# DY 43: Anomalous diffusion / Brownian motion

Time: Thursday 10:00–13:15 Location: H3

DY 43.1 Thu 10:00 H3

**Fractional electron transfer kinetics and a quantum breaking of ergodicity** — •Igor Goychuk — Institute for Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam-Golm, Germany

The dissipative curve-crossing problem provides a paradigm for electron-transfer (ET) processes in condensed media. It is studied both analytically and numerically for subdiffusive or sub-Ohmic dynamics of the reaction coordinate in the contact approximation, both from the ensemble and single-trajectory perspectives [1]. Depending on the electron coupling strength, the transfer occurs either in non-adiabatic or in a solvent-controlled adiabatic regime. It is shown that the relaxation of electronic populations has universally a power law tail even in a deeply non-adiabatic regime. For a sufficiently strong tunnel coupling, it is described by a Mittag-Leffler function. The statistics of electron transitions is, however, very different from both the ensemble and single-trajectory perspective. For large sojourn times, it is featured by a stretched exponential Weibull distribution and not by a power law dependence. Moreover, a profound difference occurs for the distribution of residence times in the electronic states on the ensemble level and on the level of single trajectories. Ergodicity is broken dynamically even in a more spectacular way than in the memoryless case [2].

[1] I. Goychuk, arXiv:1811.03838 [cond-mat.stat-mech] (2018).
[2] I. Goychuk, Phys. Chem. Chem. Phys. **19**, 3056 (2017).

DY 43.2 Thu 10:15 H3

**Dynamics of ellipsoidal particles in random light fields** — Rene Hermann[1], Christoph Zunke[1], •Florian Platten[1], Arjun G. Yodh[2], and Stefan U. Egelhaaf[1] — [1]Heinrich Heine University Duesseldorf — [2]University of Pennsylvania, Philadelphia, USA

Ellipsoidal polystyrene particles are exposed to a random light field applying different laser power, and the particle motions are tracked by video microscopy. From the particle trajectories, mean-squared (angular) displacements are analyzed. Initial and long-time diffusion, as well as transient intermediate sub-diffusive behavior, are observed for the center-of-mass and angular displacements.

DY 43.3 Thu 10:30 H3

**Ideal circle microswimmers in crowded media** — •Oleksandr Chepizhko and Thomas Franosch — University of Innsbruck, Innsbruck, Austria

Microswimmers in nature move in crowded environments and their transport properties depend in a subtle way on the interaction with obstacles. Here, we study a model for a single ideal circle swimmer exploring a two-dimensional disordered array of impenetrable obstacles. The microswimmer moves on ideal circular orbits in the freely accessible space and follows the surface of an obstacle for a certain time upon collision. Depending on the obstacle density and the radius of the circular orbits, the microswimmer displays either long-range transport or is localized in a finite region. We show that there are transitions from two localized states to a diffusive state each driven by an underlying static percolation transition. We determine the non-equilibrium state diagram and calculate the mean-square displacements and diffusivities by computer simulations. Close to the transition lines transport becomes subdiffusive which is rationalized as a dynamic critical phenomenon. Additionally, we discuss the influence of inclusion of a stochastic noise term into the equation of orbital motion.

DY 43.4 Thu 10:45 H3

**Anomalous transport in the soft Lorentz model of crowded media** — •Charlotte Petersen and Thomas Franosch — Institute for Theoretical Physics, University of Innsbruck, Austria

Transport in heterogeneous crowded environments occurs in many situations, including inside of cells, in catalysts, and in porous rock during oil recovery. Both experimentally, and in simple models, the transport in complex crowded media can be subdiffusive. The origin of this anomalous diffusion has been explained theoretically for the paradigmatic Lorentz model. Here, a single particle moves with Newtonian dynamics through a random array of identical fixed obstacles. The moving particle has specular collisions with the obstacles. At the percolating density of the obstacles, the mean square displacement grows subdiffusively. We extend the Lorentz model towards realistic systems by relaxing the hard-exclusion interaction assumption, and find that they system exhibits a percolation transition dependent on the energy of the probe particle, and the dynamics remain anomalous at the percolation point.

