DY 37: Brownian Motion and Anomalous Diffusion

Time: Thursday 15:00–17:15 Location: H43

DY 37.1 Thu 15:00 H43

A universal class of exactly solvable diffusions — •Costantino Di Bello[1], Edgar Roldan[2], and Ralf Metzler[1] — [1]Potsdam University, Institute of Physics and Astronomy, Potsdam-Golm, Germany — [2]ICTP, Quantitative Life Sciences section, Trieste, Italy

We consider a general one-dimensional overdamped diffusion model described by the Ito stochastic differential equation (SDE) $dX_t = \mu(X_t, t)dt + \sigma(X_t, t)dW_t$, where W_t is the standard Wiener process. We obtain a specific condition that μ and σ must fulfill in order to be possible to solve the SDE via mapping the generic process, using a suitable space-time transformation, into the simpler Wiener process. By taking advantage of this transformation, we obtain the propagator in the case of open, reflecting, and absorbing boundary conditions for a large class of diffusion processes. With the same technique, we were also able to derive the first passage time (FPT) statistics of a large class of models. Moreover, as many physical observables in stochastic thermodynamics are described by an SDE of the same form, our result can provide the analytical expression of the probability distribution of many observables like work, entropy et similia. We stress the fact that our results are valid for many non-autonomous, non-linear and non-homogeneous processes.

DY 37.2 Thu 15:15 H43

Thermodynamic bounds on generalized transport: From single-molecule to bulk observables — •Cai Dieball and Aljaž Godec — Mathematical bioPhysics Group, Max Planck Institute for Multidisciplinary Sciences, 37077 Göttingen, Germany

We prove that the transport of any scalar observable in d-dimensional non-equilibrium systems is bounded from above by the total entropy production scaled by the amount the observation "stretches" microscopic coordinates. The result, a time-integrated generalized speed limit, reflects the thermodynamic cost of transport of observables, and places underdamped and overdamped stochastic dynamics as well as deterministic motion on equal footing. Our work fills an important gap in thermodynamic inference, since microscopic dynamics is, at least for short times, underdamped. Requiring only averages but not sample-to-sample fluctuations, the proven transport bound is practical and applicable not only to single-molecule but also bulk experiments where only averages are observed, which we demonstrate by examples.

[1] Phys. Rev. Lett. 133, 067101 (2024)

DY 37.3 Thu 15:30 H43

Foundation of classical dynamical density functional theory: uniqueness of time-dependent density–potential mappings — Michael Andreas Klatt[2,3,1], •Christian Bair[1], Hartmut Löwen[1], and René Wittmann[1,4] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität, Düsseldorf, Germany — [2]Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für KI Sicherheit, Ulm, Germany — [3]DLR, Institut für Materialphysik im Weltraum, Köln, Germany — [4]Institut für Sicherheit und Qualität bei Fleisch, Max Rubner-Institut, Kulmbach, Germany

When can we uniquely map a classical density profile to an external potential? In equilibrium, without time dependence, the one-body density is known to uniquely specify the external potential that is applied to the many-body system. This mapping from a density to the potential is the cornerstone of classical density functional theory (DFT). Here, we consider non-equilibrium, time-dependent many-body systems that evolve from a given initial condition. We derive explicit conditions, for example, no flux at the boundary, that ensure that the mapping from the density to a time-dependent external potential is unique. We thus prove the underlying assertion of dynamical density functional theory (DDFT) - without resorting to the so-called adiabatic approximation often used in applications. By ascertaining uniqueness for all n-body densities, we ensure that the proof - and the physical conclusions drawn from it - hold for general superadiabatic dynamics of interacting systems.

DY 37.4 Thu 15:45 H43

Phase locking and fractional Shapiro steps in collective dynamics of microparticles — •Seemant Mishra[1], Artem Ryabov[2], and Philipp Maass[1] — [1]Institut für Physik, Universität Osnabrück, Germany — [2]Charles University, Faculty of Mathematics and Physics, Czech Republic

Nonlinear systems under time-periodic driving often exhibit phase locking, where synchronization between the system's dynamics and driving leads to robust stationary states. In this work, we show that phase-locked dynamics in a driven system of hardcore-interacting microparticles arises from running solitary cluster waves. Such cluster waves were recently predicted to occur in overdamped Brownian motion [1,2] and shortly after confirmed in experiments [3]. Particle currents are related to soliton velocities due to a unit displacement law saying that the total average shift of all particle positions per soliton period equals one wavelength of the periodic potential. The collective particle dynamics synchronize with the driving for certain particle diameters only. Based on an effective potential for solitary wave propagation, we derive dynamical phase diagrams of integer and fractional synchronization modes.

[1] A. P. Antonov, A. Ryabov, P. Maass, Phys. Rev. Lett. 129, 080601 (2022).
[2] A. P. Antonov, A. Ryabov, P. Maass, Chaos, Solitons & Fractals 132, 115079 (2024).
[3] E. Cereceda-López, A. P. Antonov, A. Ryabov, P. Maass, and P. Tierno Nat. Commun. 14, 6448 (2023).

DY 37.5 Thu 16:00 H43

Modeling charge attachment induced ion transport in glasses — •Quinn Emilia Fischer and Philipp Maass — Department of Physics, Universität Osnabrück, Germany

In charge attachment induced ion transport (CAIT), material foreign mobile ions can replace native mobile ions near the surface of a glass below the glass transition temperature. Insight into the ion dynamics during CAIT experiments is provided by measurements of near-surface concentration profiles.

