DY 59: Brownian Motion and Anomalous Diffusion

Time: Friday 9:30–13:00 Location: BH-N 334

DY 59.1 Fri 9:30 BH-N 334

Being heterogeneous is advantageous: Extreme Brownian non-Gaussian searches — •Vittoria Sposini — Faculty of Physics, University of Vienna, Vienna (Austria)

Diffusing diffusivity models, polymers in the grand canonical ensemble and polydisperse, and continuous time random walks, all exhibit stages of non-Gaussian diffusion. Is non-Gaussian targeting more efficient than Gaussian? In this talk I will show that non-Gaussian rare fluctuations in Brownian diffusion dominates extreme searches, introducing drastic corrections to the known Gaussian behavior. Our demonstration entails different physical systems and pinpoints the relevance of diversity within redundancy to boost fast targeting.

Joint work with Sankaran Nampoothiri, Aleksei Chechkin, Enzo Orlandini, Flavio Seno, and Fulvio Baldovin.

DY 59.2 Fri 9:45 BH-N 334

Non-Gaussian displacements in active transport on a carpet of motile cells — •Robert Grossmann[1], Lara S. Bort[1], Ted Moldenhawer[1], Setareh Sharifi Panah[1], Ralf Metzler[1,2], and Carsten Beta[1] — [1]University of Potsdam, Potsdam, Germany — [2]Asia Pacific Center for Theoretical Physics, Pohang, Republic of Korea

In this talk, we discuss the dynamics of micron-sized particles on a layer of motile cells [1]. This cell carpet acts as an active bath that propels passive tracer particles via direct mechanical contact. The resulting nonequilibrium transport shows a crossover from superdiffusive to normal-diffusive dynamics. The particle displacement distribution is distinctly non-Gaussian even in the limit of long measurement times—different from typically reported Fickian yet non-Gaussian transport, for which Gaussianity is restored beyond some system-specific correlation time. We obtain the distribution of diffusion coefficients from the experimental data and introduce a model for the displacement distribution that matches the experimentally observed non-Gaussian statistics. We argue why similar transport properties are expected for many composite active matter systems.

[1] Großmann, Bort, Moldenhawer *et al.* (2023) arXiv:2311.05377

DY 59.3 Fri 10:00 BH-N 334

Brownian particle in a Poisson-shot-noise active bath: exact statistics, effective temperature, and inference — •costantino di bello[1], rita majumdar[2,3], rahul marathe[2], ralf metzler[1,4], and edgar roldan[3] — [1]Institute of Physics & Astronomy, University of Potsdam, Germany — [2]Department of Physics, Indian Institute of Technology, New Delhi, India — [3]ICTP - The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy — [4]Asia Pacific Centre for Theoretical Physics, Pohang, Republic of Korea

This work studies the fluctuating, nonequilibrium dynamics of an optically trapped Brownian particle within a dilute solution of active particles. The authors propose a stochastic model in which the particle moves in a harmonic potential and experiences both thermal and Poisson shot-noise kicks with specified amplitude distribution due to moving active particles in the bath. A variety of exact analytical results for the particle position statistics are derived, like mean, variance, skewness and excess kurtosis. Interestingly, the positions' distribution, for any choice of the parameters of the system, is leptokurtic, in accordance with recent experimental studies.

The work also sheds light on when and how to use the notion of effective temperature in such active systems.

DY 59.4 Fri 10:15 BH-N 334

Run-and-trap motility of self-propelled particles — •Agniva Datta, Sönke Beier, Veronika Pfeifer, Carsten Beta, and Robert Grossmann — University of Potsdam, Potsdam, Germany

In many experimental manifestations of active matter, self-propelled particles have been observed to exhibit dynamic transitions between different states of motility that are characterized by various features such as velocity and rotational diffusion coefficients as well as their duration. These multi-state motility behaviors often result in non-Gaussian statistics, anomalous diffusion and ergodicity breaking. We introduce a comprehensive dynamical motility model for self-propelled particles whose active run motility is intermittently interrupted by a trap state as it is observed, for example, for active motion in disordered media. Thereby, we provide a unified framework to study Lévy walks, classical continuous-time random walks and active diffusion models such as active Brownian motion, run-and-tumble or run-and-reverse. We analytically derive expressions for essential quantities, including mean-squared displacements and diffusion coefficients, crucial for understanding the intricacies of these processes. We illustrate the applicability of our model to experimental data using the example of soil bacteria spreading in agar.

