DY 26: Brownian Motion, Transport and Anomalous Diffusion

Time: Tuesday 10:00–13:15 Location: HÜL 186

DY 26.1 Tue 10:00 HÜL 186

Topological solitons driven through grain boundaries — •Xin Cao[1], Emanuele Panizon[1,2], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, 78464 Konstanz, Germany — [2]International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy

Topological solitons, or kinks, widely exists in materials and at interfaces. They play important roles in the elastic deformation of metals and alloys and in the mobility of nano contacts. Here, by driving such solitons through grain boundaries in colloidal crystals, we study the influence of such boundaries to the dynamics of solitons. We show that when small solitons are travelling through the grain boundaries, their motion is delayed at the grain boundary with the delay time depending on the driving force. In contrast large extended solitons are splitted upon approaching grain boundaries. Afterwards they split into several smaller solitons due to variations in the delay times at different regions of the grain boundary. At small driving forces, solitons are not able to cross grain boundaries which leads to their accumulation (pile up) at these locations. In addition to the time delay, splitting and pile up of solitons, we also found that the grain boundary can reflect incoming solitons when driving forces are parallel to the grain boundary. Such reflections strongly depend on the mismatch of lattice orientations at the grain boundary and can be used for the controlled guiding of solitons.

DY 26.2 Tue 10:15 HÜL 186

Transport and Constrictivity in Porous Media — •Johannes Hauskrecht and Rudolf Hilfer — Institute for Computational Physics, University of Stuttgart, Germany

Geometric quantities such as porosity and physical quantities such as permeability determine transport in porous media. The constrictivity, on the other hand, which is intended to describe the influence of cross-sectional variations of the pore space on transport, is a less-used quantity. It is therefore an interesting question whether transport in porous media can be characterized additionally with the help of this quantity.

Existing definitions of constrictivity from the literature and their relation to the macroscopic transport coefficients have been investigated. In general, they can be divided into physical and geometrical definitions. The physical definitions directly relate the constrictivity to the transport coefficients, the geometrical definitions, on the other hand, calculate the constrictivity directly from the pore structure. However, most of the geometrical definitions are only defined for simplified models of the pore space and are ill defined for general pore spaces. In addition, it is shown for homogeneous and isotropic media that the existing geometrical definitions of constrictivity can be expressed as a variation of porosity.

DY 26.3 Tue 10:30 HÜL 186

Heterogeneous diffusion with(out) stochastic resetting — •Trifce Sandev[1,2,3], Viktor Domazetoski[1], Aleksei Chechkin[2,4], Ljupco Kocarev[1,3], and Ralf Metzler[2] — [1]Macedonian Academy of Sciences and Arts — [2]University of Potsdam — [3]Ss. Cyril and Methodius University in Skopje — [4]Akhiezer Institute for Theoretical Physics, Kharkov

We analyze diffusion processes with finite propagation speed in heterogeneous media in terms of the telegrapher's or Cattaneo equation with position-dependent diffusion coefficient. In the diffusion limit of infinite-velocity propagation we recover the results for diffusion equations with position-dependent diffusivity. We observe various diffusive regimes including hyperdiffusion, ballistic motion, superdiffusion, normal diffusion and subdiffusion. We further consider heterogeneous diffusion process under stochastic resetting. We find exact results for the mean squared displacement and the probability density function for three different stochastic interpretations of the multiplicative process. The stationary distributions reached in the long time limit are derived as well. The obtained results are verified by numerical simulations employing the Langevin equation with position dependent diffusivity in different stochastic calculi.

DY 26.4 Tue 10:45 HÜL 186

Cooperatively enhanced reactivity and stabilitaxis of dissociating oligomeric proteins — •Jaime Agudo-Canalejo[1], Pierre Illien[2], and Ramin Golestanian[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), D-37077 Göttingen, Germany — [2]Sorbonne Université, CNRS, Laboratoire PHENIX, UMR CNRS 8234, 75005 Paris, France — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

Many functional units in biology, such as enzymes or molecular motors, are composed of several subunits that can reversibly assemble and disassemble. This includes oligomeric proteins composed of several smaller monomers, as well as protein complexes assembled from a few proteins. By studying the generic spatial transport properties of such proteins, we investigate here whether their ability to reversibly associate and dissociate may confer them a functional advantage with respect to nondissociating proteins. In uniform environments with position-independent association-dissociation, we find that enhanced diffusion in the monomeric state coupled to reassociation into the functional oligomeric form leads to enhanced reactivity with distant targets. In non-uniform environments with position-dependent association-dissociation, caused e.g. by spatial gradients of an inhibiting chemical, we find that dissociating proteins generically tend to accumulate in regions where they are most stable, a process that we term 'stabilitaxis'.

