DY 30: Reaction-Diffusion Systems

Time: Thursday 10:15–12:30 Location: ZEU 118

DY 30.1 Thu 10:15 ZEU 118

Interaction of a pair of scroll waves — •Dennis Kupitz and Marcus Hauser — Abteilung Biophysik, Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Scroll waves are the three-dimensional counterparts of spiral waves occurring in excitable media. Single scroll waves may undergo a series of instabilities that play an important role in the formation of cardiac arrhythmias, like ventricular tachycardia. While the dynamics of single scroll waves have attracted some experimental effort, the interaction of scroll waves has so far received much less attention.

We present an experimental study of the interaction of two scroll waves created in a Belousov-Zhabotinsky reaction medium and observed by optical tomography with a parallel beam technique. The scroll waves may either rotate in the same or in an opposite sense of rotation, thus leading to situations with different topological charges. The organising centres of the scrolls, the so-called filaments, were originally straight, and depending on the selected experimental conditions, they may either describe a circular or a meandering trajectory. The dynamics of pairs of co- and counter-rotating scroll waves were studied for both rigidly rotating and meandering filaments, leading to different types of collective filament behaviour.

DY 30.2 Thu 10:30 ZEU 118

A reactive-flow model of phase separation in fluid binary mixtures with continuously ramped temperature — Izabella Benczik and •Jürgen Vollmer — Max Planck Institute for Dynamics and Self-Organization, 37073 Göttingen

We suggest to revisit the phase separation of binary mixtures subjected to a sustained change of temperature from the point of view of reactive flows. Exploiting this new perspective, we describe the demixing dynamics by a spatial model of advection-reaction-diffusion completed with nucleation and coaguation of droplets. In this approach several features of the dynamics — in particular an oscillatory variation of the droplet density — become numerically and analytically accessible. Hence, this model helps to clarify why the oscillation frequency is hardly affected by the flow.
I.J. Benczik and J. Vollmer, EPL **91** (2010) 36003.

DY 30.3 Thu 10:45 ZEU 118

Reaction-diffusion system with continuous distributions of binding energies — •Andrea Wolff[1], Ingo Lohmar[2], Joachim Krug[1], and Ofer Biham[2] — [1]Institut für theoretische Physik, Universität zu Köln — [2]Racah Institute of physics, The Hebrew University, Jerusalem, Israel

We study pair reactions on a periodic square lattice with continuous deposition, diffusion, and spontaneous desorption of particles. The characteristic quantity of the system's steady state is the efficiency, which is the fraction of incoming particles, that react before desorption.

Since spatial inhomogeneity is of theoretical and applied interest, we want to study the influence of disorder in the process rates systematically. We start with binary disorder, where each site has one of two possible different binding energies. The behaviour of this system has been well-understood qualitatively and quantitatively [1]. In contrast, the case of continuously distributed binding energies cannot be treated exactly anymore. We use the knowledge of the binary system to derive a mapping from the system with a continuous distribution to an effective binary model, where all the different binding energies are pooled into two effective ones. Comparison of this effective model with Monte Carlo simulations shows remarkable agreement.

[1] A. Wolff, I. Lohmar, J. Krug, Y. Frank, O. Biham, Phys. Rev. E 81, 061109 (2010)

DY 30.4 Thu 11:00 ZEU 118

Reentries generated by a random heterogeneous region in cardiac tissue — •Sergio Alonso and Markus Bär — Physikalisch-Technische Bundesanstalt

Wave propagation in the heart has a discrete nature due to the discrete intercellular connections via gap junctions. Cardiac diseases may result on the reduction of conductivities of the gap junctions. The distribution of the disrupted connections can be inhomogeneous and some part of the heart can accumulate a major density.

We study the effect on homogeneous wave propagation with a region where a random distribution of connectivities between cells are eliminated. This region can produce the appearance of reentries. We consider the Fenton-Karma model for cardiac tissue to perform a systematic study of the reentry generation depending on the topology of the connectivity network.

DY 30.5 Thu 11:15 ZEU 118

Coupling of pacemakers and irregular excitation patterns in reaction-diffusion systems — •Claudia Lenk[1], Mario Einax[2], J. Michael Koehler[1], and Philipp Maass[2] — [1]Institut für Physik, Technische Universität Ilmenau, Germany — [2]Fachbereich Physik, Universität Osnabrück, Germany

Reaction-diffusion (RD) systems describe pattern formation in many areas as, e.g., chemical reactions, population dynamics, and the propagation of electrical excitations in the brain or heart. They allow one also to study the mechanisms that lead to irregular, chaos-like excitation patterns and related pathological states in physiologic applications. In this talk we report on the generation of irregular excitation patterns due to coupling of different pacemakers in two types of spatially separated RD-systems, the Belousov-Zhabotinsky reaction (BZR) and a simple model for atrial fibrillation. Theoretical calculations are carried out for two different RD-models, the FitzHugh-Nagumo equations and the minimal model of Bueno-Orovio *et al* [1]. Experiments of the BZR are conducted in a gel system with periodic pattern of the catalyst Ferroin. The regularity of the excitation patterns is analyzed by the entropy of the frequency distribution and by the synchronization properties between the two pacemakers.

