DY 60: Statistical Physics in Biological Systems III

Time: Friday 10:00–11:45 Location: H3

DY 60.1 Fri 10:00 H3

Charting the hydrophobic effect: Computing spatially resolved absolute hydration shell entropies — •Leonard Heinz and Helmut Grubmüller — Department of Theoretical and Computational Biophysics, Max Planck Institute for Biophysical Chemistry, Göttingen

Biophysical systems are governed by their free energy and thus depend on a fine-tuned interplay between enthalpy and entropy. E.g. for protein folding, the solvation contributions are crucial, as they give rise to the hydrophobic effect. A quantitative understanding of the thermodynamics of solvation, and in particular the associated entropies, is therefore essential. While a variety of methods allow assessing the solute entropy, solvation shell entropies are notoriously difficult to obtain from computer simulations, because the shallow energy landscape requires sampling of an extremely large configuration space. Here we solve the sampling problem by exploiting the permutation symmetry of the solvent particles which reduces the configuration space that needs to be sampled by the Gibbs factor 1/N!, leaving the physics of the system unchanged. We perform a mutual information expansion to obtain translational and rotational solvent entropy values from the permutationally reduced trajectory. The expansion yields entropy contributions of individual solvent particles as well as of groups of particles, such as different solvation shells, thereby providing spatial resolution. We tested our method by assessing the solvation of small molecules, such as n-alkanes and small peptides and obtained agreement with other methods and experimental values.

DY 60.2 Fri 10:15 H3

GTPase cascades can perform as both robust switches and biochemical oscillators — •Andreas Ehrmann, Basile Nguyen, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

GTPases regulate a wide range of cellular processes, such as intracellular vesicular transport, signal transduction, and protein translation. These hydrolase enzymes operate as biochemical switches by toggling between an active guanosine triphosphate (GTP)-bound state and an inactive guanosine diphosphate (GDP)-bound state. We compare two switch models, a single-species switch and an interlinked switch that consists of two species coupled through positive and negative feedback loops. We find that interlinked switches are closer to the ideal all-or-none switch and are more robust against input fluctuations. While the single-species switch can only achieve bistability, interlinked switches can be converted into oscillators by tuning the cofactor concentrations. These regimes can only be achieved with sufficient chemical driving, which is associated with GTP hydrolysis. In this study, we provide a minimal thermodynamically consistent model that can achieve bistability and oscillations with the same feedback structure.

DY 60.3 Fri 10:30 H3

Force-dependent diffusion coefficient of molecular Brownian ratchets — •Matthias Uhl and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

We study the mean velocity and diffusion constant in models of molecular Brownian ratchets. Brownian ratchets can be used to describe translocation of biopolymers through nanopores in cells in the presence of molecules that prevent backwards transitions if bound to the polymer strand. We provide an analytical expression for the diffusion constant in the classical model of a translocation ratchet that was first proposed by Peskin et al. [1]. This model is only applicable if the binding and unbinding of the blocking molecules are much faster than the diffusion of the strand. We propose a modified model that is also applicable if the (un)binding rates are finite [2]. Our analysis shows that for large pulling forces the predictions of both models can differ strongly even if the (un)binding rates are large in comparison to the diffusion timescale but still finite. Implications of the thermodynamic uncertainty relation on the efficiency of Brownian ratchets are also discussed.

[1] C. S. Peskin, G. M. Odell, and G. F. Oster, Biophys. J. 65, 316 (1993).
[2] M. Uhl and U. Seifert, Phys. Rev. E 98, 022402 (2018).

DY 60.4 Fri 10:45 H3

Structures and Dynamics of Growing Semi-Flexible Polymer Chains — •Jörn Appeldorn and Reiner Kree — Inst. f. Theo. Physik, Univ. Göttingen, Friedrich-Hund Pl. 1, 37077 Göttingen

Numerous studies have investigated both, the conformational dynamics of semi-flexible polymer chains with fixed length and the dynamics of the chemical growth separately. Here, we study the combined effects, if both processes are characterized by comparable time scales.
We consider irreversible chain growth of a Gaussian semi-flexible polymer with growth laws $\langle N(t)\rangle = \left(\frac{t}{\tau_0}\right)^{\alpha}$ characterized by a power law exponent $0 < \alpha \leq 1.1$. In particular, we study the end-to-end distance, mean square radius of gyration, mean square displacement of monomers, and center of mass position. Results are obtained from numerical simulations using a modified Brownian dynamics algorithm, which makes use of the exact solvability of the Gaussian dynamics and allows us to perform simulations on very long timescales.
For small growth parameters, the polymer chains reach their equilibrium state in between the growth events for all bending stiffnesses. With increasing α, the conformational properties are influenced by the chemical growth and the polymer chains never reach their equilibrium state. The resulting non-stationary properties are systematically studied as a function of ν and α .