DY 43.5 Thu 11:00 H3

**First passage statistics for Brownian yet non-Gaussian diffusion.** — •Vittoria Sposini[1,2], Aleksei V. Chechkin[1,3], and Ralf Metzler[1] — [1]Institute for Physics and Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany — [2]Basque Center for Applied Mathematics, 48009 Bilbao, Spain — [3]Akhiezer Institute for Theoretical Physics, 61108 Kharkov, Ukraine

A rapidly increasing number of systems is identified in which the stochastic motion of tracer particles follows the Brownian law $\langle \mathbf{r}^2(t) \rangle \simeq Dt$ yet the distribution of particle displacements is strongly non-Gaussian. A central approach to describe this effect is the diffusing diffusivity (DD) model in which the diffusion coefficient itself is a stochastic quantity, mimicking heterogeneities of the environment encountered by the tracer particle on its path. In this talk I will discuss how to quantify, in terms of analytical and numerical approaches, the first passage behaviour of the DD model. We observe significant modifications compared to Brownian-Gaussian diffusion, in particular that the DD model may have a more efficient first passage dynamics. Moreover we find a universal crossover point of the survival probability independent of the initial condition.

[1] Chechkin A V, Seno F, Metzler R & Sokolov I 2017 Brownian Yet Non-Gaussian Diffusion: From Superstatistics to Subordination of Diffusing Diffusivities *Phys. Rev. X* **7** 021002.

[2] Sposini V, Chechkin A V & Metzler R 2018 First passage statistics for diffusing diffusivity *arXiv:1809.09186 [cond-mat.stat-mech].*

DY 43.6 Thu 11:15 H3

**Bayesian statistics for models of diffusion: theory and applications** — •Samudrajit Thapa[1], Michael A. Lomholt[2], Jens Krog[2], Andrey G. Cherstvy[1], and Ralf Metzler[1] — [1]Institute for Physics & Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany — [2]MEMPHYS, Department of Physics, Chemistry & Pharmacy, University of Southern Denmark, 5230 Odense M, Denmark

Particle diffusion in heterogeneous systems poses the following question: Can a single model describe the entire dynamics of a particle in complex biological, soft matter systems? Indeed, often several different physical mechanisms are at work and it is more insightful to rank them based on the likelihood of them explaining the dynamics. This talk will discuss—within the Bayesian framework—,(a) how maximum-likelihood model selection can be done by assigning probabilities to each feasible model and (b) how to estimate the parameters of each model. In particular, the implementation of this powerful statistical tool using the Nested Sampling algorithm to compare—at the single trajectory level-models of Brownian motion, viscoelastic anomalous diffusion and normal yet non-Gaussian diffusion will be discussed. Finally, the application of this method to experimental data of tracer diffusion in polymer-based hydrogels (Mucin) will be presented.

[1] S. Thapa, M. A. Lomholt, J. Krog, A. G. Cherstvy, & R. Metzler, *Bayesian analysis of single-particle tracking data using the nested-sampling algorithm: maximum-likelihood model selection applied to stochastic-diffusivity data*,Phys. Chem. Chem. Phys., **20** 29018 (2018).

**15 min. break**

DY 43.7 Thu 11:45 H3

**Flat-to-curved transition during clathrin-mediated endocytosis** — •Felix Frey[1], Delia Bucher[2], Kem A. Sochacki[3], Susann Kummer[2], Jan-Philip Bergeest[4], William J. Godinez[4], Hans-Georg Kräusslich[2], Karl Rohr[4], Justin W. Taraska[3], Steeve Boulant[2], and Ulrich S. Schwarz[1] — [1]ITP, Heidelberg University — [2]Department of Virology, University Hospital Heidelberg — [3]NHLBI, NIH, Bethesda, U.S.A. — [4]IPMB, Heidelberg University