DY 59.5 Fri 10:30 BH-N 334

Machine-Learning-Based Classification of Anomalous Diffusion - How well does it generalize? — •Henrik Seckler[1], Janusz Szwabiński[2], and Ralf Metzler[1] — [1]University of Potsdam, Germany — [2]Wrocław University of Science and Technology, Poland

Single-particle traces of the diffusive motion of molecules, cells, or animals are by now routinely measured, similar to stochastic records of stock prices or weather data. Deciphering the stochastic mechanism behind the recorded dynamics is vital in understanding the observed systems. Typically, the task is to decipher the exact type of diffusion and/or to determine the system parameters. The tools used in this endeavor are currently being revolutionized by modern machine-learning techniques. As such methods are often criticized for their lack of interpretability, we focus on means to include uncertainty estimates and feature-based approaches, both improving interpretability and providing concrete insight into the learning process of the machine. We expand the discussion by examining predictions on different out-of-distribution data.

DY 59.6 Fri 10:45 BH-N 334

First-passage area distribution and optimal fluctuations of fractional Brownian motion — •Alexander K. Hartmann[1] and Baruch Meerson[2] — [1]University of Oldenburg, Germany — [2]Hebrew University of Jerusalem, Israel

We study the probability distribution $P(A)$ of the area $A=\int_0^T x(t)dt$ swept under fractional Brownian motion (fBm) $x(t)$ until its first passage time T to the origin. The process starts at $t=0$ from a specified point $x=L$. We show that $P(A)$ obeys the exact scaling relation $P(A)=\frac{D^{\frac{1}{2H}}}{L^{1+\frac{1}{H}}}\,\Phi_H\left(\frac{D^{\frac{1}{2H}}A}{L^{1+\frac{1}{H}}}\right)$, where $0<H<1$ is the Hurst exponent characterizing the fBm, D is the coefficient of fractional diffusion, and $\Phi_H(z)$ is a scaling function. The small-A tail of $P(A)$ has been recently predicted [1] as having an essential singularity at $A=0$. Here [2] we determine the large-A tail of $P(A)$. It is a fat tail, with the average value A diverging for all H. We also verify the predictions for both tails by performing simple-sampling as well as large-deviation Monte Carlo [3] simulations. The verification includes measurements of $P(A)$ up to probability densities as small as 10^{-190}. We also perform direct observations of paths conditioned on the area A. For the steep small-A tail of $P(A)$ the "optimal paths", *i.e.* the most probable trajectories of the fBm, dominate the statistics. Finally, we discuss extensions of theory to a more general first-passage functional of the fBm.

[1] B. Meerson and G. Oshanin, Phys. Rev. E **105**, 064137 (2022).
[2] A.K. Hartmann and B. Meerson, preprint arXiv:2310.14003 (2023).
[3] A.K. Hartmann, Phys. Rev. E **89**, 052103 (2014).

DY 59.7 Fri 11:00 BH-N 334

Density fluctuation analysis of biological matter — •Conrad Möckel[1,2,3], Abin Biswas[1,2,4], Simone Reber[4], Vasily Zaburdaev[2,3], and Jochen Guck[1,2,3] — [1]Max Planck Institute for the Science of Light, 91058 Erlangen, Germany — [2]Max Planck Zentrum für Physik und Medizin, 91058 Erlangen, Germany — [3]Friedrich Alexander Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [4]Max Planck Institute for Infection Biology, 10117 Berlin, Germany

The characterization of the dynamical properties of biological matter plays an important role in unraveling its complexity and associated functions. Here we employ differential dynamic microscopy in combination with bright field microscopy to probe and evaluate the inherent density fluctuations at present in the sample under study. Using theoretical models, this approach allows for quantification of the time and length scale dependent viscoelastic properties of optically transparent systems as demonstrated for high speed supernatant (HSS) *Xenopus laevis* egg extract. We find that upon microtubule formation, the HSS exhibits subdiffusive characteristics at two distinct time scales which can be connected to dynamical caging and escape events. Our findings illustrate the relevance of this methodology for characterizing dynamical heterogeneities of cytoplasm non-invasively, beyond multiple particle tracking.

