DY 9: Statistical Physics 2 - organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) und Thomas Speck (Mainz)

Time: Monday 11:00–13:00 Location: DYb

DY 9.1 Mon 11:00 DYb

Path integral approach to strong fluctuations in chemical reaction network dynamics using the Plefka expansion — •Moshir Harsh and Peter Sollich — Institut für Theoretische Physik, Georg-August-Universität, Göttingen, Germany

Biochemical reaction networks such as *gene* regulation, *protein* interaction and signalling pathways involve the participation of just a few copies of some key molecular species. With the advent of modern capabilities in live quantitative fluorescence microscopy and spectroscopy, the dynamics of a number of molecular species in these networks can be observed experimentally. However, inferring dynamical parameters from such data remains a challenge as the trajectories of low copy number species show large fluctuations, causing approximate approaches like the Fokker-Planck equation and moment closure to fail in this regime, while the in principle exact master equation has no general analytical solution.

Here we present an alternative method based on constructing the path integral for the dynamics of a generic reaction network, which is then treated within a Gaussian approximation by constraining the first and the second order statistics of the field variables using the systematic Plefka expansion of the dynamical free energy. We develop the method to treat any system of reactions in full generality and show its applicability and accuracy across a range of example systems. The approximate path integral can also form the basis for making inferences from experimentally measured dynamics.

DY 9.2 Mon 11:20 DYb

Negative dissipation and instability in systems with distributed delay — •Sarah A.M. Loos[1], Simon Hermann[2], and Sabine H.L. Klapp[3] — [1]Universität Leipzig — [2]Humboldt-Universität zu Berlin — [3]Technische Universität Berlin

Many natural and artificial systems are subject to some sort of delay, which can be in the form of a single discrete delay or distributed over a range of times. Here, we discuss the impact of this distribution on (thermo-)dynamical properties of time-delayed stochastic systems. To this end, we study a simple model with white and colored noise, and focus on the class of Gamma-distributed delays which includes a variety of distinct delay distributions typical for feedback experiments and biological systems. A physical application is a colloid subject to time-delayed feedback control, which is, in principle, experimentally realizable by co-moving optical traps. We uncover several unexpected phenomena in regard to the system's linear stability and its thermodynamic properties. First, increasing the mean delay time can destabilize, or stabilize the process, depending on the distribution of the delay. Second, for all considered distributions, the heat dissipation of the controlled system (e.g., the colloidal particle) can become negative, which implies that the delay force extracts energy of the heat bath. This refrigerating effect is particularly pronounced for exponential delay. The exponential delay further yields the largest stable parameter regions. In this sense, exponential delay represents the most effective and robust type of delayed feedback.

DY 9.3 Mon 11:40 DYb

On the fluctuation-dissipation theorem of a buckminster fullerene — •Andreas Baer[1], David Smith[2], and Ana-Sunčana Smith[1,2] — [1]PULS Group, Institute for Theoretical Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Division of Physical Chemistry, Ruđer Bošković Institute, Zagreb, Croatia

The fluctuation-dissipation theorem goes back to the first half of the last century with a lot of work in statistical physics sharpening the limits of applicability [1]. The Stokes-Einstein relation is a direct consequence of the fluctuation-dissipation theorem and was recently, within an experimental study, argued to be valid for dissolved buckminster fullerenes [2], while theoretical and simulation studies deny the applicability at such small scales [3]. We perform both equilibrium and constrained molecular dynamics studies of a buckminster fullerene dissolved in toluene. Retrieving velocity and force autocorrelation functions, we can directly show the failure of the fluctuation-dissipation theorem. Additionally, transport coefficients obtained via the Green-Kubo formalism can be compared to the friction coefficient retrieved from the ratio of pulling force and resulting velocity to test the Stokes-Einstein relation. We outline the most important assumptions of the theory not fulfilled and provide a solution to the apparent contradiction with experimental studies.

[1] Zwanzig, R., *Annu. Rev. Phys.* 1965, **16**, 67-102
[2] Pearson, J. et al., *J. Phys. Chem. Lett.* 2018, **9**, 6345-6349
[3] Schmidt J. R. et al., *J. Phys. Chem. B* 2004, **108**, 21, 6767-6771

DY 9.4 Mon 12:00 DYb

Quantifying configurational information for a stochastic particle in a flow-field — •Evelyn Tang[1] and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

Flow-fields are ubiquitous systems that are able to transport vital signaling molecules necessary for system function. While information regarding the location and transport of such particles is often crucial, it is not well-understood how to quantify the information in such stochastic systems. Using the framework of nonequilibrium statistical physics, we develop theoretical tools to address this question. We observe that rotation in a flow-field does not explicitly appear in the generalized potential that governs the rate of system entropy production. Specifically, in the neighborhood of a flow-field, rotation contributes to the information content only in the presence of strain – and then with a comparatively weaker contribution than strain and at higher orders in time. Indeed, strain and especially the flow divergence, contribute most strongly to transport properties such as particle residence time and the rate of information change. These results shed light on how information can be analyzed and controlled in complex artificial and living flow-based systems.

DY 9.5 Mon 12:20 DYb

Asymmetric nascent Dirac delta functions and their application to probability and mechanics — •Jens Christian Claussen — Department of Mathematics, Aston University, Birmingham, UK

The Dirac delta distribution is ubiquitious from quantum mechanics and statistical physics to Fourier analysis. In theoretical physics lectures, a commonly presented approach uses a series of nascent delta functions which are normalized and localized and converge point-wise to zero except at the origin. For simplicity, nascent delta functions are usually chosen to be even, i.e. $\delta_n(x) = \delta_n(x)$. However, this is not a necessary assumption, and in physical interactions as the inelastic collision of two rigid bodies, the force between the particles as a function of time may follow an asymmetric profile; nevertheless with the total momentum transferred in a Dirac delta pulse in the limit of an infinesimal short interaction time.

Here I discuss asymmetric nascent Dirac delta functions and their implications in probability and physics. The gross advantage of asymmetric nascent delta functions is found in their application to probability theory. By introduction of totally asymmetric nascent delta functions, the inconsistencies of using the Dirac delta in mixed discrete-continuous probability spaces when arriving at the cumulative distribution function are resolved. It is anticipated that asymmetric nascent delta functions find further applications in mathematical physics and the theory of measurement.

DY 9.6 Mon 12:40 DYb

Hilbert space average of transition probabilities — •Nico Hahn, Thomas Guhr, and Daniel Waltner — Faculty of Physics, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

The typicality approach and the Hilbert space averaging method as its technical manifestation are important concepts of quantum statistical mechanics. Extensively used for expectation values we will extend them to transition probabilities. We find that the transition probability of two random uniformly distributed states is connected to the spectral statistics of the considered operator. We will demonstrate our quite general result for a kicked spin chain.