Biological cells constantly transport material and information across

their plasma membrane. The most important pathway for the uptake of nutrients and receptors is clathrin-mediated endocytosis (CME). Although CME has been studied for decades, the exact sequence of molecular and structural events remains elusive. Two basic models have been suggested for the way CME proceeds, namely the constant curvature and the constant area models [1]. Here, we combine correlative electron and light microscopy, super-resolution microscopy, single particle tracking and simple mathematical grow laws to estimate the temporal sequence of ultrastructural rearrangements of the clathrin coat. Our quantitative analysis shows that neither model is correct and that clathrin-coated structures initially grow flat but start to acquire curvature when on average 70% of the final clathrin content is reached [2]. [1] Haucke, Volker, and Michael M. Kozlov. "Membrane remodeling in clathrin-mediated endocytosis." J. Cell Sci. (2018), 131(17):jcs216812. [2] Bucher, Delia, et al. "Clathrin-adaptor ratio and membrane tension regulate the flat-to-curved transition of the clathrin coat during endocytosis." Nat. Commun. (2018), 9(1):1109.

DY 43.8 Thu 12:00 H3

**Long-time tails of correlation functions of Brownian particles** — Suvendu Mandal[1], •Lukas Schrack[2], Hartmut Löwen[1], Matthias Sperl[3], and Thomas Franosch[2] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany — [2]Institut für Theoretische Physik, Leopold-Franzens-Universität, Technikerstraße 21A, 6020 Innsbruck, Austria — [3]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Linder Höhe, 51147 Köln, Germany

The dynamics of Brownian particles of a hard-sphere fluid can be described by generalized Langevin equations. Starting with the microscopic motion of the colloids we use the Zwanzig-Mori projection operator formalism to derive equations of motion for correlation functions. To close the equations, suitable mode-coupling approximations (slowing down of the dynamics due to the caging by neighboring particles) are used. Introducing a logarithmically spaced wavevector grid we investigate the long-wavelength behavior of the system. The velocity autocorrelation function of a tagged particle decays algebraically as $\propto t^{-5/2}$ rather than exponentially due to repeated interactions. Comparing the collective dynamics with the self-dynamics for different packing fractions near the glass transition we find that contrary to the self-dynamics the collective dynamics do not slow down.

DY 43.9 Thu 12:15 H3

**Controlled dispersion in periodic microchannels and regular obstacle parks** — •Matthieu Mangeat[1,2], Thomas Guérin[1], and David S. Dean[1] — [1]Univ. Bordeaux and CNRS, LOMA, Talence, France — [2]Universität des Saarlandes, Saarbrücken, Germany

The dispersion of Brownian particles in heterogeneous media is a widely studied problem which appears in many contexts (chemical reactions, biological systems, zeolites, porous media, pollutant spreading, ...). A cloud of particles disperses over time without reaching the Boltzmann equilibrium distribution and its spreading is then characterized by an effective long-time diffusivity $D_e$ lower than the microscopic diffusivity. The analytical expression of $D_e$ is given by an exact Kubo-type formula [Phys. Rev E **92**, 062103 (2015)] for periodic systems. The dispersion in periodic microchannels is controlled by the confinement geometry via an entropic trapping. Three different dispersion regimes are then identified for continuous and discontinuous channels [EPL **118**, 40004 (2017)]. The expression of $D_e$ is thus well-described by the Fick-Jacobs' approximation, narrow escape problems or the diffusion problem in comb-like geometries in each regime. This analysis can be extended to the dispersion in regular obstacle parks. The presence of short-range attractive potential on the surface of obstacles enhance the dispersion of Brownian particles. The optimal value of $D_e$ is then analytically characterized in the dilute limit of obstacles.