15 min. break

DY 59.8 Fri 11:30 BH-N 334

The Role of Cross-Correlations in the Fluctuation-Dissipation-Theorem of the Generalized Langevin Equation — •Niklas Wolf, Viktor Klippenstein, and Nico van der Vegt — TU Darmstadt, 64287 Darmstadt, Germany

In molecular dynamics, the development of dynamically consistent coarse-grained models revolves around modeling friction and random forces to reintroduce fluctuations in the force that are lost when choosing a more coarse description of a problem/system. Modeling these fluctuations with Markovian approaches like the Langevin equation or dissipative particle dynamics assumes time scale separation between the degrees of freedom in the atomistic and coarse model. Usually, this is not given in condensed matter systems but can be accounted for with non-Markovian models like the generalized Langevin equation (GLE), which we focused on in this work.

Recent works[1, 2] have demonstrated that for a GLE with position-independent friction, the usual second fluctuation-dissipation theorem connecting friction and random force should be modified with a cross-correlation term. We investigated these cross-correlations and their effect on dynamic properties in several model systems and found that discarding them does generally not lead to a correct description of the dynamics. To remedy this, we discuss different approaches to include cross-correlations in a GLE equation of motion.

[1] V. Klippenstein, N. F. A. van der Vegt, *J. Chem. Phys.* **154**, 191102 (2021)

[2] H. Vroylandt, *EPL* **140**, 62003 (2022)

DY 59.9 Fri 11:45 BH-N 334

Iterative parameterization of Markovian embedded generalized Langevin equations for molecular dynamics — •Viktor Klippenstein, Niklas Wolf, and Nico F. A. Van Der Vegt — Technical University of Darmstadt, Darmstadt, Germany

In molecular dynamics, coarse-grained (CG) models which aim to describe dynamic properties consistently with the underlying fine-grained (FG) system, typically introduce some dissipative thermostat to account for friction and fluctuations due to removed degrees of freedom. In many cases, the time scales of CG and FG degrees of freedom are not separated which necessitates a non-Markovian (NM) description typically based on a generalized Langevin equation (GLE).

To keep the CG models tractable, we augment the Hamiltonian equation of motion by individually coupling every coarse-grained particle to an isotropic GLE thermostat, where NM friction is fully characterized by a single scalar function termed memory kernel. For computational efficiency, the NM GLE thermostat can be mapped on a Markovian auxiliary variable thermostat (aux-GLE). While our recently introduced method (iterative optimization of memory kernels (IOMK)[1]) allows for efficient optimization of the GLE the parameterization of the aux-GLE is by itself non-trivial, and potentially both error-prone and computationally expensive. To sidestep this problem, we propose a Gauss-Newton type method (IOMK-GN), which allows us to directly optimize the aux-GLE parameters.

[1] Klippenstein V., van der Vegt N. F. A., *J. Chem. Theory Comput.* 2023, 19, 4, 1099-1110

DY 59.10 Fri 12:00 BH-N 334

Concentration-of-measure in time-average statistical mechanics — •Rick Bebon and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

Nowadays, state-of-the-art single-molecule or particle-tracking experiments provide direct access to path-dependent observables by probing individual trajectories. Obtained by means of time-averaging a limited number of individual realizations each with a finite duration, inferred estimates are typically afflicted by large systematic uncertainties, making a correct interpretation *a priori* non-trivial. Recent theoretical advances motivate a deeper understanding of fluctuating path-observables, as the latter would allow for decoding important and otherwise hidden information about the underlying microscopic dynamics. Reliably interpreting sample-to-sample fluctuations of time-averaged functionals of noisy trajectories therefore remains a crucial but challenging task, especially in the presence of subsampling. Instigated by these difficulties, we propose a non-asymptotic concentration-of-measure perspective on functionals of overdamped Langevin dynamics that allows a general and correct rationalization of time-averaged observables and their fluctuations for arbitrary times. Subsequently, we demonstrate how bounding the probability that an individual realization deviates from the mean value by more than any fixed amount provides a new outlook on time-averaged observables.

