DY 56: Brownian Motion and Anomalous Diffusion

Time: Friday 9:30–12:45 Location: ZEU 160

DY 56.1 Fri 9:30 ZEU 160

Odd Diffusion of Interacting Particles — •Erik Kalz[1], Hidde Derk Vuijk[2], Iman Abdoli[2], Jens-Uwe Sommer[2,3], Hartmut Löwen[4], Ralf Metzler[1], and Abhinav Sharma[2,3] — [1]Universität Potsdam, Institut für Physik und Astronomie — [2]Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere — [3]Technische Universität Dresden, Institut für Theoretische Physik — [4]Heinrich Heine-Universität Düsseldorf, Institut für Theoretische Physik II: Weiche Materie

It is generally believed that collisions of particles reduce the self-diffusion coefficient, closely related to autocorrelation functions, which are assumed to decay monotonously in the overdamped limit. We show that these beliefs are only limiting cases in odd-diffusive systems, which are characterized by diffusion tensors with antisymmetric offdiagonal elements. We show that in the dilute limit, particle interactions can reduce, unalter and even enhance the self-diffusion. The underlying particle dynamics thereby can be captured by the force autocorrelation function. We show that this autocorrelation function exhibits a variety of behaviour: (a) even in the dilute limit where collisions are rare, the correlation can become negative, (b) despite the overdamped dynamics, the force autocorrelation can exhibit temporal oscillations and (c) the long-time power-law decay of the force autocorrelation depends on the odd-diffusion parameter. Odd diffusivity, therefore, shines new light on fundamental beliefs in overdamped systems.

Kalz, Erik, et al. Collisions enhance self-diffusion in odd-diffusive systems. Physical Review Letters 129.9 (2022): 090601.

DY 56.2 Fri 9:45 ZEU 160

Bounding Uncertainty of Empirical First-Passage Times of Reversible Markov Processes — •Rick Bebon and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

First-passage phenomena are ubiquitous in nature and are at the heart of, e.g. reaction kinetics, cell signaling, gene regulation, foraging behavior of animals, and stock option dynamics. Whereas theoretical studies typically focus on predicting statistics for a given process, practical applications often aim at inferring, e.g. mean first-passage times (i.e. inverse kinetic rates) from experimental or simulation data. The inference of mean first-passage times is challenging because only a small number of realizations is usually available, in turn leading to high uncertainties and non-Gaussian errors. We derive universal concentration inequalities for first-passage times of ergodic reversible Markov processes on discrete and continuous-state spaces. For a sample of $n \geq 1$ independent realizations of the first-passage process, we prove a Cramér-Chernoff-type bound on the probability that the inferred sample mean deviates from the true mean first-passage time by more than any given amount. We further construct reliable non-asymptotic estimation guarantees, such as confidence intervals valid for all sample sizes n. Our findings allow for a rigorous uncertainty quantification of inferred first-passage times and lay grounds for a systematic understanding of finite-sample effects avoiding asymptotic approximations or biases due to prior-distribution assumptions.

DY 56.3 Fri 10:00 ZEU 160

Single-trajectory spectral analysis as a criterion of anomalous diffusion — •Vittoria Sposini — University of Vienna, Austria

The departure of the spreading dynamics of diffusing particles from the traditional law of Brownian-motion is a signature feature of a large number of complex soft-matter and biological systems. This anomalous diffusion can emerge due to a variety of physical mechanisms, e.g., trapping interactions or the viscoelasticity of the environment. Demonstrating that a system exhibits normal- or anomalous-diffusion is highly desirable for a vast host of applications. In this talk I will present a criterion for anomalous-diffusion based on the method of power-spectral analysis of single trajectories. The robustness of this criterion is studied for trajectories of fractional-Brownian-motion, a ubiquitous stochastic process for the description of anomalous-diffusion, in the presence of two types of measurement errors. In particular, I will report results from various tests on surrogate data in absence or presence of additional positional noise demonstrating the efficacy of this method in practical contexts.

[1] V Sposini, D Krapf, E Marinari, R Sunyer, F Ritort, F Taheri, C Selhuber-Unkel, R Benelli, M Weiss, R Metzler & G Oshanin, Comms. Phys. 5, 305 (2022).

