DY 28: Extreme Events, Glasses and Miscellaneous

Time: Wednesday 11:15–13:00 Location: H19

DY 28.1 Wed 11:15 H19

Symmetries and zero modes in sample path large deviations — •Timo Schorlepp[1], Tobias Grafke[2], and Rainer Grauer[1] — [1]Institute for Theoretical Physics I, Ruhr-University Bochum, Bochum, Germany — [2]Mathematics Institute, University of Warwick, Coventry, United Kingdom

Sharp large deviation estimates for stochastic differential equations with small noise, based on minimizing the Freidlin-Wentzell action functional under appropriate boundary conditions, can be obtained by integrating certain matrix Riccati differential equations along the large deviation minimizers or instantons, either forward or backward in time. Previous works in this direction often rely on the existence of isolated minimizers with positive definite second variation. By adopting techniques from field theory and explicitly evaluating the large deviation prefactors as functional determinant ratios using Forman's theorem, we extend the approach to general systems where degenerate submanifolds of minimizers exist. The key technique for this is a boundary-type regularization of the second variation operator. This extension is particularly relevant if the system possesses continuous symmetries that are broken by the instantons. We find that removing the vanishing eigenvalues associated with the zero modes is possible within the Riccati formulation and amounts to modifying the initial or final conditions and evaluation of the Riccati matrices. We apply our results in multiple examples including a dynamical phase transition for the average surface height in short-time large deviations of the one-dimensional Kardar-Parisi-Zhang equation with flat initial profile.

DY 28.2 Wed 11:30 H19

Diffusivity dependence of the transition path ensemble — Lukas Kikuchi, Ronojoy Adhikari, and •Julian Kappler — DAMTP, Cambridge University, Cambridge, UK

Transition pathways of stochastic dynamical systems are typically approximated by instantons. Here we show, using a dynamical system containing two competing pathways, that at low-to-intermediate temperatures, instantons can fail to capture the most likely transition pathway. We construct an approximation which includes fluctuations around the instanton and, by comparing with the results of an accurate and efficient path-space Monte Carlo sampling method, find this approximation to hold for a wide range of temperatures. Our work delimits the applicability of large deviation theory and provides methods to probe these limits numerically.

DY 28.3 Wed 11:45 H19

Sampling Rare Event Energy Landscapes via a Birth-Death Process — •Benjamin Pampel[1], Simon Holbach[2], Lisa Hartung[2], and Omar Valsson[1,3] — [1]Max-Planck-Institute für Polymerforschung, Ackermannweg 10, 55128 Mainz — [2]Institut für Mathematik, Johannes Gutenberg-Universität Mainz, Staudingerweg 9, 55099 Mainz — [3]Department of Chemistry, University of North Texas, Denton, TX, USA

We investigate a novel sampling algorithm that augments Langevin dynamics with birth-death moves. This is a modification of a previously proposed algorithm [arXiv:1905.09863] that provides an approximation of a stochastic birth-death process for a particle-based implementation. The method connects multiple parallel Langevin dynamics simulations of the same system with a birth-death scheme to facilitate global sampling according to the equilibrium distribution. We investigate the algorithm theoretically, implement it into a custom molecular simulation code, and test it via numerical simulations. We also examine the behavior of the algorithm under change of parameters. In this process, we observe the desired sampling for all tested systems. We find that the performance of the method is independent of the intrinsic time scales and barriers of the system, which is favorable for systems with processes on long time scales.

DY 28.4 Wed 12:00 H19

MD simulations of partially frozen water in silica nanopores — •Sebastian Kloth and Michael Vogel — TU Darmstadt, Institut für Physik kondensierter Materie, Hochschulstr. 6, 64289, Darmstadt, Germany

The properties of confined water are of enormous importance in nature and technology. In particular, the effects of partial freezing on structure and dynamics is highly relevant for, e.g. geology, cryopreservation and our understanding of the glass transition of water [1]. A powerful tool to study structural and dynamical properties of confined liquids are MD simulations [2]. We use this method to gain a better understanding of the effect of partial crystallization on the properties of confined water. A series of silica confinements with and without an artificially frozen crystalline core were prepared and the remaining liquid water layer was analyzed. Dynamics and structures of liquid layers with various thicknesses and their temperature dependencies are determined and compared to those with interfacial layers in the absence of a frozen crystalline core. We show that partial crystallization has substantial effects on the properties of confined water. Additionally the simulation results are used to calculate spectral densities of water dynamics for comparison with results of experimental studies. In particular, we explore which model for the functional form of the spectral density should be used in NMR spin-lattice relaxation studies on the dynamics of completely liquid or partially frozen water in nanopores.
[1] Cerveny, S. et al., Chem. Rev., **2016**, *116* (13) 7608-7625
[2] Horstmann, R. et al., Langmuir, **2022**, 10.1021/acs.langmuir.2c00521