DY 43.10 Thu 12:30 H3

**Orientational and directional locking of colloidal clusters driving across periodic surfaces** — •Xin Cao[1], Emanuele Panizon[2], Andrea Vanossi[2,3], Nicola Manini[4], and Clemens Bechinger[1] — [1]Fachbereich Physik, University Konstanz, 78464 Konstanz, Germany — [2]International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy — [3]CNR-IOM Democritos National Simulation Center, Via Bonomea 265, 34136 Trieste, Italy — [4]Dipartimento di Fisica, Universita degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy

When isolated particles are driven over atomically corrugated crystalline surfaces, their trajectories do not necessarily follow the applied force but become locked to directions imposed by the substrate symmetry. Such directional locking is relevant for the manipulation and steering of nano-objects on surfaces. Contrary to previous studies which have been performed for single particles, here we study the motion of extended crystalline clusters composed of colloidal particles on a periodic surface. We observe that both their orientational and their center-of-mass motion become locked in the presence of a driving force. Contrary to single particles, the locking directions do not coincide with the substrate symmetry, but are determined by the geometrical moiré superstructure of the cluster-substrate contact. For certain incommensurabilities, competing locking directions exist and a cluster may spontaneously switch from one direction to another depending on its size. Our research provides insights to the transport of crystalline islands on top of crystalline surfaces.

DY 43.11 Thu 12:45 H3

**The cage effect in systems of hard spheres** — •Hans Joachim Schöpe[1] and William van Megen[2] — [1]Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10,72076 Tübingen, Germany — [2]Department of Applied Physics, Royal Melbourne Institute of Technology, Melbourne, Victoria 3000, Australia

The cage effect is generally invoked when discussing the delay in the decay of time correlation functions of dense fluids. In an attempt to examine the role of caging more closely we consider the temporal evolution of the displacement distributions of Brownian particles. In an equilibrium fluid these distributions are necessarily biased by the presence of neighbouring particles. Accommodation of this bias by those neighbours conserves the displacement distribution locally and it presents a collective mechanism for exploring configuration space that is more efficient than the intrinsic Brownian motion. In contrast caging of some particles incurs a delayed, non-local collective transport process due to the fact that of the displacement distribution must be conserved globally. Both collective mechanisms incur delay or stretching of time correlation functions, in particular the particle number and flux densities [1]. We identify and distinguish these mechanisms in existing data from experiments [2,3] and computer simulations [4] on systems of particles with hard sphere interactions.

[1] J. Chem. Phys. 146, 104503 (2017) [2] Phys. Rev. Lett. 103 (25) (2009) [3] 4th International Symposium on Slow Dynamics in Complex Systems: Tohoku Univ, edited by M. Tokuyama and I. Oppenheim (2013), Vol. 1518, pp. 214-221 [4] Nature Comm. 5 (2014)

DY 43.12 Thu 13:00 H3

**Memory-induced acceleration and slowdown of barrier crossing** — •Julian Kappler[1,2], Jan O. Daldrop[1], Florian N. Brünig[1], Moritz D. Boehle[1], and Roland R. Netz[1] — [1]Freie Universität Berlin, 14195 Berlin, Germany — [2]Cambridge University, Cambridge CB3 0WA, United Kingdom

We study the mean first-passage time $\tau_{\mathrm{MFP}}$ for the barrier crossing of a single massive particle with non-Markovian memory by Langevin simulations in one dimension. Compared to the Markovian case, we find barrier crossing to be accelerated for intermediate memory time, while for long memory time, barrier crossing is slowed down and $\tau_{\mathrm{MFP}}$ increases with $\tau_\Gamma$ as a power law $\tau_{\mathrm{MFP}} \sim \tau_\Gamma^2$. A simple and globally accurate heuristic formula for $\tau_{\mathrm{MFP}}$ in terms of all relevant time scales of the system is presented and used to establish a scaling diagram featuring the Markovian overdamped and the Markovian inertial regimes, as well as the non-Markovian intermediate memory time regime where barrier crossing is accelerated and the non-Markovian long memory time regime where barrier crossing is slowed down.