DY 56.4 Fri 10:15 ZEU 160

Apparent anomalous diffusion and non-Gaussian distributions in a simple mobile-immobile transport model with poissonian switching — •Timo J. Doerries[1], Aleksei V. Chechkin[1,2,3], and Ralf Metzler[1] — [1]Institute of Physics & Astronomy, University of Potsdam, Germany — [2]Faculty of Pure and Applied Mathematics, Hugo Steinhaus Center, Wrocław University of Science and Technology, Wrocław, Poland — [3]Akhiezer Institute for Theoretical Physics National Science Center “Kharkiv Institute of Physics and Technology", Kharkiv, Ukraine

We analyse mobile-immobile transport of particles that switch between mobile and immobile states with finite rates. Despite this seemingly simple assumption of Poissonian switching we unveil rich transport dynamics including significant transient anomalous diffusion and non-Gaussian displacement distributions. Our discussion is based on experimental parameters for tau proteins in neuronal cells, but the results obtained here are expected to be of relevance for a broad class of processes in complex systems. Concretely, we obtain that when the mean binding time is significantly longer than the mean mobile time, transient anomalous diffusion is observed at short and intermediate time scales, with a strong dependence on the fraction of initially mobile and immobile particles. We unveil a Laplace distribution of particle displacements at relevant intermediate time scales and the mean squared displacement of mobile tracers displays a plateau. Adding advection to the mobile phase, corresponding to a biosensor with flow, generates a cubic regime of the MSD for high Péclet numbers.

Invited Talk DY 56.5 Fri 10:30 ZEU 160

Transport and self-organization in living fluids — •Matthias Weiss — Experimental Physics I, University of Bayreuth, Bayreuth, Germany

Intracellular fluids, e.g. the eukariotic cytoplasm, are crowded with a plethora of macromolecules, bearing similarities to semidilute polymer solutions. Since many of the macromolecules are actively driven by ATP hydrolysis, these crowded living fluids are also equipped with genuine non-equilibrium properties. Using model systems from culture cells to extracts, we have explored fluctuation-driven transport and the self-organized formation of compartments in living fluids. As a result, we have observed via extensive single-particle tracking experiments that the generic mode of motion in the cytoplasm appears to be a driven, anti-persistent, and partially intermittent fractional Brownian motion process. On larger length scales, we have observed that a spontaneous, ATP-driven compartmentalization in cell extracts without priming template structures, features geometric properties and a dynamic coarse-graining like two-dimensional foams. Altogether, our experimental observations suggest that fluctuation-driven transport and self-organized space compartmentalization in living biofluids are well captured by few but robust physico-chemical principles.

15 min. break

DY 56.6 Fri 11:15 ZEU 160

Brownian solitons in periodic structures — •Alexander P. Antonov[1], Artem Ryabov[2], and Philipp Maass[1] — [1]Fachbereich Physik, Universität Osnabrück, Osnabrück, Germany — [2]Charles University, Faculty of Mathematics and Physics, Department of Macromolecular Physics, Prague, Czech Republic

Solitons are known in systems with inertia as waves propagating without dispersion due to nonlinear effects. We show that solitons can occur in the absence of inertia for fully overdamped Brownian dynamics of hard spheres in periodic potentials at high particle densities [1,2]. The solitons manifest themselves as periodic sequences of different particle assemblies moving even in the zero-noise limit, where transport of single particles is not possible. To uncover the hard sphere dynamics at zero noise, a new simulation technique has been developed that can be applied for arbitrary external force fields [3]. At low temperature, the solitons give rise to particle currents appearing in band-like structures around certain particle diameters. At high temperatures, currents occur for all particle diameters. The variation of the current magnitudes with particle diameter and driving force reflects the inherent soliton formation.

[1] A. P. Antonov, A. Ryabov, P. Maass, Phys. Rev. Lett. 129, 080601 (2022).
[2] A. P. Antonov, D. Voráč, A. Ryabov, P. Maass, New J. Phys 24, 093020 (2022).
[3] A. P. Antonov, S. Schweers, A. Ryabov, P. Maass, Phys. Rev. E 106, 054606 (2022).

DY 56.7 Fri 11:30 ZEU 160

Large beam X-ray Photon Correlation Spectroscopy — •Fabian Westermeier, Nimmi Das A, Vijay Kartik, Zhe Ren, Wojciech Roseker, Rustam Rysov, Daniel Weschke, Han Xu, and Michael Sprung — Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

The Coherence Applications Beamline P10 at PETRA III is dedicated to coherent X-ray scattering experiments such as X-ray Photon Correlation Spectroscopy (XPCS) and Coherent Diffraction Imaging (CDI). In an XPCS experiment, either the speckle visibility or the temporal changes of a series of scattering patterns are used to measure the dynamics of a sample.

At beamline P10, two 12 m long experimental hutches (EH1 and EH2) house various experimental setups. Among them, two setups are optimized to perform XPCS experiments. One of them is a SAXS/WAXS instrument, where the detector can be translated between 0° and 30° at a sample to detector distance of 5 m. This setup also offers the possibility to use a range of different focal sizes to adjust to the needs of the experiment. The other configuration is an ultra-small angle X-ray scattering (USAXS) setup, where the detector is positioned at a sample to detector distance of around 21 m. This long pathway allows it to use a large fraction of the coherent flux in an unfocused X-ray beam, while providing a fairly strong speckle visibility. Exemplary experimental results obtained at both setups will be shown illustrating the possibilities of XPCS at the beamline.

