DY 32: Focus Session: Physics of Fluctuating Paths (joint session DY/CPP)

State-of-the-art experiments probe physical observables, such as heat, work or entropy production, empirical densities and currents, on the level of individual, stochastic paths. Such experiments are typically analysed by averaging along a limited number of individual realisations, which leads to substantial uncertainties in estimates. The systematic sample-to-sample fluctuations of such path-observables encode important information about the underlying, microscopic dynamical processes and are therefore a frontier of experimental, theoretical, and computational physics. Recently there has been a surge in the development and applications of path-based concepts across many fields of physics. This focus session complements a symposium and contains contributed talks.

Organized by Aljaz Godec, Udo Seifert, and Peter Sollich

Time: Wednesday 15:00–18:15 Location: ZEU 160

DY 32.1 Wed 15:00 ZEU 160

Towards a stochastic thermodynamics of fields and tracers — •Sarah A.M. Loos[1], Davide Venturelli[2], Benjamin Walter[3], Edgar Roldan[4], and Andrea Gambassi[2] — [1]DAMTP, University of Cambridge, Cambridge, UK — [2]SISSA, Trieste, Italy — [3]Imperial College London, UK — [4]ICTP, Trieste, Italy

Many results of stochastic thermodynamics, including the close connection between entropy production and stochastic heat dissipation, rely on physical assumptions, e.g., break down if there is no clear separation into "fast equilibrium bath degrees of freedom" and "slow nonequilibrium degrees of freedom". In this talk, I will discuss some insights into thermodynamic notions of nonequilibrium systems that do not fall into the usual paradigm of stochastic thermodynamics. In particular, we develop a thermodynamic description for systems consisting of tracer particles coupled to correlated scalar fields with thermal fluctuations in terms of trajectory-wise energy flows of the particle and the field, as well as the joint entropy production rate measured by path-probability ratios. As an illustration, we consider the case in which the particle is dragged by a harmonic trap through a complex medium described by a fluctuating Gaussian field. Using a perturbative approach, we uncover three dynamical regimes with distinct scaling behavior of the power and discuss the heat dissipation occurring within the field.

DY 32.2 Wed 15:15 ZEU 160

Fluctuation theorem for time reversal markers — •Gabriel Knotz, Till M. Muenker, Timo Betz, and Matthias Krüger — Fakultät für Physik, Georg-August-Universität, Göttingen, Germany

The analysis of particle trajectories is of high theoretical and experimental interest. Especially if hidden degrees are present, detecting broken detailed balance is a challenging task. We introduce and analyze a class of observables with certain symmetry properties under time reversal of trajectories that detect the breakage of detailed balance. Further, these observables fulfill a new form of fluctuation theorem and, under certain conditions, this fluctuation theorem provides bounds and relations for the total change in entropy. These findings are not limited to Markov or overdamped dynamics.

DY 32.3 Wed 15:30 ZEU 160

Necessity for Coarse Graining Empirical Densities and Currents in Continuous Space — •Cai Dieball and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Goettingen, Germany

We present general results on fluctuations and spatial correlations of the coarse-grained empirical density and current of diffusion in equilibrium or non-equilibrium steady states on all time scales. The time averaging and coarse graining hardwired in the definition of the functionals under consideration give rise to experimentally relevant but highly non-trivial statistics. We unravel a deep connection between current fluctuations and generalized time-reversal symmetry. We highlight the essential role of coarse graining in space from mathematical, thermodynamical, and experimental points of view. Spatial coarse graining is required to uncover salient features of currents that break detailed balance, and a thermodynamically "optimal" coarse graining ensures the most precise inference of dissipation. Defined without coarse graining, the fluctuations of empirical density and current are proven to diverge on all time scales in dimensions higher than one, which has far-reaching consequences for large-deviation limits in continuous space and for continuum limits of Markov-jump processes. Our findings provide new intuition about time-averaged observables and allow for a more efficient analysis of single-molecule experiments.

References: Phys. Rev. Lett. 129, 140601 (2022) and Phys. Rev. Research 4, 033243 (2022)

DY 32.4 Wed 15:45 ZEU 160

How Stickiness Can Speed Up Diffusion in Confined Systems — Arthur Alexandre[1], Matthieu Mangeat[2], •Thomas Guérin[1], and David Dean[1] — [1]Laboratoire Ondes et matière d'Aquitaine, CNRS/University of Bordeaux, F-33400 Talence, France — [2]Center for Biophysics and Department for Theoretical Physics, Saarland University, D-66123 Saarbrücken, Germany