We discuss the modeling of concentration profiles by coupling the Poisson equation to kinetic equations of linear irreversible thermodynamics. Solving the kinetic equations requires knowledge on the dependance of both the Onsager coefficients and chemical potentials of the mobile ions on the ion concentrations.

We show how chemical potentials can be derived for a model, where mobile ions occupy sites in a disordered energy landscape, and how Fermi energies are generalized to a system of multiple ion types. We further explain the determination of Onsager coefficients by modeling thermally activated hopping motion in the energy landscape and the relation between the coefficients and ion mobilities.

The dependence of both the Onsager coefficients and the chemical potentials on mobile ion concentration is sensitive to the form of the energy landscape. It is argued that this sensitivity needs to be taken into account in a consistent theoretical modeling of CAIT experiments, which requires solutions of the coupled Poisson and kinetic equations to reproduce measured concentration profiles.

DY 37.6 Thu 16:15 H43

Local and Diffusive Dynamics of Interlayer Lithium ions in Synthetic Fluoro-Hectorites: ^{2}H and^{7}Li NMR-Study — •Jepsinraj Kakkuzhiyulla Parambath and Michael Vogel — TU Darmstadt, Institut for Condensed Matter Physics, Hochschulstr. 6, 64289, Darmstadt, Germany

Investigating ion transport is a crucial part of developing robust devices for energy storage and sensors. Fluoro-Hectorite, a clay mineral of the Smectite group serves as a model material for this investigation, specifically Lithium Hectorite with the structural formula of $Li_{0.5}[Mg_{2.5}Li_{0.5}]Si_4O_{10}F_2$ and a layered structure. Due to the swelling properties of the Hectorites, the interlayer spacing and thus the degree of confinement can be varied with water content. The charge transports results from interlayer lithium ions, which are dissolved in water. The Hectorite confinements provide mechanical stability and guide the charge carriers over long distances, leading to fast ion transport [Hiebl et al., Chem. Mater. 2020, 32, 7445]. We use ^{2}H and ^{7}Li NMR to study the dynamics of the interlayer water molecules and lithium ions. Spin lattice relaxometry studies of local dynamics, including field cycling and static field gradient(SFG) measurements of diffusive dynamics show a strong dependence on the interlayer spacing.

DY 37.7 Thu 16:30 H43

Random Walks of Intermittently Self-Propelled Particles — Agniva Datta[1], Carsten Beta[1,2], and •Robert Grossmann[1] — [1]University of Potsdam, Potsdam, Germany — [2]Kanazawa University, Kanazawa, Japan

We present a dynamical model of intermittently self-propelled particles: active particles that recurrently switch between two modes of motion, namely an active run-state and a turn state, in which self-propulsion is absent. The durations of these motility modes are drawn from arbitrary waiting-time distributions. We derive the expressions for exact forms of transport characteristics like mean-square displacements and diffusion coefficients to describe such processes. Furthermore, the conditions for the emergence of sub- and superdiffusion in the long-time limit are presented. We give examples of some important processes that occur as limiting cases of our system, including run-and-tumble motion of bacteria, Lévy walks, hop-and-trap dynamics, intermittent diffusion and continuous time random walks. We eventually apply this modeling framework to describe bacterial swimming in polysaccharide matrices.

DY 37.8 Thu 16:45 H43

First-passage time for generalized telegrapher's processes under stochastic resetting — •Trifce Sandev — Macedonian Academy of Sciences and Arts, Skopje, Macedonia — Ss. Cyril and Methodius University in Skopje, Macedonia — Korea University, Seoul, Korea

We consider different generalizations of the telegrapher's process. One possible generalization is the so-called subordinated telegrapher's process, which can be obtained from the standard telegrapher's process subordinated by Lévy noise. Another possible generalization is a heterogeneous telegrapher's process which is a stochastic process with a multiplicative dichotomic noise and a position-dependent velocity. For both cases we analyze the non-equilibrium stationary states approached in the long time limit, as well as the survival probability, the first-passage time density and the mean first-passage time in the presence of Poissonian stochastic resetting of the particle to the initial position.

1 T. Sandev, A Iomin, *Phys. Rev. E* **110**, 024101 (2024)

2 K. Górska, F. J. Sevilla, G. Chacón-Acosta, T. Sandev, *Entropy* **26**, 665 (2024)

3 P. Jolakoski, P. Trajanovski, A. Iomin, L. Kocarev, T. Sandev, sibmitted (2024)

DY 37.9 Thu 17:00 H43

Diffusion and Homogeneous Linewidth – Phthalocyanine on Solid Rare-Gas Clusters — •Philipp Elsässer, Arne Morlok, Ulrich Bangert, Li Yilin, Felix Riedel, Lukas Bruder, Frank Stienkemeier, and Tanja Schilling — Institute of Physics, University of Freiburg, Hermann-Herder-Straße 3, 79104 Freiburg, Germany

Doped clusters are an important tool in the spectroscopy of organic molecules and the study of basic properties of confined quantum systems. It is crucial in these structures to understand the characteristics of the configurations between dopant and cluster. The binding sites may vary over time due to diffusion. Because of this, the diffusion behavior is valuable to characterize doped clusters.

We have studied the diffusion of free-base phthalocyanine (H_2Pc) on solid, icosahedral, rare-gas clusters of argon and neon by molecular dynamics simulations. We observe on both systems that the spacial motion of H_2Pc is confined on a single face of the icosahedron. The rotational movement of the molecule shows a cluster-size dependent anomalous-diffusive behavior on a picosecond timescale. This overall anomalous diffusion is in agreement with the homogeneous line width broadening observed in action-based two-dimensional electronic spectroscopy experiments.