DY 16: Statistical Physics in Biological Systems (joint session DY/ BP)

Time: Wednesday 9:30–12:00 Location: ZEU 160

DY 16.1 Wed 9:30 ZEU 160

Statistics of local multiple sequence alignments — •Pascal Fieth and Alexander K. Hartmann — Institute of Physics, University of Oldenburg

To assess the significance of alignment scores obtained by comparing DNA or amino acid sequences using sequence alignment, knowledge of the score distribution in the biologically relevant high-scoring region is necessary. The score distribution can analytically be shown to follow a Gumbel extreme value distribution for gapless local alignments. For gapped alignments, however, the distribution can only be obtained numerically. To cover the rare-event region of the distribution, studies of the score distribution of pairwise local alignments were done utilising parallel tempering[1]. They showed that, unlike predicted by previous simple sampling approaches, a Gaussian correction to the Gumbel distribution is necessary in case of finite sequence lengths. Here, this study is expanded to sum-of-pair scores of multiple sequence alignments, i.e. the alignments of more than two sequences, with gaps. Results will be shown for the score distributions of local multiple alignments and compared to previous results for global multiple alignments, where regions with probabilities smaller than 10^{-70} could be obtained.

[1] S. Wolfsheimer, B. Burghardt, A.K. Hartmann, *Local sequence alignment statistics: deviations from Gumbel statistics in the rare-event tail*, Algorithms for Molecular Biology (2007)

DY 16.2 Wed 9:45 ZEU 160

Optimising the spatial structure of BLN protein models by means of "partial distortion"-quench cycles — •Florian Günther[1,2,3], Arnulf Möbius[2], and Michael Schreiber[3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [3]Institute of Physics, Technical University Chemnitz, Germany

The prediction of the spatial structure of a protein based on its amino acid sequence is a challenging problem. Corresponding theoretical studies of the protein folding require highly efficient structure optimisation tools. Here we investigate whether and to what extent the thermal cycling (TC) algorithm [1] is appropriate for determining low energy structures of the BLN protein model by J.D. Honeycutt and D. Thirumalai [2]. In our simulations for 46-, 58-, and 69-bead sequences, the TC algorithm reliably finds the global minimum within reasonable computing time. In comparison to the multi-start local search and simulated annealing approaches, TC turns out to be far more efficient.

In the present work, the BLN model with rigid bonds is studied in detail for the first time. Comparing these results to data for the extended model by Berry *et al.* [3], where stiff springs are substituted for the rigid bonds, we observe several level crossings when varying the spring constant, even for quite hard springs.

[1] A. Möbius *et al.*, Phys. Rev. Lett. **79** (1997) 4297.
[2] J.D. Honeycutt and D. Thirumalai, Biopolymers **32** (1992) 695.
[3] R.S. Berry *et al.*, Proc. Natl. Acad. Sci. USA **94** (1997) 9520.

DY 16.3 Wed 10:00 ZEU 160

Stochastic Processes with Delays and Their Application to Gene Regulation and Epidemics — •Tobias Brett and Tobias Galla — The University of Manchester, Manchester, United Kingdom

Many of the systems modeled in biology have memory: not all of the effects of interactions can be well approximated as occurring instantaneously. Examples are transcriptional and translational delays in gene regulation, or recovery periods in the context of infectious diseases. We focus on chemical reaction models with delays. For such processes it is not straightforward to formulate Master equations, and it is not clear how to derive systematic Gaussian approximations. We demonstrate that progress can be made using a path-focused view, based on generating functionals. These do not describe the time-evolution of one-time probability distributions, instead they capture the probabilities of entire paths. We derive analytical expressions for Gaussian approximations for a wide class of delay systems, and apply these to two biological problems in which delay is relevant. One is the susceptible-infective-recovered model in epidemiology and the other a model of delayed autoinhibition in gene regulation. This allows us to characterise the phenomena arising from the combination of intrinsic noise and delayed dynamics.

Reference: T. Brett, T. Galla, Phys. Rev. Lett. **110**, 250601 (2013)

DY 16.4 Wed 10:15 ZEU 160

Environmental effects on DNA denaturation — •Christian von Ferber[1] and Yurij Holovatch[2] — [1]AMRC, Coventry University, Coventry, UK — [2]Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, Lviv, Ukraine

We re-consider the Poland and Scheraga model for the DNA denaturation transition where the double DNA strands locally and then globally detach as the transition temperature is attained. Applying a polymer field theory approach we discuss in particular variants of this transition that may occur due to the properties of the environment. We show that different environments may shift the transition further or less towards a first order transition. Effects we discuss are: the presence of (1) uncorrelated and (2) power-law long-range correlated disorder where the latter influences the transition as function of the power law exponent,(3) quality of the solution which may affect the self- and mutual interaction of both single and double strands, and (4) combinations of these effects. We find that the effects studied significantly influence the transition.

15 min break

DY 16.5 Wed 10:45 ZEU 160

Pattern formation in individual-based systems with time-varying parameters — •Peter Ashcroft and Tobias Galla — The University of Manchester, Manchester, UK

We study the patterns generated in finite-time sweeps across symmetry-breaking bifurcations in individual-based models of evolutionary dynamics and cell differentiation. Similar to the well-known Kibble-Zurek scenario of defect formation, large-scale patterns are generated when model parameters are varied slowly, whereas fast sweeps produce a large number of small domains. The symmetry breaking is triggered by intrinsic noise, originating from the discrete dynamics at the microlevel. Based on a linear-noise approximation, we calculate the characteristic length scale of these patterns. We demonstrate the applicability of this approach in a model of evolutionary game theory with a time-dependent fitness structure, and in a model of cell differentiation, which we relate to Waddington's epigenetic landscape. Our theoretical estimates are confirmed in simulations. In further numerical work, we observe a similar phenomenon when the symmetry-breaking bifurcation is triggered by population growth.

