DY 7: Reaction-Diffusion-Systems

Time: Monday 16:45–18:30 Location: MA 144

DY 7.1 Mon 16:45 MA 144

Influence of boundaries on the intrinsic dynamics of excitation waves — •Jan Frederik Totz[1], Oliver Steinbock[2], and Harald Engel[1] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, EW 7-1, D-10623 — [2]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL-32306-4390

Three-dimensional excitation waves are thought to play a fundamental role in serious cardiac diseases such as tachycardia and fibrillation. We employ the well-studied Belousov-Zhabotinsky-Reaction as a chemical model system to investigate the altered dynamics of scrollrings close to boundaries, using an experimental setup as described in [1]. We observed four different scenarios of the scrollring evolution dependent upon the distance to the nearest zero-flux boundary: Annihilation at the boundary, weakly & strongly boundary-affected scrollring contraction rates and even vanishingly small contraction. The experimental findings are in good agreement with previous numerical results [2].

[1] Z. A. Jiménez, B. Marts, O. Steinbock, Phys. Rev. Lett. 102, 244101 (2009)

[2] M. Bray, J.P. Wikswo, Phys. Rev. Lett. 90, 23 (2003)

DY 7.2 Mon 17:00 MA 144

Spiral wave selection in excitable media with a phase wave at the wave back — •Vladimir Zykov, Noriko Oikawa, and Eberhard Bodenschatz — Max Planck Institute for Dynamics and Self-Organization, D-37077 Goettingen, Germany

Universal relationships between the medium excitability and the angular velocity and the core radius of rigidly rotating spiral waves in excitable media are derived for situations where the wave front is a trigger wave and the wave back is a phase wave [1]. Such trigger-phase (TP)-waves are equally important for applications as commonly studied trigger-trigger (TT)-waves. Two universal limits restricting the region of existence of spiral TP-waves in the parameter space are demonstrated. The predictions of the free-boundary approach are in good quantitative agreement with results from numerical reaction-diffusion simulations performed on the Kessler-Levine model.

The proposed free-boundary approach opens perspectives to analyze TP-spiral waves in different kind of models including such important applications as chemical or cardiac excitable media.

1. V.S. Zykov, N. Oikawa, and E. Bodenschatz, Phys. Rev. Lett., accepted.

DY 7.3 Mon 17:15 MA 144

Speed-up of a clock reaction with microfluidic methods — •Robert Niedl, Igal Berenstein, and Carsten Beta — Biological Physics, Universität Potsdam, Germany

The focus of our research is a combination of nonlinear kinetics and microfluidics to amplify chemical input signals. We study the dynamics of the autocatalytic iodate-arsenite reaction in PDMS-based microfluidic devices under continuous flow conditions. If a critical amount of initializer is present, a reaction is triggered by a nonlinear autocatalytic process. In our experimental setup two different scenarios are implemented to initiate the reaction. On the one hand, we use diffusive micromixing to systematically investigate the kinetics of the clock depending on the various input concentrations, flow velocities, and fluid viscosities. On the other hand, we introduce a Pt electrode into the microchannel that acts as a local chemical source in the flow. This setup allows us to explore the interplay of mixing kinetics and nonlinear reaction that may lead to accelerated reaction rates in specific microfluidic configurations.

DY 7.4 Mon 17:30 MA 144

Parameter estimation for reaction-diffusion systems — •Andreas Ruttor and Manfred Opper — Technische Universität Berlin

Spatial fluctuations of the particle density in reaction-diffusion systems are often modelled by dividing the system into small compartments. In this case, additional transfer reactions describe the diffusion, so that methods for homogeneous reactions systems can be used in order to estimate parameters. However, finding a suitable discretization is not easy: if the compartments are too big, important spatial structure contained in the observations is lost. But using smaller compartments increases the complexity of the calculations. In order to solve this problem, we propose a more fundamental approach. Instead of using compartments directly, we transform the model into Fourier space and calculate the continuum limit analytically. As before, the dynamics of the system is described by its Fokker-Planck equation. We then apply system size and weak noise expansions, which lead to a Gaussian approximation suitable for efficient parameter estimation. It turns out that only low-frequency moments are relevant here, while higher frequencies mostly contain noise. This also applies to the observations, as it is impossible to measure all details of the spatial fluctuations. Consequently, only a small number of moments in Fourier space are needed for calculating the total likelihood, usually less than in the case of compartment models.

DY 7.5 Mon 17:45 MA 144

Non-equilibrium reaction-diffusion structures in Poiseuille flows: A Lattice Boltzmann study — •Segun Gideon Ayodele — Max-Planck Institute für Eisenforchung, Düsseldorf, Germany.

Solutions of the reaction-diffusion equations are know to exhibit a wide variety of spatially and/or temporally varying structures [S.G. Ayodele et. al. Phys.Rev.E. 80,016304 (2009), S.G. Ayodele et. al. Phys.Rev.E. 83,016702 (2011)]. In this work we study spatially varying structures arising from the interaction of advective transport with an autocatalytic reaction-diffusion process under an imposed Poiseuille flow. Structures resulting from the interaction of the 2D Poiseuille flow with the reaction-diffusion process takes place via two mechanisms. A differential advection induced instability and a flow independent Turing instability. The differential advection mechanism leads to traveling stripes with a velocity dependent wave vector parallel to the flow direction. The second mechanism similar to the Turing instability produces longitudinal stripes aligning along the streamlines with a velocity independent wave vector perpendicular to the flow direction. The symmetry of the patterns in the case of Turing instability are found to be similar to the symmetry of the underlying advective fields. We observe a parameter range where a competition between the two mechanism produces mixed modes comprising of transverse and longitudinal stripes. Using predictions from linear and weakly-nonlinear theory we propose an explanation of this behaviour in terms of the effective diffusivities due to Taylor dispersion.

DY 7.6 Mon 18:00 MA 144

Proton-transfer barriers in low-temperature hexagonal ice from computer simulations — •Christof Drechsel-Grau and Dominik Marx — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany

Hexagonal ice exhibits remarkable properties. For instance, the proton positions remain disordered down to low temperatures ($\approx 10\,\mathrm{K}$), thereby giving rise to the residual entropy of ice, which stems from many configurations of the hydrogen-bond network even in the absence of defects. Collective proton-transfer or proton-tunnelling events may connect different (defect-free) proton configurations. Unravelling the proton dynamics would not only shed light on properties of ice, but might also contribute to our understanding of liquid water. In this contribution we investigate whether the barriers between different configurations are sufficiently low for proton dynamics to occur even at low temperature. In particular, we describe the electronic structure via density-functional theory and take into account nuclear quantum effects by means of path-integral simulations. First results indicate that the classical barrier is significantly higher than its quantum counterpart, thereby underlining the importance of nuclear quantum effects.

DY 7.7 Mon 18:15 MA 144

Reaction-Diffusion-Systems with various Distributions of Binding Energies — •Andrea Wolff[1], Ingo Lohmar[2], and Joachim Krug[1] — [1]Institut für theoretische Physik, Universität zu Köln, Deutschland — [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 behavior 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 [2]. 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)

[2] A. Wolff, I. Lohmar, J. Krug, O. Biham, J. Stat. Mech. 10, P10029 (2011)