT 2: Tutorial: Ferroics (DF with MA/TT)

This tutorial introduces the field of domain and domain-wall engineering, key concepts and materials, and launches our 3-days focus on ferroic domain walls. The tutorial will provide a forum for non-specialists to get informed / involved and, at the same time, aims at inspiring topical discussions to stimulate a vivid scientific exchange during the following Sypmosium (SYDW), the three Focus Sessions and a Poster Session.

Organizers: Elisabeth Soergel (Universität Bonn) and Dennis Meier (ETH Zürich)

Time: Sunday 16:00–18:30 Location: H 0107

Tutorial TUT 2.1 Sun 16:00 H 0107

Fundamentals of ferroelectric materials — •Susan Trolier-McKinstry — Penn State University, University Park, PA, USA

This tutorial will cover the fundamental phenomena that underpin the field of ferroelectricity, with an emphasis on the relationship between crystal structure and the allowed domain states. An introduction will be made to ferroelectricity, pyroelectricity, piezoelectricity, and the origins of the dielectric response. The crystal structures of key materials, including perovskites, $LiNbO_3$, the tungsten bronzes, and polymer ferroelectrics will be introduced, along with the link between the loss of symmetry elements and the allowed domain states. The tutorial will conclude with an introduction to the movement of domain walls, and the influence that this has on the properties of ferroelectric materials.

Tutorial TUT 2.2 Sun 16:50 H 0107

Domain walls in multiferroics as functional oxide interfaces — •Manfred Fiebig — Department of Materials, ETH Zürich, Vladimir-Prelog-Weg 4, 8093 Zurich, Switzerland

The functionality of any ferroic material depends on its domains. Consequently, their shape and manipulation in external fields are of major research interest. In compounds uniting magnetic and electric order in the same phase, the magnetoelectric coupling on the level of the domains is, however, largely unexplored. For such so-called multiferroics it is therefore not known how exactly electric or magnetic fields affect the multiferroic domains and their walls. In my talk I will discuss this issue and focus on the influence of the multiferroic order on the ferroelectric state and its domain walls. Examples I will include are: (i) multiferroics with geometric ferroelectricity such as hexagonal $YMnO_3$ where the domain walls exhibit anisotropic conductance and can therefore be regarded as "tunable oxide interfaces"; (ii) multiferroics with magnetically induced ferroelectricity such as $MnWO_4$ or $TbMnO_3$ where the electric polarization within the wall is expected to rotate instead of passing through zero, as in conventional displacive ferroelectrics; (iii) multiferroics with strain-induced ferroelectricity like $SrMnO_3$ where the interplay of strain and oxygen vacancies leads to polar state in which domain walls act as insulating boundaries to the conducting domains.

Tutorial TUT 2.3 Sun 17:40 H 0107

Ferroelastic templates for multiferroic domain boundaries — •Ekhard Salje — University of Cambridge, Cambridge, UK

The field of Domain Boundary Engineering is introduced. Ferroelastic domain pattern are derived and their dynamical behaviour is deducted from experimental observations and computer simulations. It is then shown that twin boundaries are particularly easily modified to possess functional properties that do not exist in the bulk. Such functional properties include (super-) conductivity, ferroelectricity, and ferromagnetism. In addition, chemical mixing inside domain walls can generate novel chemical compounds. This effect is refereed to as 'Chemical Mixing in Confined Spaces'. Functionalities often generate chiralities and vortex structures in domain boundaries. It is shown that chirality (in order parameter space) leads to Bloch lines and vortex points as one- and zero-dimensional domain walls embedded in two-dimensional ferroelastic domain walls and are hence walls in walls. Examples in $CaTiO_3$ and $SrTiO_3$ are discussed.