DY 28.5 Wed 12:15 H19

Driven aging dynamics on sparse networks — •Benedikt Johannes Grüger[1], Diego Tapias[1], and Peter Sollich[1,2] — [1]Institute for Theoretical Physics, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [2]Department of Mathematics, King's College London, London WC2R 2LS, UK

We investigate the interaction of two paradigmatic ways of being out of equilibrium, aging and driving, in simple models of glassy dynamics. We specifically consider the Bouchaud model, where a system jumps between the numerous minima of a rough energy landscape in configuration space. As the temperature decreases, the system undergoes a dynamical phase transition, at which the relaxation time diverges. With an additional field, we then drive the system by biasing its dynamics towards higher/lower jumping activity. We investigate the spectrum of the (biased) master operator in that framework, using a population dynamics algorithm based on cavity theory that allows us to deduce statements about the thermodynamic limit. Combining this with extensive diagonalization we identify novel regimes in the bias-temperature phase diagram that are distinguished by the occurrence of different kinds of eigenvector localization and are linked to the existence of a spectral gap. We also present methodological advances in the form of novel strategies for operating the population dynamics algorithm.

DY 28.6 Wed 12:30 H19

Moiré-pattern evolution couples rotational and translational friction at crystalline interfaces — •Xin Cao[1], Andrea Silva[2,3], Emanuele Panizon[4], Andrea Vanossi[2,3], Nicola Manini[5], Erio Tosatti[2,3,4], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, 78464 Konstanz, Germany — [2]CNR-IOM, Consiglio Nazionale delle Ricerche - Istituto Officina dei Materiali, c/o SISSA, Via Bonomea 265, 34136, Trieste, Italy — [3]International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy — [4]The Abdus Salam International Centre for Theoretical Physics (ICTP), Strada Costiera 11, 34151 Trieste, Italy — [5]Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy

We experimentally and theoretically study the rotational dynamics and depinning of two-dimensional colloidal crystalline clusters on periodically corrugated surfaces under well-controlled torques. We demonstrate that the traversing of locally commensurate areas of the moiré pattern through the edges of clusters, which is hindered by potential barriers during cluster rotation, eventually controls its rotational depinning. The experimentally measured depinning thresholds as a function of cluster size strikingly collapse onto a universal theoretical curve which predicts a superlow-static-torque state for large clusters. We further reveal a cluster-size-independent rotation-translation depinning transition when lattice-matched clusters are driven jointly by a force and a torque. Our work provides guidelines to the design of nanomechanical devices that involve rotations on atomic surfaces.

DY 28.7 Wed 12:45 H19

Accurate dynamics from memory in chemical reactions with

small copy numbers — •Moshir Harsh and Peter Sollich — Institut für Theoretische Physik, Georg-August-Universität Göttingen

Chemical reactions in the regime of small copy numbers of species such as *gene* regulation or *protein* interaction networks show large fluctuations, making mean field solutions as given by mass action kinetics unreliable. Accurate calculations of the one and two-time quantities of these stochastic processes remain a challenging problem; numerical solutions to the master equation or stochastic simulations can be deployed, but these are computationally intensive and do not allow likelihood inference from dynamical trajectories.

Here, we present a method that captures the fluctuations beyond mean field using self-consistently determined *memory*: by integrating information from the past we can systematically improve our approximation for the dynamics of chemical reactions. This memory is not added ad-hoc, but can be shown to arise naturally by considering the effective action of the Doi-Peliti field theory of chemical reactions. The effective action is treated perturbatively but we can self-consistently resum a very large class of diagrams resulting in a stable expansion. We demonstrate this method and its accuracy on single and multi-species binary reactions across a range of parameter values. We show how this approach also opens a route to making inferences from experimentally measured dynamics.