DY 60.5 Fri 11:00 H3

Reactive paths and record statistics in complex energy landscapes — David Hartich and •Aljaz Godec — Mathematical Biophysics Group, Max-Planck-Institute for Biophysical Chemistry, Göttingen (GER)

When considering reaction kinetics in a single-molecule setting paradigmatic kinetic rate-based approaches often fail, and an explicit consideration of trajectory-to-trajectory fluctuations is required for a correct theoretical description. Exploiting a recently proven duality between relaxation and first passage processes (Hartich & Godec, *New J. Phys.* **20**, 112002 (2018)) we will review our recent results on the full statics of reactive trajectories. We will demonstrate that traditional rate-based approaches counter-intuitively reflect delocalized and indirect reactive trajectories. We will highlight the striking difference between diffusion-controlled reactions in chemical systems and kinetics in the so-called few-encounter limit relevant for nucleation-limited phenomena. As a second application of the duality we will present large deviation results for the statistics of records. On the hand of selected examples we will discus the relevance of our results for emerging biophysical phenomena at low-copy numbers.

DY 60.6 Fri 11:15 H3

NK Fitness Landscapes Interpolated between K=2 and K=3 — James E Sullivan, Dmitry Nerukh, and •Jens Christian Claussen — Department of Mathematics, Aston University, Birmingham B4 7ET, U.K.

The NK model was introduced by Stuart Kauffmann and coworkers [1] as a model for fitness landscapes with tunable ruggedness, to understand epistasis and pleiotropy in evolutionary biology. It has also raised interest in combinatorial optimisation, study of spinglasses and in organizational theory. In the original formulation, fitness is defined as a sum of fitness functions for each locus, each depending on the locus itself and K other loci. Varying K from $K = 0$ to $K = N - 1$ leads to different ruggedness of the landscape. Here we introduce a generalization that allows to interpolate between integer values of K by allowing K_i to assume different values for each locus. We focus on the interpolation between the most widely studied cases of $K = 2$ and $K = 3$ and characterize the landscapes by study of their local minima. While we largely see a linear interpolation, small deviations are observed. Finally we discuss applications of this approach in economic systems and biology.

[1] Kauffman, S.; Levin, S., Journal of Theoretical Biology. 128, 11 (1987); Kauffman, S.; Weinberger, E., Journal of Theoretical Biology. 141, 211 (1989).

DY 60.7 Fri 11:30 H3

Transport and Free Energy Transduction in Chemical Reaction Pathways far from Equilibrium — •Artur Wachtel and Massimiliano Esposito — Complex Systems and Statistical Mechan-

ics, Physics and Materials Science, University of Luxembourg

The metabolism of living cells extracts useful energy and matter from their food. Recent progress in the understanding of the nonequilibrium thermodynamics of chemical reaction networks [1, 2, 3] allows us to address the thermodynamics in biochemical reaction pathways in a systematic and rigorous way.

In this talk I address two important points: transport far from thermodynamic equilibrium and the transduction of free energy. For the first point I draw a similarity to electrical circuits. This similarity is remarkable because the reactions may operate far from the linear regime, thus currents and thermodynamic forces are no longer linearly related.

Transduction is the defining feature of all thermodynamic machines. In living systems it allows building up of nonequilibrium free energy against its natural tendency to degrade. Here, I provide a systematic identification of free energy transduction in nonlinear biochemical reaction pathways, which also leads to a formal definition of its efficiency.

[1] Polettini & Esposito, J Chem Phys 141, 024117 (2014)
[2] Rao & Esposito, Phys Rev X 6, 041064 (2016)
[3] Wachtel, Rao, & Esposito, New J Phys 20, 42002 (2018)