DY 54: Statistical Physics of Biological Systems I (joint session BP/DY)

Time: Thursday 9:30–13:00 Location: H 2013

DY 54.1 Thu 9:30 H 2013

Thermodynamic bounds on the ultra- and infra-affinity of Hsp70 for its substrates — •Basile Nguyen[1,2], David Hartich[1], Paolo De Los Rios[2], and Udo Seifert[1] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, Stuttgart, Germany — [2]Laboratory of Statistical Biophysics, Institute of Physics, School of Basic Science and Institute of Bioengineering, School of Life Sciences, École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

The 70 kDa heat shock protein Hsp70 has several essential functions in living systems, such as protecting cells against protein aggregation, assisting protein folding, remodeling protein complexes, and driving translocation into organelles. These functions require high affinity for nonspecific amino acid sequences that are ubiquitous in proteins. It has been recently shown that this high affinity, called ultra-affinity, depends on a process driven out of equilibrium by ATP hydrolysis. Here, we establish the thermodynamic bounds for ultra-affinity, and further show that the same reaction scheme can in principle be used both to strengthen and to weaken affinities (leading in this case to infra-affinity). We show that cofactors are essential to achieve affinity beyond the equilibrium range. Finally, we consider small GTPases which can benefit from infra-affinity to optimize intracellular signal transduction.

[1] B. Nguyen, D. Hartich, U. Seifert and P. De Los Rios (2017), *Biophys. J.* 113, 362-370

DY 54.2 Thu 9:45 H 2013

A reaction center driven by entropy — •Franz-Josef Schmitt, Zuleyha Yenice Campbell, Mai Vi Bui, and Thomas Friedrich — Technische Universität Berlin, Sekr. PC 14, Straße des 17. Juni 135, 10623 Berlin

The phototrophic cyanobacterium *Halomicronema hongdechloris* contains chlorophyll *a* and *f* in photosystem II. The ratio of Chl *f* to Chl *a* is reversibly changed from 1:8 under illumination with far red light (720-730 nm) to a very low level of Chl *f* under white-light culture conditions. Phycobiliproteins exhibit highly efficient excitation energy transfer (EET) to Chl *a* and from there to Chl *f* within 200 ps apparent transfer time if *H. hongdechloris* grown under far red light is illuminated with 630 nm laser radiation which is absorbed by phycobilisomes. However excitation energy localized on Chl *f* shows long lifetime of more than 1 ns. Questions arise about composition of the reaction center and possible primary charge separation driven by Chl *f*. Our Simulations and thermodynamic considerations suggest that the time- and wavelength-resolved ps fluorescence data can be explained assuming light-induced far red-shifted traps of excitation energy localized on Chl *f* in the light harvesting antenna while the large majority of Chl *a* is strongly coupled to these Chl *f* traps driving the uphill EET from Chl *f* to Chl *a* by entropic force.

DY 54.3 Thu 10:00 H 2013

Shape of pinned polymer loops in an external force field — •Wenwen Huang[1], Yen Ting Lin[2], and Vasily Zaburdaev[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Los Alamos National Laboratory, New Mexico, USA

We studied the shapes of pinned polymer loops subjected to a constant external force field. We show that the polymer density profile can be calculated analytically in agreement with the simulation results. Moreover, we calculated the distribution of gyration radius and found it to vary non-monotonically with the strength of the external force field: the distribution is broader for moderate forces and more narrow for strong and weak forces. Furthermore, we analyzed the gyration tensor of the polymer loop characterizing its overall shape and in particular two parameters called asphericity and the nature of asphericity. These parameters, along with the gyration radius, can be used to quantify experimental data.

DY 54.4 Thu 10:15 H 2013

The labyrinth-like shapes of nasal cavities arise from physical and geometrical constraints — •David Zwicker[1,2], Rodolfo Ostilla-Mónico[2], Daniel E. Lieberman[2], and Michael P. Brenner[2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Harvard University, Cambridge, USA

Although the nasal cavity is vital for heating and humidifying inhaled air in all vertebrates, its shape varies widely across animals. To understand this variability, we here connect nasal geometry to its function by theoretically studying the airflow and the associated scalar exchange that describes heating and humidification. We show that optimal geometries, which have minimal resistance for a given exchange efficiency, are narrow with a uniform gap width. Our prediction for the gap width matches measured values over a large range of animal sizes. Moreover, we show that geometric constraints imposed by the head can be satisfied with the observed labyrinth-like geometries, which perform almost as well as the optimal shapes without the constraints. Taken together, our theory explains the geometric variations of natural nasal cavities quantitatively and we hypothesize that the trade-off between high exchange efficiency and low resistance to airflow is the main driving force shaping the nasal cavity.