The paradigmatic model for heterogeneous media used in diffusion studies is built from reflecting obstacles and surfaces. It is well known that the crowding effect produced by these reflecting surfaces slows the dispersion of Brownian tracers. In this talk, using a general adsorption desorption model with surface diffusion, we present an analytical theory showing that making surfaces or obstacles attractive can accelerate dispersion. In particular, we show that this enhancement of diffusion can exist even when the surface diffusion constant is smaller than that in the bulk. Even more remarkably, this enhancement effect occurs when the effective diffusion constant, when restricted to surfaces only, is lower than the effective diffusivity with purely reflecting boundaries. We give analytical formulas for this intriguing effect in periodic arrays of spheres as well as undulating microchannels. Our results are confirmed by numerical calculations and Monte Carlo simulations. [Ref: How Stickiness Can Speed Up Diffusion in Confined Systems, Phys Rev Lett 128 210601 (2022)]

DY 32.5 Wed 16:00 ZEU 160

From trajectories to models: data-driven approaches to decipher the stochastic dynamics of living systems — •Pierre Ronceray — Turing Centre for Living Systems, CINaM, CNRS, Aix-Marseille University, France

Stochastic differential equations are often used to model the dynamics of living systems, from Brownian motion at the molecular scale to the dynamics of cells and animals. How does one learn such models from experimental data? This task faces multiple challenges, from information-theoretical limitations to practical considerations. I will present a recent and ongoing effort to develop new methods to reconstruct such stochastic dynamical models from experimental data, with a focus on robustness and data efficiency. This provides a generic means to quantify complex behavior and unfold the underlying mechanisms of an apparently erratic trajectory.

DY 32.6 Wed 16:15 ZEU 160

Entropons as vibrational excitations in active solids — •Lorenzo Caprini[1], Umberto Marini Bettolo Marconi[2], Andrea Puglisi[3], and Hartmut Löwen[1] — [1]Heinrich-Heine-Universität Düsseldorf — [2]Scuola di Scienze e Tecnologie, University of Camerino — [3]Istituto dei Sistemi Complessi, CNR

We study the vibrational properties of non-equilibrium active crystals, i.e. solids formed by active particles, that are intrinsically out of equilibrium and governed by entropy production. As known in solid-state physics, equilibrium crystals are characterized by basic collective excitations with thermal origins that are named phonons. In this talk, I will show that active crystals are described by additional vibrational excitations that we called 'entropons' because each of them represents a mode of spectral entropy production. Entropons coexist with phonons and dominate over them for large activity, i.e. when the solid is far from equilibrium, while they vanish in equilibrium conditions. Their existence can be verified in experiments on dense self-propelled colloidal Janus particles and granular active matter, as well as in living systems such as dense cell monolayers.

15 min. break

DY 32.7 Wed 16:45 ZEU 160

Inferring Fractional Processes Using Path Integrals — •Johannes A. Kassel[1], Benjamin Walter[2], and Holger Kantz[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Imperial College London, London, UK

We present a method for inferring overdamped nonlinear Langevin equations driven by multiplicative fractional Gaussian noise from single-trajectory time series. Constructing a maximum-likelihood estimator, we simultaneously infer the nonlinear deterministic force term and the space-dependent diffusion term. We illustrate our method using artificial time series. We observe that Markovian modeling of long-range correlated data leads to a substantial underestimation of the deterministic force term while for anti-correlated data it leads to an overestimation of the force term.

DY 32.8 Wed 17:00 ZEU 160

Kinetics of Imperfect Reactions for non-Markovian Random Walks — •Toni Vieira Mendes and Thomas Guérin — Laboratoire Ondes et Matière d'Aquitaine, Université de Bordeaux

Most transport influenced reactions between two random walkers are usually imperfect, i.e., they do not occur at first contact between the reactants. For such imperfect reactions, recent work has been made to determine the statistics of first reaction time for Markovian random walkers in confinement. However, a lot of physical random walks are actually non-Markovian, i.e., their movement in the future depend on the trajectory they have followed up to then, thus displaying memory effects. These memory effects can be seen, for example, for beads moving inside complex fluids where the force fields do not equilibrate instantly. In this contribution, we describe an analytical theory giving access to the mean reaction time for imperfect reactions for random walkers with memory in confinement. Our theory clearly shows that, contrary to the Markovian case, the reaction time is not the sum of the mean first passage time and the time to react once within reactive distance. We show that the results of our theory match the results of simulations for both one and two dimensions. Then, the equations are analytically solved in the limit of weakly non-Markovian processes. Remarkably, in the limit of weakly reactive targets for fractional Brownian Motion, we find that the mean reaction time displays a non-trivial scaling as a function of the reactivity.

