DY 5: Statistical Physics of Biological Systems II (joint session of BP + DY)

Time: Monday 14:00–17:00 Location: H45

Invited Talk DY 5.1 Mon 14:00 H45

Nonlinear dynamics and control of migraine waves — •Markus Dahlem — Institut f. Theo. Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Migraine is a dynamical disease. A mechanism is presented by which traveling wave patterns, which cause migraine, are formed in the 2D folded human cortex. The predicted wave is maintained only transiently but with a characteristic form (shape and size). Such patterns contradict the established image of a migraine wave engulfing one cortical hemisphere, but we found that they are in agreement with our results obtained from a study using functional magnetic resonance imaging. The mechanism is based on an unstable particle-like wave solution that exists in generic reaction-diffusion media of activator-inhibitor type. This solution can vanish in a saddle-node bifurcation if excitability is globally controlled. This creates a bottleneck region in phase space that sucks in all sufficiently largely perturbed cortical states (ignition phase in migraine). While, as a consequence, recovery is slowed down, a pattern with universal space and time scales emerges. Our bifurcation analysis is also supported by numerical simulations. Moreover, it is shown analytically that such confined waves favor certain cortical geometries. Consequences are discussed for the design and application of biomedically engineered devices that can be used in therapeutic approaches to intelligently target migraine waves by changing the bottleneck passage time and thus more quickly revive the physiological state of the cortex.

DY 5.2 Mon 14:30 H45

Using GFRD to Study Pattern Formation due to the Interplay of Active and Passive Transport — •Thomas Sokolowski, Nils Becker, Laurens Bossen, Thomas Miedema, and Pieter Rein ten Wolde — FOM Institute AMOLF, Science Park 113, 1098 XG Amsterdam, The Netherlands

Cells exploit the interplay of active transport along cytoskeletal tracks and cytosolic passive diffusion to establish a wide range of spatial patterns of functional proteins, mRNA and specialized organelles. Such systems are not well-stirred, so standard simulation techniques can be very expensive while coarse-graining may be inappropriate.

Green's function reaction dynamics (GFRD) is an exact event-driven chemical simulation scheme based on analytical solutions of the Smoluchowski equation with appropriately chosen boundary conditions. For sufficiently low particle concentrations up to 1uM it allows for spatially resolved stochastic simulations of many-particle-systems with an efficiency orders of magnitude higher as compared to common Brownian dynamics schemes.

Based on GFRD we develop a framework which allows for a spatio-temporal stochastic simulation of both active and diffusive movement in different geometries to study pattern formation arising from the interplay the two transport types.

DY 5.3 Mon 14:45 H45

Prokaryotic Chromosome Organization in the Context of Entropy, Confinement and Tethering Interactions — •Miriam Fritsche and Dieter W. Heermann — Institute for Theoretical Physics, University of Heidelberg, Philosophenweg 19, 69120 Heidelberg, Germany

Prokaryotic chromosomes are physically organized and condensed into an intricately structured DNA-protein complex called a nucleoid. The large-scale physical structure might arise from protein mediated interactions that can form both inter and intra-chromosome tethers as well as anchoring the chromosome to the membrane of the nucleoid or to protein scaffolds [1]. Motivated by recent experiments that capture E. coli nucleoid structure using three spectrally distinct, fluorescently-labeled genetic loci [2], we analyze single-locus and two-locus positioning distributions in the theoretical framework of a coarse-grained polymer model taking into account excluded volume, confining geometries as well as tethering interactions therewith shedding light into the mechanisms governing E.coli nucleoid structure between replication cycles.