DY 26.5 Tue 11:00 HÜL 186

Influence of fractional hydrodynamic memory on superdiffusion and supertransport in tilted washboard potentials — •Igor Goychuk — Friedrich-Alexander Universität Erlangen-Nürnberg — Universität Augsburg, Germany

Diffusion in tilted washboard potentials can paradoxically exceed free normal diffusion [1]. The effect becomes much stronger in the underdamped case due to inertial effects [2]. What happens upon inclusion of usually neglected fractional hydrodynamics memory effects (Basset-Boussinesq frictional force), which result in a heavy algebraic tail of the velocity autocorrelation function of the potential-free diffusion making it transiently superdiffusive? Will a giant enhancement of diffusion become even stronger, and the transient superdiffusion last even longer? These are the basic questions which we answer [3] based on an accurate numerical investigation. We show that a resonance-like enhancement of normal diffusion becomes indeed much stronger and sharper. Moreover, a long-lasting transient regime of superdiffusion, including Richardson-like diffusion, $\langle \delta x^2(t) \rangle \propto t^3$ and ballistic supertransport, $\langle \delta x(t) \rangle \propto t^2$, is revealed.

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[2] I. G. Marchenko and I. I. Marchenko, EPL **100**, 50005 (2012); B. Lindner and I. M. Sokolov, Phys. Rev. E **93**, 042106 (2016).
[3] I. Goychuk, Phys. Rev. Lett. **123**, 180603 (2019), Editors' Suggestion.

DY 26.6 Tue 11:15 HÜL 186

Hydrodynamics of Active Levy Matter — Andrea Cairoli and •Chiu Fan Lee — Imperial College, London, U.K.

Collective motion emerges spontaneously in many biological systems such as bird flocks, insect swarms and tissue under dynamic reorganization. This phenomenon is often modeled within the framework of active fluids, where the constituent active particles, when interactions with other particles are switched off, perform normal diffusion at long times. However, single-particle superdiffusion and fat-tailed displacement statistics are also widespread in biology. The collective properties of interacting systems exhibiting such anomalous diffusive dynamics – which we call active Levy matter – cannot be captured by current active fluid theories. Here, we formulate a hydrodynamic theory of active Levy matter by coarse-graining a microscopic model of aligning polar active particles performing superdiffusive Levy flights. We then perform a linear stability analysis at the onset of collective motion and find that in contrast to its conventional counterpart, the order-disorder transition can become critical. We further support our analytical predictions with simulation results. This work not only highlights the need for more realistic models of active matter integrating both anomalous diffusive motility and inter-particle interactions, but also potentially enriches the universal properties of active systems.

15 min. break.

DY 26.7 Tue 11:45 HÜL 186

Subdiffusion in the Anderson model on random regular graph — •Giuseppe De Tomasi[1], Soumya Bera[2], Antonello Scardicchio[3], and Ivan Khaymovich[4] — [1]TUM Munich/Cambridge University — [2]IIT Bombay — [3]ICTP Trieste — [4]MPIPKS Dresden

We study the finite-time dynamics of an initially localized wave-packet in the Anderson model on the random regular graph (RRG) and show the presence of a subdiffusion phase coexisting both with ergodic and putative non-ergodic phase. The full probability distribution Π(x,t) of a particle to be at some distance x from the initial state at time t, is shown to spread subdiffusively over a range of disorder strengths. The comparison of this result with the dynamics of the Anderson model on Z^d lattices, $d > 2$, which is subdiffusive only at the critical point implies that the limit d $\to \infty$ is highly singular in terms of the dynamics. A detailed analysis of the propagation of Π(x,t) in space-time (x,t) domain identifies four different regimes determined by the position of a wave-front $X_{\mathrm{front}}(t)$, which moves subdiffusively to the most distant sites $X_{\mathrm{front}}(t) \sim t^{\beta}$ with an exponent $\beta < 1$.

