DY 60: Anomalous Diffusion (joint session DY/BP)

Time: Thursday 10:00–13:15 Location: BH-N 334

DY 60.1 Thu 10:00 BH-N 334

Frequency-dependent Hydrodynamic Interaction Between Two Nanocolloids — •Gerhard Jung and Friederike Schmid — Institut für Physik, Staudingerweg 9, 55128 Mainz

The dynamics of fluids are subject of extensive research since over 300 years. In the second book of the "Principa" Newton investigates the dynamics of viscous fluids to disprove the Cartesian idea that the planetary orbits are created by fluid vortices. Since then this problem has drawn the attention of many great physicists and mathematicians. However, there are still many fundamental questions in the field of fluid dynamics like for example the understanding of hydrodynamic interactions between two particles submerged in a fluid. The first and most basic analytic derivation was published by Oseen describing the interaction between two point particles in a steady-state Stokes flow.

Based on work by Ardekani et al. we extended this approach by considering finite-sized particles in an unsteady compressible flow, described by the linearized Navier-Stokes equations [1]. This theoretical extension enables us to compare results from hydrodynamic theory to molecular dynamics simulations of nanocolloids in a Lennard-Jones fluid. We show that the simulation data agree qualitatively and quantitatively with our theoretical findings. The analytic results can therefore be used to include dynamically consistent hydrodynamic interactions into non-Markovian coarse-grained models.

[1] G. Jung, F. Schmid, accepted by the Journal Physics of Fluids

DY 60.2 Thu 10:15 BH-N 334

Anomalous Diffusion in Complex Dynamical Systems: Diffusing Diffusivity Models — •Rohit Jain and Kizhakeyil L Sebastian — Indian Institute of Science, Bangalore 560012, India

Diffusion inside a crowded, rearranging environment has attracted a lot of attention recently [1]. In such systems, the mean square displacement of diffusing particle remains Fickian obeying $\langle x^2 \rangle \propto T$, yet the distribution of displacements is not Gaussian. Following the work of Chubynsky and Slater [2], we have proposed a class of analytically solvable models where the diffusion coefficient becomes a random function of time [3]. The results obtained with our model are in very good agreement with the simulations of Chubynsky and Slater (see also [4]).

In a different model [5], we have analyzed a case where diffusivity evolves as a Lévy flight process. That is, the distribution of diffusivity decays as power-law of the form $D^{-1-\alpha}$ with $0 < \alpha < 1$, for large D. The distribution of displacements with this model is found to be a Lévy stable distribution with a time dependent width. With this model, the dynamics is Brownian at short times and superdiffusive at long times.

References:
[1] Wang et. al., Proc. Natl. Acad. Sci. U.S.A., **106**, 15160 (2009).
[2] Chubynsky and Slater, Phys. Rev. Lett. **113**, 098302 (2014).
[3] Jain and Sebastian, J. Phys. Chem. B **120**, 3988 (2016).
[4] Chechkin et. al., Phys. Rev. X **7**, 021002 (2017).
[5] Jain and Sebastian, Phys. Rev. E **95**, 032135 (2017).

DY 60.3 Thu 10:30 BH-N 334

First-passage properties of Gaussian interfaces — •Markus Gross — MPI-IS Stuttgart / Uni Stuttgart

Fluctuating interfaces are relevant in various circumstances, such as liquid phase separation, nanofluidics, or surface growth. An effective description of the interfacial dynamics is provided by the Edwards-Wilkinson and the stochastic Mullins-Herring equations, corresponding to non-conserved and conserved dynamics. Despite the Gaussian nature of these models, their first-passage properties are highly nontrivial due to the presence of long-range correlations along the interface. We study here the full spatio-temporal evolution of an interface until it reaches a given maximum height for the first time. Analytical predictions, obtained within weak-noise theory, are contrasted to results of numerical Langevin simulations of the first-passage problem. It is shown the averaged profile shape is accurately captured by weak-noise theory, but the time evolution (specifically, the dynamic exponent) is not. The latter can instead be accounted for within a reduced model based on a fractional Brownian walker, which describes the anomalous diffusion of a tagged monomer of the interface as it approaches an absorbing boundary.

References: M. Gross, arXiv:1708.03466, 1708.03467

DY 60.4 Thu 10:45 BH-N 334

Sinai type diffusion in Gaussian random potentials with decaying spatial correlations — •Igor Goychuk[1], Vasyl O. Kharchenko[2], and Ralf Metzler[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany — [2]Institute of Applied Physics, Natl. Acad. Sci. Ukraine, Sumy, Ukraine

Logarithmic subdiffusion is usually associated with random force disorder and non-stationary potential fluctuations whose root mean squared amplitude grows with distance. We show that such Sinai type diffusion also universally emerges at sufficiently low temperatures in stationary Gaussian random potentials with spatially decaying correlations, known to exist in a broad range of physical systems. Combining results from extensive simulations with a scaling approach we elucidate the physical mechanism of this unusual subdiffusion. In particular, we explain why with growing temperature and/or time a first crossover occurs to standard, power-law subdiffusion and then a second crossover occurs to normal diffusion with a disorder-renormalized diffusion coefficient. Interestingly, the initial, nominally ultraslow diffusion turns out to be much faster than the universal de Gennes-Bässler-Zwanzig limit of the renormalized normal diffusion, which realistically cannot be attained at sufficiently low temperatures and/or for strong disorder. The ultraslow diffusion is also shown to be non-ergodic and it displays a local bias phenomenon. Our simple scaling theory not only explains our numerical findings, but also has a predictive character.