Reference: P. Ashcroft and T. Galla, Phys. Rev. E 88, 062104 (2013)

DY 16.6 Wed 11:00 ZEU 160

A time-continuous model for E. coli's motion using shot noise — •Oliver Pohl[1], Marius Hintsche[2], Carsten Beta[2], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institut für Physik und Astronomie, Universität Potsdam, 14476 Potsdam, Germany

The bacterium Escherichia coli moves with alternating runs and tumbles that occur with a mean tumble rate. In the presence of gradients of a chemoattractant, E. coli performs chemotaxis [1]. It adjusts the tumble rate in response to the time-integrated concentration in order to increase the uptake of the chemical.

We set up a time-continuous model that describes runs and tumbles as a stochastic process of the bacterium's swimming direction and speed. The swimming direction updates according to rotational Brownian motion and additional shot noise, which initiates tumbling events. The speed is not constant as in previous models but is determined by the random shots as well. By analyzing experimental data on swimming trajectories, we adjust the parameters of our model. First, we determine the shot noise from higher moments of the experimental trajectories. Second, we present a novel approach to determine the chemotactic response function, which E.Coli uses to integrate the chemical concentration in time. Finally, we want to use our model to explore the behavior of E. Coli in different chemical concentration profiles.

[1] H.C. Berg, "E.Coli in motion", Springer, New York, (2003)

DY 16.7 Wed 11:15 ZEU 160

Self-propelled particles with alignment and anti-alignment — •Robert Grossmann[1], Pawel Romanczuk[1], Markus Bär[1], and Lutz Schimansky-Geier[2] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]Department of Physics, Humboldt-Universität zu Berlin, Germany

It was recently suggested that the observations of vortex structures in the local polarization of dense bacterial suspensions can be explained by a negative viscosity in the hydrodynamic equation for the polar order parameter [1]. Here, we propose a simple model of self-propelled particles interacting via a short-ranged alignment and a long-ranged anti-alignment, which may exhibit negative viscosity. This simple model allows us to systematically derive a coarse-grained description via a one-particle Fokker-Planck equation [2], and to analyze the relation of hydrodynamic transport coefficients on the microscopic parameters of the model. We explore the impact of different approximations required in the derivation of the coarse-grained theory on the validity of the linearized equations. Furthermore, we verify our results by comparing numerical simulations of the microscopic model with predictions of the coarse-grained theory.

[1] Dunkel, J. et al., New J. Phys., 15, 045016 (2013)
[2] Grossmann, R. et. al, New J. Phys., 15, 085014 (2013)

DY 16.8 Wed 11:30 ZEU 160

Constructing a Stochastic Model of Bumblebee Flights from Experimental Data — Friedrich Lenz[1], Aleksei V. Chechkin[2], and •Rainer Klages[1] — [1]Queen Mary U. of London, School of Math. Sci., UK — [2]Inst. f. Theor. Physics, NSC KIPT, Kharkov, Ukraine

The movement of organisms is subject to a multitude of influences of widely varying character: from the bio-mechanics of the individual, over the interaction with the complex environment many animals live in, to evolutionary pressure and energy constraints. As the number of factors is large, it is very hard to build comprehensive movement models. Even when movement patterns in simple environments are analysed, the organisms can display very complex behaviours. While for largely undirected motion or long observation times the dynamics can sometimes be described by isotropic random walks, usually the directional persistence due to a preference to move forward has to be accounted for, e.g., by a correlated random walk. We generalise these descriptions to a model in terms of stochastic differential equations of Langevin type, which we use to analyse experimental search flight data of foraging bumblebees [1]. Using parameter estimates we discuss the differences and similarities to correlated random walks. From simulations we generate artificial bumblebee trajectories which we use as a validation by comparing the generated ones to the experimental data [2]

[1] T.C.Ings, L.Chittka, Curr. Biol. **18**, 1520 (2008)
[2] F.Lenz, A.V.Chechkin, R.Klages, PLoS ONE **8**, e59036 (2013)

DY 16.9 Wed 11:45 ZEU 160

Swarming of self-propelled agents with selective attraction-repulsion interaction - From microscopic dynamics to coarse-grained theories — •Pawel Romanczuk[1], Robert Grossmann[1], and Lutz Schimansky-Geier[2] — [1]Physikalisch-Technische Bundesanstalt, Berlin — [2]Department of Physics, Humboldt Universität zu Berlin

We propose a model of stochastic self-propelled agents interacting via selective attraction-repulsion interaction, where individuals respond differently to their neighbours depending on their relative state of motion (approach versus movement away) [1]. This kind of social response is directly motivated by visual sensory information available to individuals (e.g. looming stimuli). We show that the model exhibits various modes and collective behaviour and derive a coarse-grained description via a non-linear Fokker-Planck equation, which allows us to formulate hydrodynamic equations for the density and velocity fields of the Toner-Tu type [2]. Finally, we compare the predictions on the linear stability from our coarse-grained theory with the results of individual-based simulations of the microscopic model, and discuss the limitations of the hydrodynamic theory and its region of validity.

[1] Romanczuk P. and Schimansky-Geier L., Interface Focus 2, 746-756 (2012)
[2] Grossmann R., Schimansky-Geier L., Romanczuk P., New J Phys 15, 085014, (2013)