DY 26.8 Tue 12:00 HÜL 186

Entropic contribution to surface diffusion barriers of oligophenyls — •Mila Miletic[1], Karol Palczynski[1,2], and Joachim Dzubiella[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universität, Freiburg, Germany

Surface diffusion is usually described by Arrhenius laws, with a diffusion energy barrier in the exponent and a prefactor. The prefactor contains not only the jump length and attempt frequency but also contributions of the system's entropy to the diffusion. However, the decomposition into these three contributions is often unclear, which hampers the interpretation of the prefactor. We successfully perform such a decomposition for single oligophenyl molecules of different length on an amorphous silica surface using atomistic molecular dynamics simulations, and find meaningful values for the jump length, attempt frequency and entropy of the adsorbates. We systematically increase the molecular length, from a single phenyl ring, up to six phenyl rings and study the influence of the increase in length on surface diffusion and binding. First, we find a substantial difference in entropy of about one order of magnitude between the shortest and longest adsorbates and entropy contributions to the diffusion barrier of about 20-30%. Second, as for the binding to the surface, we find that longer molecules display higher binding free energies with substantial entropic contributions coming from the increase in internal degrees of freedom with the molecular length. Our results demonstrate that it is essential for investigations of surface diffusion to consider entropic effects.

DY 26.9 Tue 12:15 HÜL 186

A finite-radius stochastic action — •Julian Kappler and Ronojoy Adhikari — Department of Applied Mathematics and Theoretical Physics, Cambridge University, Cambridge, United Kingdom

A fundamental question associated with Langevin dynamics is to quantify the (relative) probability of individual trajectories. Due to the singular nature of an individual stochastic trajectory, quantifying its probability is both technically challenging, and the result is not directly related to any physical observable. We regularize the singular concept of an individual trajectory by considering the tubular ensemble, which consists of all stochastic trajectories that remain within a ball of small but finite radius, and with moving center given by a smooth reference path. We derive the finite-radius generalization of the Onsager-Machlup stochastic action, characterize explicitly the stochastic dynamics within the tubular ensemble, and generalize the well-known single-trajectory entropy to the tubular ensemble. Our work thus establishes the finite-radius tubular ensemble as a useful extension of a single stochastic trajectory. In particular, introducing a finite threshold distance in the discussion of path probabilities, and relating experimental observables to the Onsager-Machlup action, brings the latter within reach of direct measurement.

DY 26.10 Tue 12:30 HÜL 186

Infinite-densities and the Moses, Noah and Joseph effects in Levy walks — •Erez Aghion[1], Vidushi Adlakha[2], Kevin Bassler[2], Holger Kantz[1], and Philipp Meyer[1] — [1]mpiPKS, Dresden, Germany — [2]U. Huston, Dep. of Physics, USA

When one is presented with an ensemble of data sets, each obtained as a time series, for example in an experiment, which anomalous diffusion, it is often not possible to know exactly the details of the underlying dynamics that produced it. The braking of the CLT can be decomposed into three root causes: temporal correlations in the process, statistical aging, and power-law distributions, known respectivley as the Joseph, Moses and Noah effects. These effects, are quantified individually, and measured individually from the time series.

We study this decomposition using numerical simulations, which are compared with analytical results, for a coupled Levy walk model, where the particle's velocity v at each step is decays nonlinearly with the step-duration Tau. The step durations are independent, identically distributed random variables, taken from the fat tailed distribution where the mean <Tau> is divergent. Here, recently it was shown [Akimoto et al., 2019] that the velocity distribution of the particles converges to a non-normalizable infinite-invariant density, when t approaches infinity. This scenario is tantamount to a sort-of "temporal equilibrium", when we rescale the probability density properly with time. We study how this leads to a different manifestation of the three effects, depending on whether infinite-ergodic theory describes the time-average of |v| or v^2.

DY 26.11 Tue 12:45 HÜL 186

Hydrodynamic resistance matrices of colloidal particles with various shapes* — Johannes Voss and •Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

The hydrodynamic resistance matrix encodes the shape- and size-dependent hydrodynamic properties of a colloidal particle that is suspended in a liquid. It determines the particle's diffusion tensor and is typically needed when modeling the motion of purely Brownian, externally driven, or self-propelled colloidal particles or the behavior of dilute suspensions of such particles on the basis of Langevin equations, Smoluchowski equations, dynamical density functional theory, or other appropriate methods. So far, however, the hydrodynamic resistance matrix is available only for selected particle shapes. In this talk, we present and compare the hydrodynamic resistance matrices for various additional particle shapes that are relevant for current research, including apolar and polar as well as convex and partially concave shapes. The elements of the hydrodynamic resistance matrices are given as functions of shape parameters like the aspect ratio of the corresponding particle so that the results apply to continuous sets of particle shapes. This opens up new possibilities for studying the dynamics of colloidal particles with anisometric and even variable shapes.
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DY 26.12 Tue 13:00 HÜL 186

Hot Brownian Motion in the Ballistic Timescale — •Xiaoya Su[1], Alexander Fischer[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 times. Yet, the ballistic 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 5ns. We show how the mean squared displacement of the particle from the nanoseconds to the seconds 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.