[1] A. Bueno-Orovio, E. M. Cherry, F. H. Fenton, JTB **253**, 544 (2008).

DY 30.6 Thu 11:30 ZEU 118

Dynamics of scroll rings interacting with boundaries — •Arash Azhand, Peter Kolski, and Harald Engel — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Undamped propagation of three-dimensional travelling waves has been observed in a variety of dissipative active media including chemical waves, temperature waves in solid fuel combustion and waves of electric activity during cardiac arrhythmias, for example. Here, we present experimental and numerical results for the dynamics of scroll rings in thin layers of the photosensitive Belousov-Zhabotinsky reaction. The study is focused on boundary effects that modify the intrinsic dynamics of the scroll ring under these geometrically confined conditions. The experimental findings are compared to results obtained by numerical simulations with the underlying Oregonator model. The reported results do not depend, however, on a particular kinetics but apply to a large class of excitable media.

DY 30.7 Thu 11:45 ZEU 118

Control of spatiotemporal chaos by flow in a reaction-diffusion-advection system — •Igal Berenstein and Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Germany

We report spatiotemporal chaos in the Oregonator model of the Belousov-Zhabotinsky (BZ) reaction. Uniform oscillations and traveling waves are unstable and spatiotemporal chaos spontaneously develops in a regime, where the underlying local dynamics show stable limit cycle oscillations (diffusion-induced turbulence). We show that spatiotemporal chaos can be suppressed by a unidirectional flow in the system. With increasing flow velocity, we observe a transition scenario from spatiotemporal chaos via a regime of travelling waves to a stationary steady state. At large flow velocities we recover the known regime of flow distributed oscillations (stationary structure). We also investigated systems with a gradient in one of the parameters. We show that in such systems, localized domains of spatiotemporal chaos can be found if the gradient is sufficiently small, i.e., if the size of the chaotic domain is large compared to the diffusive length scale. Finally, we show that spatiotemporal chaos can be suppressed by allowing diffusive exchange of the activator between the reaction- diffusion system and a non-reacting layer. The type of pattern that is formed is independent of a flow in the non-reactive layer.

DY 30.8 Thu 12:00 ZEU 118

Hysteresis in the pinning-depinning transition of a spiral wave close to a circular defect — •Jan Frederik Totz and Harald Engel — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

A non-monotonous dependence of the rotation period on the defect radius with coexistence between freely rotating and pinned spiral waves in a certain parameter range has been reported first by Pertsov et al. [1]. Recently, these results were confirmed in a detailed numerical bifurcation analysis using the continuation software AUTO [2]. Within a free-boundary formulation the role of curvature and dispersion effects has been clarified [3]. By doing so, quantitative agreement between theoretical predictions and results obtained by numerical simulations was achieved. The experimental verification of the hysteresis phenomenon in an open gel reactor with the photosensitive Belousov-Zhabotinsky reaction is the topic of the talk.

[1] A. M. Pertsov, E. A. Ermakova, A. V. Panfilov, Physica D 14, 117 (1984).

[2] G. Bordyugov, H. Engel, Physica D 228, 49 (2007).

[3] V. Zykov, G. Bordyugov, H. Lentz, H. Engel, Physica D 239, 797 (2010).

DY 30.9 Thu 12:15 ZEU 118

Activation parameters of model redox reactions and their variation from classical molecular simulation — •Christof Drechsel-Grau and Michiel Sprik — University of Cambridge, Department of Chemistry, Cambridge, CB2 1EW, United Kingdom

Transition states are dynamical bottlenecks of chemical reactions, and an understanding of their energetic properties and location can provide insight into the reactions' mechanism. In particular, the variation of the activation free energy with temperature yields the activation entropy and the activation energy, whereas the variation of the activation free energy with reaction free energy defines the charge-transfer symmetry factor, which indicates the location of the transition state relative to the stable states. The calculation of activation parameters is not only computationally demanding, but traditionally also relies on knowledge of the reaction coordinate, which is usually unavailable. Thus, we employ transition path sampling, which does not require knowledge of the reaction coordinate, to compute activation energies and their variation with reaction free energy for a model system. Exploiting knowledge of the reaction coordinate for the model system, we also calculate the activation free energies and the charge-transfer symmetry factor from umbrella integration and from free energy perturbation simulations. We find that the activation energies are smaller than the activation free energies. In addition, the variation of the latter with reaction free energy is larger than that of the former.