[1] W.F. Marshall, Current Biology 12, 158 (2002)

[2] P.A. Wiggins, K. Cheveralls, J.S. Martin, R. Lintner, J. Kondev, private communication

DY 5.4 Mon 15:00 H45

Velocity distributions of foraging bumblebees in the presence of predators — •Friedrich Lenz[1], Thomas C. Ings[2], Lars Chittka[2], Aleksei V. Chechkin[3], Holger Kantz[4], and Rainer Klages[1] — [1]Queen Mary University of London, School of Math. Sci., UK — [2]Queen Mary University of London, School of Biol. & Chem. Sci., UK — [3]Inst. for Theo. Physics, NSC KIPT, Kharkov, Ukraine — [4]Max Planck Institute for the Physics of Complex Systems, Dresden

We analyse changes in the flight behaviour of foraging bumblebees under varying environmental conditions, measured in a laboratory experiment by Ings and Chittka[1]. We estimate parameters for different plausible velocity distributions by maximising their likelihood and compare their goodness of fit by applying the Akaike Information Criterion. Using Quantile-Quantile-plots we check for deviations between the estimated probability distributions and the data. We also discuss differences in these distributions for different individual bumblebees. On this basis, we look for systematic changes of the distributions due to the presence of different kinds of artificial spiders.

[1] Thomas C. Ings and Lars Chittka. Current Biology, 18(19):1520-15 24 (2008)

DY 5.5 Mon 15:15 H45

Modelling a flexible sheet swimmer with stochastic rotation dynamics — •Sujin Babu and Holger Stark — Institut für Theoretische Physik Technische Universität Berlin

The dynamics of microorganisms in a viscous fluid has recently received considerable attention in the physics community. It has been reported that some microorganisms (such as the African Trypanosome) make use of hydrodynamic flow fields to evade attack from antibodies. The flexible cell body of the African Trypanosome possesses some bending rigidity due to its cytoskeleton. To mimic the cell body of such an organism, we introduce a flexible sheet that is impenetrable to the surrounding fluid. The flow fields around such a sheet are simulated by stochastic rotation dynamics. I will explain how we couple the flexible sheet to the viscous fluid. Then I will discuss the drag coefficients of the sheet and investigate how it swims under the influence of appropriately applied forces.

15 min. break

DY 5.6 Mon 15:45 H45

The first passage problem for diffusion through a cylindrical pore with sticky walls — •Nicholas A. Licata[1,2] and Stephan W. Grill[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

We calculate the first passage time distribution for diffusion through a cylindrical pore with sticky walls. A particle diffusively explores the interior of the pore through a series of binding and unbinding events with the cylinder wall. Through a diagrammatic expansion we obtain first passage time statistics for the particle's exit from the pore. Connections between the model and nucleocytoplasmic transport in cells are discussed.

DY 5.7 Mon 16:00 H45

A growth model for bacterial flagella — •Maximilian Schmitt, Reinhard Vogel, and Holger Stark — Institut für Theoretische Physik, TU Berlin

Bacterial flagella of e.g. E.coli consist of up to 30000 flagellin molecules which are arranged in a hollow tube with outer and inner diameters of 20nm and 3nm, respectively, and a length of up to 20μm. When the flagellum grows, flagellin molecules are transported through the hollow core of the filament and attached at its tip.

As a model for this growth process, we extend one model system of non-equilibrium statistical mechanics, the ASEP (Asymmetric Simple Exclusion Process), to an exclusion process on a growing lattice. In this one-dimensional model, particles enter the lattice with rate α, travel forward with jump rate q and backward with rate p. At the tip particles can transform into a new lattice site with rate γ.

Monte Carlo simulations and mean-field approximations both give the same phase diagram in (α, γ) phase space with distinct low density, high density and maximal current phases. In case of symmetric dy-

namics ($q = p$) both low density and high density phase vanish, which is in agreement with the SSEP (Symmetric Simple Exclusion Process). Special attention is put on the tip velocity with which the length L of the flagellum grows. It shows an unstable fixed point at $q = p$. For $q > p$ the model is ballistic with $\langle L^2 \rangle \sim t^2$, for $q = p$ diffusive with $\langle L^2 \rangle \sim t$, and for $q < p$ sub-diffusive with a tip velocity slower than single-file diffusion: $\langle L^2 \rangle \sim t^{1/6}$.