[1] E.K.H. Salje, Ferroelastic Materials, Annual Review of Materials Research, 42, 265-283 (2012)
[2] E.K.H. Salje and K.A. Dahmen, Crackling Noise in Disordered Materials, Annual Review of Condensed Matter Physics, 5, 233-254 (2014)
[3] E.K.H. Salje, Multiferroic Domain Boundaries as Active Memory Devices: Trajectories Towards Domain Boundary Engineering, Chem. Phys. Chem., 11, 940-950 (2010)
[4] D.D. Viehland and E.K.H. Salje, Domain boundary-dominated systems: adaptive structures and functional twin boundaries, Advances in Physics, 63, 267-326 (2014)

TUT 3: Tutorial: Nonequilibrium Renormalization Group Methods (TT)

This tutorial provides introductions to three essentially analytic renormalization-group-like approaches to the quantum many-body problem in non-equilibrium. They constitute versatile tools to investigate driven steady states as well as the nonequilibrium dynamics of correlated systems in different fields of growing interest such as, e.g., meso- and nanoscopic solid-state systems, as well as cold atomic gases.

Organizer: Volker Meden (RWTH Aachen)

Time: Sunday 16:00–18:15 Location: H 0110

Introductory Remarks

Tutorial TUT 3.1 Sun 16:05 H 0110

From Lunar Motion to Real Time Evolution of Quantum Many-Body Systems — •Stefan Kehrein — Institute for Theoretical Physics, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

While studying the real time evolution of quantum many-body systems is a fairly new topic in physics, the real time evolution of classical systems is an old one. In fact, this topic goes back to the very beginning of classical mechanics, namely its application to celestial mechanics. One of the important lessons learned in this classical setting is that naive application of perturbation theory can lead to secular terms in time which quickly invalidate the expansion. This observation gave rise to the development of canonical perturbation theory with much improved convergence properties.

In this lecture I will show how similar progress can be made for the calculation of the real time evolution of quantum systems by using unitary perturbation theory [1,2,3]. In addition, this approach permits one to deal with models with a nontrivial renormalization flow and to see how this affects the real time dynamics away from equilibrium.

[1] A. Hackl and S. Kehrein, Phys. Rev. B **78**, 092303 (2008)
[2] A. Hackl and S. Kehrein, J. Phys. C **21**, 015601 (2009)
[3] F. Essler, S. Kehrein, S. Manmana, and N. Robinson, Phys. Rev. B **89**, 165104 (2014)

5 min. break

Tutorial TUT 3.2 Sun 16:50 H 0110

Functional Renormalization Group Approach to Nonequilibrium Transport through Mesoscopic Systems — •Severin Georg Jakobs — Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany

The transport properties of quantum dots and wires are strongly influenced by correlation effects like the Kondo effect or Luttinger liquid behavior. The theoretical description of these effects requires methods beyond plain perturbation theory or mean-field theory. In the last decade, the functional renormalization group (fRG) has been used extensively and successfully to investigate such situations. It is applicable if the interaction on the dot is weak to intermediate compared to the hybridization with the leads. This makes the method complementary to the real-time RG which applies to the opposite regime and which is described in the tutorial by Herbert Schoeller. The particular formulation of the fRG in the framework of Keldysh formalism allows to study time-dependent and steady-state nonequilibrium situations. In this tutorial I introduce the basic concepts of that method and discuss the choice of appropriate flow parameters. I discuss examples for steady-state transport at finite bias voltage and for the time-dependent transient regime.

5 min. break

Tutorial TUT 3.3 Sun 17:35 H 0110

Real-Time RG: Nonequilibrium Properties of Open Quantum Systems — •Herbert Schoeller — Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany — JARA-Fundamentals of Future Information Technology

A tutorial introduction is presented for the description of nonequilibrium properties of few-level quantum sytems coupled to reservoirs as e.g. realized by quantum dot, spin boson or Kondo models. Within a quantum field theoretical framework in Liouville space it is shown how formally exact kinetic equations can be derived which can be systematically studied in terms of an effective Liouvillian. By using special resummation techniques via self-consistent perturbation theory and renormalization group methods it is shown how the time evolution and the stationary state can be studied in a nonequilibrium set-up. Various applications in the weak and strong coupling limit are presented.