DY 32.9 Wed 17:15 ZEU 160

Instantons and the Path to Intermittency in Turbulent Flows — •André Fuchs[1], Corentin Herbert[2], Joran Rolland[3], Matthias Wächter[1], Freddy Bouchet[2], and Joachim Peinke[1] — [1]Institute of Physics and ForWind, University of Oldenburg, Küpkersweg 70, 26129 Oldenburg, Germany — [2]Université de Lyon, Ens de Lyon, Université Claude Bernard, CNRS, Laboratoire de Physique, F-69364 Lyon, France — [3]Université de Lille, CNRS, ONERA, Arts et Métiers Institute of Technology, Centrale Lille, UMR 9014 - LMFL - Laboratoire de Mécanique des fluides de Lille - Kampé de Fériet, F-59000 Lille, France

Processes leading to anomalous fluctuations in turbulent flows, referred to as intermittency, are still challenging. We consider cascade trajectories through scales as realizations of a stochastic Langevin process for which multiplicative noise is an intrinsic feature of the turbulent state. The trajectories are conditioned on their entropy exchange. Such selected trajectories concentrate around an optimal path, called instanton, which is the minimum of an effective action. The action is derived from the Langevin equation, estimated from measured data. In particular instantons with negative entropy pinpoint the trajectories responsible for the emergence of non-Gaussian statistics at small-scales.

DY 32.10 Wed 17:30 ZEU 160

A nonadiabatic generalized-dividing-surface instanton rate theory — •Rhiannon A. Zarotiadis, Joseph E. Lawrence, and Jeremy O. Richardson — Lab. für Physikalische Chemie, ETH Zürich, Zürich, Switzerland.

The accurate prediction of quantum rate processes is fundamental to our understanding of chemical reactions, but exact calculations are extremely costly. To make them tractable many chemical processes are described within the Born-Oppenheimer (BO) approximation, which assumes strong coupling between the diabatic states, and BO instanton theory is known to capture nuclear quantum effects for these systems well [1]. Alternatively, some systems are better captured by Fermi's golden rule, which is appropriate in the opposite limit of weak coupling.

Nevertheless, many reactions are in neither of these two limits, and so a universal rate theory is desirable. We introduce a new nonadiabatic generalized-dividing-surface instanton approach rigorously derived from the flux-flux correlation function. Our new theory correctly recovers the weak- and strong-coupling limits and goes beyond existing, ad hoc attempts to describe general, nonadiabatic rate processes.

Instanton rate theories [1] have already resolved many longstanding discrepancies between experiment and theory [2] and this new rate theory will be key to address processes beyond their scope such as proton-coupled electron transfer reactions.

[1] Richardson, J. O., Int. Rev. Phys. Chem., 2018, 37:2, 171-216.

[2] Zarotiadis, R. A., Fang, W., Richardson, J. O., Phys. Chem. Chem. Phys., 2020, 22, 10687.

DY 32.11 Wed 17:45 ZEU 160

Sojourn probabilities for diffusive dynamics with state-dependent friction: Theory and experiment — Alice Thorneywork[1,2], Jannes Gladrow[2,3], Ulrich F. Keyser[2], Ronojoy Adhikari[4], and •Julian Kappler[4,5] — [1]Department of Chemistry, University of Oxford, Oxford, United Kingdom — [2]Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom — [3]Microsoft Research, Cambridge, United Kingdom — [4]Department of Applied Mathematics and Theoretical Physics, Cambridge University, Cambridge, United Kingdom — [5]Fakultät für Physik, Ludwig-Maximilians-Universität, München, Germany

The trajectories of diffusion processes are continuous but nondifferentiable, and each occurs with vanishing probability. This introduces a gap between theory, where path probabilities are used in many contexts, and experiment, where only events with nonzero probability are measurable. We bridge this gap by considering the sojourn probability, i.e. the probability for diffusive trajectories to remain within a tube of small but finite radius around a smooth path. For systems with state-dependent diffusivity, we show that the sojourn probability is characterized by a functional that is different from all previously reported multiplicative-noise stochastic actions. We corroborate our theoretical results by comparison to experimentally measured sojourn probabilities for a colloidal particle in a corrugated microchannel. Our work directly connects the discussion of path probabilities for diffusive dynamics with state-dependent friction to physical observables.

DY 32.12 Wed 18:00 ZEU 160

Optimality of non-conservative driving in discrete systems — •Jonas Fritz and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

A fundamental problem in stochastic thermodynamics is that of optimal driving. The goal is to drive a system from some specified initial state to a specified final state, while minimizing entropy production (or work performed) along the trajectory. As shown recently [1], the optimal protocol in a cyclical Markov network has a non-conservative force, i.e. non-zero cycle affinity, which is in contrast to continuous systems. However, the reduction in entropy production from such a non-conservative force has been numerically found to be at most on the order of 10^{-2} for the case of the three state cycle. We investigate why this is the case, by systematically varying step size and initial conditions numerically for the simple case of the three state cycle. Further, we try to maximize the improvement in entropy production through the non-conservative force. By increasing the number of states in the cycle, we find a possible improvement which is an order of magnitude larger than the previously known one. We attempt to find a lower bound for the possible improvement through non-conservative driving, by analyzing the scaling behavior of the underlying quantities.

[1] Benedikt Remlein and Udo Seifert, Phys. Rev. E 103, L050105