DY 54.5 Thu 10:30 H 2013

Cell polarization in elliptical geometry: how does C. Elegans determine its first axis? — •Raphaela Gessele, Jacob Halatek, and Erwin Frey — Department of Physics, Ludwig-Maximilians-Universität München, 80333 Munich, Germany

Cell polarity defines axes that guide cell differentiation and division. In the single cell state of the Caenorhabditis Elegans embryo, PAR protein patterns determine the anterior-posterior axis which further guides the first cleavage. Experiment and theory have indicated that mutual binding inhibition of (anterior) aPAR and (posterior) pPAR proteins is the key mechanism of polarity maintenance by the PAR reaction-diffusion network. Strikingly, our analysis of the reaction-diffusion dynamics in (elliptical) cellular geometry shows that mutual inhibition alone does not lead to a stable polarity along the long (anterior-posterior) axis of the cell but generically favors polarity by aPAR and pPAR protein domains aligned with the short axis. We find that the geometry adaption of the patterning process depends on an intricate interplay between attachment-detachment dynamics on the one hand, and cytosolic reactivation on the other hand. Our findings show that the local ratio of membrane surface to cytosolic bulk volume is the main geometric cue to which patterns adapt. Furthermore, an inactive phase after membrane detachment can switch the preferred polarity axis - The decisive parameter for switching is the diffusion length of the inactive phase. In conclusion, our studies reveal the crucial role of geometry for self-organized pattern formation. Geometry should be explicitly considered in models for intracellular pattern formation.

DY 54.6 Thu 10:45 H 2013

A Spheroidal Squirmer in Shear Flow — •Kai Qi[1], Elmar Westphal[2], Gerhard Gompper[1], and Roland G. Winkler[1] — [1]Theoretical Soft Matter and Biophysics, Institute for Advanced Simulation and Institute of Complex Systems, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Jülich Centre for Neutron Science, Forschungszentrum Jülich, D-52425 Jülich, Germany

Squirmers are generic models for microswimmers like bacteria and algae. The behavior of a spheroidal squirmer [1, 2] in shear flow is studied by hydrodynamic simulations via the multiparticle collision dynamics [3] approach. Due to the elongated shapes of spheroids, alignment along the shear direction is observed for both passive spheroidal colloids and squirmers in the weak shear flow. When the shear rate exceeds a critical value, alignment changes from the shear to the vorticity direction. The alignment transition reveals a clear dependence on the hydrodynamic dipole of the swimmer's flow field. Pullers with a large positive force-dipole coefficient exhibit gradual variations of the alignment direction, whereas abrupt changes are found for pushers with a large negative coefficient. Comparison between elongated and spherical squirmers reveals a significant shape dependence of their behaviors in shear flow.

[1] M. Theers, E. Westphal, G. Gompper, and R. G. Winkler, Soft Matter **12**, 7372 (2016).

[2] J. Elgeti, R. G. Winkler, and G. Gompper, Rep. Prog. Phys. **78**, 056601 (2015).

[3] G. Gompper, T. Ihle, D. M. Kroll, and R. G. Winkler, Adv. Polym. Sci. **221**, 1 (2009).

15 min. break

Invited Talk DY 54.7 Thu 11:15 H 2013

Protein Pattern Formation: Rethinking Nonlinear Dynamics — •Erwin Frey — Ludwig-Maximilians-Universität München, München, Germany

Protein pattern formation is essential for spatial organization of many intracellular processes like cell division, flagellum positioning, and chemotaxis. More generally, these systems serve as model systems for self-organization, one of the core principles of life. We present a rigorous theoretical framework able to generalize and unify pattern formation for quantitative mass-conserving reaction-diffusion models. Within this framework, separation of diffusive mass redistribution on the level of conserved species provides a general mathematical procedure to decompose complex reaction-diffusion systems into effectively distinct functional units, and to reveal the general underlying bifurcation scenarios. We apply this general framework to a range of specific intracellular pattern forming protein networks, and show how it facilitates the identification of general self-organisation principles.