TUT 4: Tutorial: Density Functional Theory: A Computational Path to Interesting Spin-textures and Novel Skyrmions (MA with TT)

Organizer: St. Blügel (FZ Jülich)

Ferromagnetic materials are important constituents of many modern hi-tech devices. In the last years one became however aware that non-collinear spin-textures could revolutionize spintronics. The focus of attention is on the spin-orbit interaction in magnetic solids with lack of inversion symmetry, that give rise to magnetic structures of particular winding sense and can lead to the formation of topological magnetization solitons, so-called magnetic skyrmions. These are then new functional magnetic units with interesting dynamical and novel spin-dependent transport properties. Density functional theory is the most powerful theoretical approach providing microscopic inside into the various magnetic interactions and spin-dependent transport properties, which is an important requisite for the design of materials and the analysis of experiments. While density function theory is practised widely, in this field new concepts and tools are coming into play. These will be introduced with the motivation that experimentalists can follow what we really calculate, what we can do, which assumption are made and how theory papers in this field can be interpreted and theory students might get some insight into this modern methodology, widening their scope or applying them to their own problems. After a brief introduction, the first tutorial focusses on the conceptual foundation of the relativistic, spin-dependent density functional theory, the second on the formation of new magnetic ground states and the third on spin-dependent transport properties.

Time: Sunday 16:00–18:30 Location: H 1012

Introductory Remarks

Tutorial TUT 4.1 Sun 16:05 H 1012

Introduction to Spin-Density-Functional Theory — •Nicole Helbig — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

Density functional theory is the most powerful framework for a microscopic analysis of electronic properties of real solids. Spin-density-functional theory (spin-DFT) extends the density functional theory framework to allow for the description of magnetic systems, possibly in the presence of an external magnetic field. In this tutorial we introduce this subject from an elementary point of view and discuss the theoretical background of spin-DFT in both its collinear and non-collinear versions. Approximations for the exchange-correlation energy, which are necessary for practical applications, are also introduced. We give examples for calculations of different magnetic structures within spin-DFT and discuss how the theoretical results compare to experiments.

Tutorial TUT 4.2 Sun 16:50 H 1012

Determining chiral magnetism from density functional theory — •Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Spin-orbit interaction in magnetic solids with bulk or structure inversion-asymmetry leads to the Dzyaloshinskii-Moriya interaction [1]. This magnetic interaction is a source of chiral magnetism and can subsequently lead to magnetic skyrmions – topological magnetization solitons – that may open a completely new vista to spintronics. A crucial issue is to find magnetic materials and ultra-thin films that combine the right properties such that these skyrmions can be formed. Density functional theory is a theoretical framework that permits the calculation of magnetic properties of materials from first-principles and is as such a tool for the analysis of experiments, for providing understanding of the magnetic interaction and for the design of the proper materials. In this endeavor your help is requested, many more *ab initio* calculations and experiments are needed. In this tutorial I explain concepts used to find these complex magnetic phases. The tutorial is conceptualized such that experimentalists can follow what we really calculate and what we can do and which assumptions are made, and theory students might get some insight into our methodology [2]. Examples are discussed mostly from the field of thin films [3].

[1] M. Bode *et al.*, Nature **447**, 190 (2007).
[2] see for example `www.juDFT.de`
[3] S. Heinze *et al.*, Nature Physics **7**, 713 (2011).

10 min. break

Tutorial TUT 4.3 Sun 17:45 H 1012

Magneto-transport properties in spiralling spin textures — •Yuriy Mokrousov — Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Spin-dependent transport properties in chiral magnets are currently of great interest both experimentally and theoretically. In this respect the skyrmion lattices comprised of topologically non-trivial whirls of magnetization which are typically stabilized at small magnetic field in the vicinity of the magnetic transition temperature are particularly