DY 56.8 Fri 11:45 ZEU 160

Dynamic finite size correction reveals the long-time hydrodynamic tail of liquid water from molecular dynamics simulations — •Laura Scalfi, Domenico Vitali, and Roland R. Netz — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Finite-size effects in molecular dynamics simulations with periodic boundary conditions have significant effects on computed static and dynamic properties. We study the effect of periodic boundary conditions on the friction memory function and on velocity autocorrelation functions of a particle in a liquid using hydrodynamic theory and molecular dynamics simulations. We show that for liquid water, the long-time decay of these functions is significantly affected by hydrodynamic finite-size effects so that the long-time power law tails are not visible for standard simulation box sizes. We develop an analytical correction scheme that corrects for hydrodynamic finite-size effects. Using this correction scheme, the long-time power-law tails of the friction memory and the velocity autocorrelation functions are clearly revealed even for relatively small simulation box sizes. Our developed method generally allows the accurate determination of the long-time behavior of time-dependent response functions from molecular dynamics simulations.

DY 56.9 Fri 12:00 ZEU 160

Fractional anomalous diffusion and Non-Darcian flow in geological system — •Qing Wei — Institute for Physics and Astronomy, University of Potsdam, 14476 Potsdam-Golm,Germany

With the non-Darcian flow and anomalous diffusion in low-permeability porous media as research subjects, the analytical models of non-Darcian flow as well as diffusive transport in low-permeability porous media was in- vestigated by invoking the fractional calculus theory. Using the fractional derivatives with different kernel, fractional diffusion models are proposed to describe radionuclide anomalous transport in geological repository sys- tems. On the basis of Darcy*s law, the memory effectiveness deduced by solid-fluid interaction is depicted by fractional derivative approach, and a fractional Swartzendruber model is proposed for the description of low velocity non-Darcian flow in porous media.

DY 56.10 Fri 12:15 ZEU 160

Universal hyper-scaling relations, power-law tails, and data analysis for strong anomalous diffusion — •Jürgen Vollmer[1], Lamberto Rondoni[2], Claudio Giberti[3], and Carlos Mejía-Monasterio[4] — [1]Inst. Theor. Physik, Univ. Leipzig, 04103 Leipzig, Germany — [2]Dept. Math. Sc., Politecnico di Torino, 10129 Torino, Italy — [3]Dept. Scienze e Metodi dell Ingegneria, Univ. Modena e Reggio E., 42100 Reggio E., Italy — [4]School of Agric. Food and Biosys. Eng., Techn. Univ. Madrid, 28040 Madrid, Spain

Strong anomalous diffusion is often characterized by a piecewise-linear spectrum of the moments of displacement. The spectrum is characterized by slopes ξ and ζ for small and large moments, respectively, and by the critical moment α of the crossover. Higher moments are asymptotically dominated by ballistic excursions; lower moments correspond to weak anomalous diffusion. We argue that ξ and ζ characterize the asymptotic scaling of the bulk and the tails of the distribution, respectively. Asymptotic theory is adopted to match the behaviors at intermediate scales. The resulting constraint entails that strong anomalous diffusion emerges if the distribution has algebraic tails, and it relates α to the corresponding power law. Our theory provides the leading-order corrections to the asymptotic power-law behavior. This insight allows us to point out sources of (at times) severe systematic errors in numerical estimates of the moments of displacement. Rather than fitting exponents we devise a robust scheme to determine ξ, ζ and α. The findings are supported by numerical and analytical results on different models exhibiting strong anomalous diffusion.

DY 56.11 Fri 12:30 ZEU 160

Bio-hybrid colloidal transport of beads on cell monolayers — Lara Bort, Setareh Sharifi Panah, •Robert Grossmann, and Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany

The erratic motion of Brownian particles at the mesoscale, driven by collisions with the surrounding fluid particles, is the paradigm of random colloidal transport within a passive environment. In this work, we describe the transport of polystyrene micro-beads whose motion is driven by a monolayer of motile cells. We use cells of the social amoeba *Dictyostelium discoideum*, which is a widely used model organism for actin-driven motility of adherent eukaryotic cells, including neutrophils and cancer cells. Given the non-specific adhesion of our model organism, the binding of such micro-cargo to the cell membrane does not require any surface-functionalization – the physical link between cargo and carrier is established spontaneously. As a particle gets in contact with a cell, it adheres to the cell membrane and is then subjected to active forces exerted by cells. The dynamics of micro-beads reveals linear scaling of the ensemble-averaged mean-square displacement and, notably, non-Gaussian displacement distributions. We rationalize these findings by assuming that each colloidal particle effectively performs normal Brownian motion, but the diffusion coefficients vary within the ensemble due to cell-to-cell variability. This superstatistics allows to reproduce the statistical features of the long-time dynamics of colloids, subject to the active cellular forces. It serves as a first step to better understand the targeted transport of foreign objects in dense tissues.