DY 40: Brownian Motion and Anomalous Diffusion

Time: Thursday 10:00–12:00 Location: H20

DY 40.1 Thu 10:00 H20

Depinning and structural transitions of confined colloidal dispersions under oscillatory shear — •Marcel Hülsberg and Sabine H.L. Klapp — ITP, Technische Universität Berlin, Germany

Strongly confined colloidal dispersions under shear exhibit a variety of dynamical phenomena, including a depinning transition, which is accompanied by lateral structural changes [1].

Here, we investigate the depinning behaviour of these systems under pure oscillatory shearing with shear rate $\dot{\gamma}(t) = \dot{\gamma}_0 \cos(\omega t)$, as it is a common scenario in rheological experiments [2].

The colloids' depinning behaviour is assessed from a microscopic level based on particle trajectories, which are obtained from overdamped Brownian Dynamics simulations. The numerical approach is complemented by an analytic one based on an effective single-particle model in the limits of weak and strong driving.

Investigating a broad spectrum of shear rate amplitudes $\dot{\gamma}_0$ and frequencies ω, we observe complete pinning as well as temporary depinning behaviour. We discover that temporary depinning occurs for shear rate amplitudes above a frequency-dependent critical amplitude $\dot{\gamma}_0^{\mathrm{crit}}(\omega)$, for which we attain an approximate functional expression.

Above $\dot{\gamma}_0^{\mathrm{crit}}(\omega)$, we further observe a variety of dynamical structures, whose stability exhibits an intriguing $(\dot{\gamma}_0, \omega)$ dependency. This might enable new perspectives for potential control schemes.

[1] S. Gerloff and S.H.L. Klapp, *Phys. Rev. E* **94**(6), 062605 (2016)
[2] S.M. Fielding, *J. Rheol.*, **64**(3), 723-738 (2020)

DY 40.2 Thu 10:15 H20

Ballistic Hot Brownian Motion — •Xiaoya Su[1], Frank Cichos[1], and Klaus Kroy[2] — [1]Peter Debye Institute for Soft Matter Physics, University Leipzig, Leipzig, Germany — [2]Institute of Theoretical Physics, University Leipzig, Leipzig, Germany

Brownian motion is the erratic motion of particles in a fluid due to the bombardment of the particle with solvent molecules providing thermal energy and viscous friction. It is fundamental for the dynamics of soft matter and defines the prototype of a fluctuation dissipation relation. While at long timescales the motion is purely stochastic, it is at shorter times influenced by hydrodynamic effects and even ballistic at ultrashort timescales. Yet, the ballistic motion, same as the stochastic motion, is still determined by the temperature of the system. Here we explore the transition to the ballistic regime for a hot Brownian particle, i.e. a microparticle which is heated by a laser in an optical trap. In this case the particle temperature is different from the solvent temperature and so far, only theoretical predictions exist for the relevant temperature determining the particle velocity.

We report the first measurements of the thermal non-equilibrium process in a specially designed optical trap which is able to resolve particle displacements of about 20 pm with a time-resolution of 10ns. We show how the mean squared displacement of the particle from the nanosecond to the second timescale changes as a function of the surface temperature of the particle and discuss the model of a frequency dependent effective temperature of hot Brownian motion.

DY 40.3 Thu 10:30 H20

Stochastic action for tubes: Connecting path probabilities to measurement — •Julian Kappler[1], Jannes Gladrow[2,3], Ulrich F. Keyser[3], and Ronojoy Adhikari[1] — [1]DAMTP, Cambridge University, Cambridge, UK — [2]Microsoft Research, Cambridge, UK — [3]Cavendish Laboratory, University of Cambridge, Cambridge, UK

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 probability of diffusive trajectories to remain within a tube of small but finite radius around a smooth path. This probability can be measured in experiment, via the rate at which trajectories exit the tube for the first time, thereby establishing a link between path probabilities and physical observables. In my contribution I will show how this link can be used to both measure ratios of path probabilities [1], and to extend the theoretical stochastic action from individual paths to tubes [2]. I will furthermore relate our results to the usual path-integral formalism.

[1] J. Gladrow, U. F. Keyser, R. Adhikari, and J. Kappler. Experimental measurement of relative path probabilities and stochastic actions. Phys. Rev. X 11, 031022 (2021). 10.1103/PhysRevX.11.031022
[2] J. Kappler and R. Adhikari. Stochastic action for tubes: Connecting path probabilities to measurement. Physical Review Research 2(2), 023407 (2020). 10.1103/PhysRevResearch.2.023407

DY 40.4 Thu 10:45 H20

Size matters for Bayesian chemotaxis — •Julian Rode[1], Maja Novak[1,2], and Benjamin M. Friedrich[1,3] — [1]cfaed, TU Dresden, Germany — [2]Department of Physics, University of Zagreb, Croatia — [3]PoL, TU Dresden, Germany

Navigation by chemical cues, e.g., chemotaxis, is employed by single biological cells and animals. The size and speed of search agents dictate noise levels and thus optimal strategies to find a target.