intensively studied in B20 compounds. The Hall signal measured in these systems contains two topology-driven contributions due to the topological Hall effect (THE) and the anomalous Hall effect (AHE). It can be shown that the THE and AHE are a consequence of the Berry phases which electrons pick up in real and reciprocal spaces, respectively, while the so-called mixed Berry phases due to coupled dynamics in real and reciprocal space would give rise to a magnetic interaction which favors the chirality of the magnetization and gives rise to the skyrmion lattice - the Dzyaloshinskii-Moriya interaction (DMI). In my talk I will show how first principles methods can be used to justify the validity of the Berry phase concepts, as well as estimate and understand the physics of transport properties and DMI in skyrmion phase of complex materials. Moreover, I will try to convey a point that advanced material-specific modelling is a unique tool, which can be used to explore the emergent field of magneto-transport in nanometer-scale non-collinear textures.

TUT 5: Tutorial: Electro Chemistry 4 Condensed Matter Physicists (HL with MM)

Organized by Erich Runge and Jörg Neugebauer on behalf of the Semiconductor Physics Division (HL) and the Metal and Material Physics Division (MM), respectively.

Time: Sunday 16:00–18:25 Location: H 1058

Invited Talk TUT 5.1 Sun 16:00 H 1058

Challenges in the theoretical description of structures and processes at electrochemical interfaces — •Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany — Helmholtz Institut Ulm, 89069 Ulm, Germany

In spite of its technological relevance in the energy conversion and storage, our knowledge about the microscopic structure of electrochemical electrode-electrolyte interfaces is still rather limited. The theoretical description of these interfaces is hampered by three challenges [1]. i) In electrochemistry, structures and properties of the electrode-electrolyte interfaces are governed by the electrode potential which adds considerable complexity to the theoretical treatment since charged surfaces have to be considered. ii) The theoretical treatment of processes at solid-liquid interfaces includes a proper description of the liquid which requires to determine free energies instead of just total energies. This means that computationally expensive statistical averages have to be performed. iii) Electronic structure methods based on density functional theory (DFT) combine numerical efficiency with a satisfactory accuracy which makes them appropriate for electrochemical systems. However, there are severe shortcomings of the DFT description of liquids, in particular water, using current functionals.

In this tutorial talk, I will give an overview over concepts and theoretical methods for the realistic description of electrochemical interfaces. Examples of insights gained from theoretical studies will be presented but open challenges will be identified as well.

[1] N.G. Hörmann *et al.*, J. Power Sources **275**, 531 (2015).

Short break

Invited Talk TUT 5.2 Sun 16:50 H 1058

Raman under water - Of photons, phonons and the fun of tuning the Fermi level — •Katrin F. Domke — MPI for Polymer Research, Ackermannweg 10, D-55128 Mainz

t.b.a.

Short break

Invited Talk TUT 5.3 Sun 17:40 H 1058

Scanning probe microscopies for electrochemical problems — •Gunther Wittstock — Carl v. Ossietzky University of Oldenburg, School of Mathematics and Science, Department of Chemistry, D-26111 Oldenburg

Electrified solid-liquid interfaces are characterized by a vertical and horizontal inhomogeneity in structure. Even well prepared single crystal electrodes show, adatoms, steps kinks and other defects. The investigation of such structures by STM has dramatically enhanced our understanding of such interfacial structures. However, the experiments were mostly performed in the absence of a Faradayic reaction (.i.e. electrolysis). With a few exceptions, electrodes are designed for controlling Faradayic reactions. High current densities are requested for efficient energy conversion devices; very low current densities are a requirement for materials that shall resist corrosion under harsh environments. Such materials (polycrystalline, multiphase or composites) show a large variation of local current densities that are neither accessible by I-V-curves nor by STM. Scanning electrochemical microscopy (SECM) provides this information. It uses the electrolysis current of a dissolved redox-active compound at a probe microelectrode to generate the signal. The electrolysis at the probe is coupled to local reaction at the sample by diffusion of reactants in the probe-sample gap. Different working modes and examples will be explained with the aim to differentiate between fundamental barriers and current instrumental limitations that might be overcome by the impact of well trained physicist.