DY 59.11 Fri 12:15 BH-N 334

Langevin Dynamics of Oriented Active Particles on Curved Surfaces — •Balázs Németh and Ronojoy Adhikari — Department of Applied Mathematics and Theoretical Physics, Centre for Mathematical Sciences, University of Cambridge, Wilberforce Road, Cambridge CB3 0WA, United Kingdom

The motion of active particles constrained to curved surfaces is an intriguing problem with wide range of applications in biological physics and soft matter, from rotating motors on membranes to Janus particles on interfaces. In this talk, we construct Langevin equations for oriented active particles on fixed surfaces using differential geometric principles. We derive the deterministic equations of motion for the translational and rotational velocities in the body frame of the particle in Hamiltonian form. We find that surface curvature couples the linear and angular momenta of the particle. To these Hamiltonian equations, we add linear friction and white noise to obtain a generalized Ornstein-Uhlenbeck process in phase space. We obtain the corresponding Fokker-Planck equation and the fluctuation-dissipation relation. The equations of Brownian dynamics are derived by adiabatically eliminating the momenta. These can be used to simulate biophysical diffusion processes on surfaces.

DY 59.12 Fri 12:30 BH-N 334

Depinning transition of self-propelled particles — Arthur Straube[1,2] and •Felix Höfling[2,1] — [1]Zuse Institute Berlin — [2]Fachbereich Mathematik und Informatik, Freie Universität Berlin

A depinning transition is observed in a variety of contexts when a certain threshold force must be applied to drive a system out of an immobile state. A well-studied example is the depinning of colloidal particles from a corrugated landscape, whereas its active-matter analogue has remained unexplored. Here, we discuss how active noise due to self-propulsion impacts the nature of the transition [1]: it causes a change of the critical exponent from 1/2 for quickly reorienting particles to 3/2 for slowly reorienting ones. In between these analytically tractable limits, the drift velocity exhibits a superexponential behavior as is corroborated by high-precision data. Giant diffusion phenomena occur in the two different regimes. Our predictions appear amenable to experimental tests, lay foundations for insight into the depinning of collective variables in active matter, and are relevant for any system with a saddle-node bifurcation in the presence of a bounded noise.

[1] A.V. Straube, F. Höfling, under review with Phys. Rev. Lett. (preprint arXiv:2306.09150).

DY 59.13 Fri 12:45 BH-N 334

Coupled long-time dynamics in binary mixtures of colloidal Yukawa-systems — •Daniel Weidig and Joachim Wagner — Institut für Chemie, Universität Rostock, 18051 Rostock, Germany

We investigate structure and dynamics of binary mixtures consisting of particles interacting via a screened Coulomb potential. In mixtures of equally charged, but differently sized particles, the partial correlation functions $g_{\mathrm{AA}}(r) = g_{\mathrm{AB}}(r) = g_{\mathrm{BB}}(r)$ and thus partial static structure factors are identical due to identical time-averaged interactions between all present species. Different particle sizes, however, yield different Stokes-Einstein diffusion coefficients with $\sigma_\mathrm{A}/\sigma_\mathrm{B} = D_{0,\mathrm{B}}/D_{0,\mathrm{A}}$. Mediated by electrostatic interactions, different mobilities of the species influence the long-time diffusion: In presence of a smaller species, the long-time diffusion of the larger species is accelerated and vice versa as visible both in self- and collective dynamics. A nearly universal dependence of the relative acceleration or deceleration of long-time self-diffusion coefficients in mixtures on the product of size-ratio $\sigma_\mathrm{A}/\sigma_\mathrm{B}$ of the larger to the smaller species and number-density ratio ϱ_i^*/ϱ_i is observed. Here, ϱ_i^* denotes the number density of species i in a suspension containing only species i and ϱ_i the number density of species i in a mixture. The magnitude of the relative acceleration or deceleration depends in first approximation on the electrostatic interaction at the maximum $r_{\max}$ of the pair correlation functions $g_{ij}(r)$.