Here, we address information theory of gradient sensing for an ideal agent and ask for optimal strategies as a baseline for real agents. We extend the seminal work on infotaxis [1], by applying its idea of maximizing information gain to agents of finite size. These agents can now measure gradients both by temporal comparison due to their active motion [1], and by spatial comparison across their diameter, prompting an optimal weighting of both information sources [2].

In the absence of noise, trajectories show stereotypic behavior; the entropy of directional uncertainty collapses onto a master curve parameterized by a signal-to-noise ratio. Unlike [1], we account for rotational diffusion, which is prevalent for microscopic agents: Its competition with information gain due to spatial comparison sets an effective measurement time (given by the inverse geometric mean of a rate constant of information gain and the rotational diffusion coefficient), which is different from the typical bound argued by Howard Berg for bacterial chemotaxis (inverse rotational diffusion coefficient) [3].

[1] M. Vergassola et al, Nature (2007); [2] A. Auconi et al., EPL, in press (arXiv:2111.09630); [3] M. Novak et al., New J Phys (2021).

15 min. break

DY 40.5 Thu 11:15 H20

Superstatistics of protein diffusion dynamics in bacteria — •Yuichi Itto — Aichi Institute of Technology, Aichi, Japan — ICP, Universität Stuttgart, Stuttgart, Germany

In recent years, non-Gaussian normal/anomalous diffusion have experimentally been observed in a wide class of living cells. Superstatistics is a "statistics of statistics" with two largely separated time scales for treating nonequilibrium complex systems. Here, a superstatistical diffusion theory [1] is presented for obtaining a q-Gaussian displacement distribution decaying as a power law found for heterogeneous diffusion phenomenon of DNA-binding proteins in bacteria [2]. This theory takes into account the joint fluctuations of both the diffusion exponent and the (inverse) temperature, which are hierarchically combined with a fractional Brownian motion describing a local stochastic process of the proteins. Correlation between the fluctuations is also discussed and its weakness is shown to be essential. The results obtained are in a good agreement with the experimental data.

[1] Y. Itto and C. Beck, J. R. Soc. Interface 18, 20200927 (2021).
[2] A.A. Sadoon and Y. Wang, Phys. Rev. E 98, 042411 (2018).

DY 40.6 Thu 11:30 H20

Generalised master equation for diffusion and reaction problems in heterogeneous media — Daniela Frömberg[1] and •Felix Höfling[1,2] — [1]Department of Mathematics and Computer Science, Freie Universität Berlin — [2]Zuse Institute Berlin

The kinetics of chemical reactions in a heterogeneous or crowded medium significantly deviates from that in a well-mixed, aqueous environment. One example is the partitioning of cell membranes and intracellular spaces, e.g., into cytoplasm and nucleus. For reaction–diffusion problems in such compartmentalised spaces, we extend a recently proposed generalised master equation (GME) for non-Markovian jump processes [1]. The GME governs the time evolution of the occupation probability of the spatial domains, its main ingredient are first-passage time densities encoding the transport behaviour in each domain. The domains can differ with respect to their diffusivity, geometry, and dimensionality, but can also refer to transport modes alternating between diffusive, driven, or anomalous motion. We discuss further the inclu-

sion of barriers and the Markovian limit of the GME.

For a cherry-pit geometry with a reactive inner domain, we obtain the first-reaction time density and infer the effective reaction rate constant. This rate constant is timescale dependent and exhibits an enhancement at intermediate times by orders of magnitude and an algebraically slow convergence to the long-time limit. Our stochastic approach does not depend on the existence of a stationary distribution and thus overcomes a limitation of the classical Smoluchowski theory.

[1] D. Frömberg and F. Höfling, J. Phys. A **54**, 215601 (2021).

DY 40.7 Thu 11:45 H20

Molecular dynamics simulations of supercooled water in silica pores — •Markus Haneke, Robin Horstmann, and Michael Vogel — TU Darmstadt, Institut für Physik kondensierter Materie, Hochschulstr. 6, 64289, Darmstadt, Germany

Being highly relevant in biology as well as in technology and other areas, water is subject to extensive research. Especially its anomalies pose questions. Commonly, it is argued that the anomalies of water originate in the supercooled state, which is therefore regularly subject to exploration. To suppress freezing in experimental studies, confinements can be employed, where silica pores proved to be very useful.

Molecular dynamic simulations are a valuable tool to take a closer look. They allow analyses with high spatial and temporal resolution while making it easy to extract dynamic and static information. [1]

Here, we perform simulations to analyse the diffusion of water in silica pores. We want to find the influence of the pore on dynamics, as well as of the capping if the water outside of the pore freezes.

Results of our analysis are, that the diffusion inside of the pore is anomalous and slowed down. The systems show to be subdiffusive. Capping not only restricts diffusion but also slows down local relaxation and yields a nearly triangular probability density of propagation distance, contradicting free 1D-diffusion.

[1] R. Horstmann, L. Hecht, S. Kloth, and M. Vogel. "Structural and Dynamical Properties of Liquids in Confinements: A Review of Molecular Dynamics Simulation Studies". In: Langmuir 2022 38 (21), 6506-6522