DY 5.8 Mon 16:15 H45

Long-range protein coupling mediated by critical low-energy modes of tubular lipid membranes — Sylvain Monnier[1,3], Sergei B. Rochal[2], •Andrea Parmeggiani[3], and Vladimir L. Lorman[1] — [1]LPTA, CNRS, University of Montpellier II, 34095 Montpellier, France — [2]Physical Department, South Federal University, 344090 Rostov-on-Don, Russia — [3]DIMNP, CNRS, University of Montpellier II, 34095 Montpellier, France

Tubular lipid membranes (TLMs) are nanoscopic cylindrical assemblies that play a fundamental role in many intracellular and intercellular processes like protein trafficking, signaling and organelle morphogenesis. TLMs can be generated by a sum of mechano-chemical actions, ranging from mechanical forces produced by motor proteins pulling at one TLM-end up to the specific chemical activity of membrane proteins.

We develop a theory of TLM instabilities under longitudinal force and pressure difference constraints. Two qualitatively different critical low-energy modes are shown to define the stability domain boundaries. The analysis allows to introduce a new framework describing TLM-protein coupling, adsorbed protein-protein interaction and protein cluster nucleation on a TLM. In particular, bare TLM mechanical instabilities strongly influence protein-TLM coupling and protein desorption from the TLM. Model predictions can be directly tested in experiments involving nanomechanical devices extracting TLM over a large spectrum of mechanochemical conditions.

DY 5.9 Mon 16:30 H45

Protein folding trajectories and free energy landscapes in a coarse-grained model — •Katrin Wolff[1], Michele Vendruscolo[2], and Markus Porto[1] — [1]Institut für Festkörperphysik, TU Darmstadt, Germany — [2]Department of Chemistry, University of Cambridge, UK

We study protein free energy landscapes and folding dynamics from completely unfolded to folded structures using a coarse-grained model biased towards the native state. Proteins are modeled as a chain of uniform thickness with bending rigidity (tube model [1]) with a bias towards the native structure based on a one-dimensional representation of the structure (structure profile). This approach is conceptually very different from those relying on the assumption of minimal frustration (such as Gō-models) since it does not favour the formation of contacts between specific residues but mediates 'connectivity' of residues, that, much like hydrophobicity, describes a residue's propensity to form contacts. We show that the 'effective connectivity' profile [2] constitutes a suitable bias towards the native structure [3] and investigate free energy landscapes, heat capacity curves and typical folding trajectories and compare our results to experimental folding behaviour and results from (much more computationally expensive) molecular dynamics simulations.

[1] T.X. Hoang *et al.*, Proc. Natl. Acad. Sci. USA **101**, 7960 (2004).
[2] U. Bastolla *et al.*, Proteins **73**, 872 (2008).
[3] K. Wolff, M. Vendruscolo, and M. Porto, PMC Biophysics **1**, 5 (2008)

DY 5.10 Mon 16:45 H45

Intrinsic fluctuations in stochastic delay models of gene regulation — •Tobias Galla — Theoretical Physics, School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, UK

We study the effects of intrinsic noise on stochastic delay systems within an expansion in the inverse system size. It is shown that the stochastic nature of the underlying dynamics can induce sustained quasi-cycles in parameter ranges where the deterministic system does not show oscillatory behaviour. We compute the power spectra of these stochastic oscillations analytically, in good agreement with simulations. The theory is applied to a simple gene regulatory system representing the basic motif of an auto-inhibitory feedback loop and motivated by its relevance to somite segmentation. Such systems often contain only a small number of molecules, leading to significant fluctuations in mRNA and protein concentrations, and the proposed mechanism of enhanced stochastic oscillations may therefore be applicable.

Reference: Tobias Galla, Phys. Rev. E 80 (2009) 021909