DY 54.8 Thu 11:45 H 2013

Self-organised length oscillations of cellular protrusions — Mareike Bojer[1,2], •Isabella Graf[1], and Erwin Frey[1] — [1]Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Munich, Germany — [2]present address: Department of Physics, Technische Universität München, Garching, Germany

We consider a stochastic non-equilibrium model which is inspired by the interplay of directed transport and diffusive motion of molecular motors in growing and shrinking cellular protrusions like filopodia. Based on this model we investigate the effect of finite diffusion in a half-closed geometry and show that it can lead to temporal patterns in the form of oscillating system length. We examine the dynamics of the system length in terms of the growth rate of the protrusion and identify two different limits: For small growth rate, the system length changes very stochastically and our analytic prediction, using a so-called adiabatic assumption, agrees well with the result from numerical simulations. For larger growth rate, however, temporal patterns occur. More concretely, we observe quasi-periodic changes in length in a parameter regime where motor mixing (diffusion) is slow compared with the shrinkage dynamics. We provide an intuitive picture for the origin of this pattern-forming mechanism which relies on the closure of the system at the dynamic end of the protrusion and the resulting particle conservation.

DY 54.9 Thu 12:00 H 2013

Force sharing between elastically coupled molecular motors — •Mehmet Can Ucar and Reinhard Lipowsky — Max Planck Institute of Colloids and Interfaces, Science Park Golm, 14476 Potsdam, Germany

Molecular motors are nano-scale machines that drive many essential processes within the living cell such as the organization of the mitotic spindle, the powering of flagella and cilia, and the long-distance transport of cellular cargos. These motor proteins frequently work in teams of multiple motors and can collectively generate large forces, but the underlying mechanism of force generation and force sharing remains controversial. Here we address this question by introducing a new model for cargo transport by elastically coupled molecular motors. For a system of two identical motors acting against an antagonistic motor or an optical trap, we find that motors share the generated forces almost equally among the members of the same team. The model furthermore provides a new explanation for observed forces in different in vitro studies.

DY 54.10 Thu 12:15 H 2013

Statistical inference of bacterial chemotaxis strategies — •Maximilian Seyrich[1], Zahra Alirezaei[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

Bacteria like *E. coli* move with alternating runs and tumbles. Modern imaging techniques provide a high-throughput access to these run-and-tumble trajectories. However, good tumble recognition analysis is still a bottleneck and needs to set a-priori threshold parameters. We present a high-throughput inference technique, which allows to infer all swimming parameters of the bacterium without such a need.

We set up a random-walk model that describes runs and tumbles as a stochastic process of the bacterium's swimming direction and speed extending our previous work [1]. The dynamics of the swimming direction is described by enhanced rotational Brownian motion during tumbling, while thermal and shot noise together with a relaxational drift analogously to an Ornstein-Uhlenbeck process govern the speed dynamics. In order to infer the relevant swimming parameters, moments and autocorrelation functions are calculated for our model and matched to the ones determined from experimental trajectories. We first show that our method identifies the classical bacterial chemotaxis strategy of *E. coli*, i.e., the tumble rate decreases when swimming along the chemical gradient. We also find evidence that a fast subpopulation of *E. coli* reduces its mean tumble angle in this direction.

[1] O. Pohl *et al.*, PLoS Comp. Biol. **13**, 1 (2017).

DY 54.11 Thu 12:30 H 2013

Chemoattractant induced transient adaptation in the oscillatory cytoskeleton of motile amoeboid cells. — •Jose Negrete JR[1,2], Alain Pumir[3,4], Christian Westendorf[4], Marco Tarantola[4], Eberhard Bodenschatz[4,5,6], and Carsten Beta[7] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [3]École Normale Supérieure de Lyon, Lyon, France — [4]Max Planck Institute for Dynamics and Selforganization — [5]University of Göttingen, Göttingen, Germany — [6]Cornell University, Ithaca, USA — [7]University of Potsdam, Potsdam, Germany

Dictyostelium discoideum presents oscillatory actin polymerization cycles which amplitude is mostly given by noise. We investigate the transient response on the actin polymerization activity in Dictyostelium discoideum induced by a short pulse of cAMP. The stimulation induces a transient response, of reduced amplitude and frequency, which time duration is stochastic and varies between cells. To model the observed actin behavior, we extend the description of noisy oscillator by introducing an inhibitory variable that acts as a timer for the transient phase.

DY 54.12 Thu 12:45 H 2013

Evolution of carrying capacity and extinction of populations in a stochastic system — •Hye Jin Park[1], Yuriy Pichugin[1], Weini Huang[2], and Arne Traulsen[1] — [1]Max Planck Institute for Evolutionary Biology, Plön, Germany — [2]Barts Cancer Institute, London, United Kingdom

Once a mutant emerges in the population, new interactions are drawn between types, which may lead to changes in the population size. Using the game theory, we implement this population dynamics in a stochastic system. Since interactions between types are described by a game payoff matrix, the emergence of a mutant is interpreted as extending the payoff matrix. New equilibria can emerge by the change of the payoff matrix. If the population settles to a new equilibrium state, the population size changes. We examine the change of population size in time and quantify the extinction risk by the mean time to extinction.