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DY 60.5 Thu 11:00 BH-N 334

Random diffusivity from stochastic equations: two models in comparison for Brownian yet non-Gaussian diffusion. — •Vittoria Sposini[1,2], Aleksei V. Chechkin[1,3], Flavio Seno[4], Gianni Pagnini[2], 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 — [4]INFN, Padova Section and Department of Physics and Astronomy 'G.Galilei', University of Padova, 35131 Padova, Italy

Recently a considerable number of systems have been discovered exhibiting a Brownian yet non-Gaussian dynamics, characterised by a linear growth in time of the mean-squared displacement yet a non-Gaussian probability density function of the particle displacement. This behaviour observed in very different physical systems has been interpreted as resulting from diffusion in inhomogeneous environments and mathematically represented through a variability of the diffusion coefficient. Indeed different models describing a fluctuating diffusivity have been studied. Here it is presented a set of stochastic equations describing a time dependent random diffusivity within a broad spectrum of distributions: the class defined as generalised Gamma distribution. Two models for particles spreading in such variable environments are then studied. The first belongs to the class of generalised grey Brownian motion while the second follows from the idea of diffusing diffusivity. We promote these two physical models for the description of stochastic particle motion in complex environments.

DY 60.6 Thu 11:15 BH-N 334

Infinite invariant densities in intermittent systems — •Philipp Meyer[1], Eli Barkai[2], and Holger Kantz[1] — [1]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, D 01187, Dresden, Germany — [2]Department of Physics, Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Ramat-Gan, 52900, Israel

Dynamical intermittency is known to generate anomalous statistical behaviour of dynamical systems, a prominent example being the Pomeau-Manneville map. The system exhibits waiting times and chaotic bursts. For a wide range of parameters no physical invariant density exists. We show how this regime can be characterised quantitatively using the techniques of infinite invariant densities and the Thaler-Dynchin limit theorem.

We obtain pseudo Brownian motion by summing up the increments created by the map. The output corresponds to stochastic processes like continuous time random walks. We are able to relate infinite ergodic theory with scale invariant transport. Here time average diffusivities are especially interesting, because they depend not only on the joint probability density function but also on the exact definition of the paths during waiting periods.

We also present a nonlinear oscillator, i.e., a physical model in continuous time, whose properties in terms of weak ergodity breaking and ageing have a one-to-one correspondence to the properties of the Pomeau-Manneville map. We see how expectation values exhibit ageing in terms of scaling in time.

15 min. break

DY 60.7 Thu 11:45 BH-N 334

Tempered dynamics from fractional Brownian motion and generalized Langevin equation: Application to lipid molecule diffusion — •Trifce Sandev[1,2,3], Daniel Molina-Garcia[4,5], Gianni Pagnini[4], Aleksei Chechkin[5], and Ralf Metzler[5] — [1]Ss. Cyril and Methodius University in Skopje, Macedonia — [2]RSD, Skopje, Macedonia — [3]MANU, Skopje, Macedonia — [4]BCAM - Basque Center for Applied Mathematics, Bilbao, Basque Country, Spain — [5]University of Potsdam, Germany

Anomalous diffusion is widely observed in many systems. Often, the system shows a crossover from initial anomalous diffusion to terminal normal diffusion. We consider tempered versions of the fractional Brownian motion and the generalized Langevin equation (GLE) to describe this crossover dynamics. For persistent input noise, the former describes the case when an initially superdiffusive particle switches to normal diffusive behavior, while the latter exhibits a subdiffusive to normal diffusive crossover. Both models are characterized by power-law correlations of the driving noise, i.e., tempered fractional Gaussian noise, which is a noise with Gaussian amplitude and power-law correlations with a cutoff at some mesoscopic time scale. In both models we employed either hard (exponential) or soft (power-law) truncation. We show excellent agreement of the analytical results for the mean squared displacement obtained from the GLE with those obtained for the lipid dynamics in simulated model membranes [1].

[1] D. Molina-Garcia, T. Sandev, G. Pagnini, A. Chechkin, and R. Metzler, in preparation.

DY 60.8 Thu 12:00 BH-N 334

Kinetics of an enzymatic reaction under anomalous diffusion - A case study — •Daniela Froemberg and Felix Höfling — Freie Universität Berlin, Department of Mathematics and Computer Science

The interior of biological cells constitutes a crowded environment in which diffusion of organelles or macromolecules is anomalous[1]. Consequently, such heterogeneous conditions also alter the kinetics of the chemical reactions taking place.

Here, we report on simulations of the reaction-diffusion dynamics of an enzyme-catalyzed reaction using a particle-based scheme. The particles diffuse in space and reactions occur with a certain microscopic propensity if the reaction partners are within a prescribed reaction distance. To mimick a crowded environment, we implement the subdiffusion by a fractional Brownian motion.

For anomalous diffusion, it is well-known that the the diffusion coefficient is a function of the lag time. Similarly, the coefficient $k(t)$ of the effective reaction rate can adopt a timescale dependence. Preliminary results from extensive simulations suggest a power law dependence of $k(t)$, slowing down the reaction as compared to the normal diffusive case.

We detail the behavior of $k(t)$, elucidate the role of the subdiffusion parameter, and test for an old prediction originally made for reactions on fractals.

[1] F. Höfling, T. Franosch, Rep. Prog. Phys. 76 (2013) 046602 (50pp)

DY 60.9 Thu 12:15 BH-N 334

Obstructed Motion – from frozen to mobile obstacles — Christoph Zunke, René Hermann, Manuel A. Escobedo-Sanchez, Jörg Bewerunge, •Florian Platten, and Stefan U. Egelhaaf — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

Many natural and industrial processes rely on transport through confined spaces. Confinement by obstacles, for example in porous materials or crowded environments, leads to anomalous diffusion. An idealized situation, the diffusion of point-like tracers through the voids between randomly-placed fixed obstacles, is described by the Lorentz model. Beyond a critical obstacle concentration, the obstacles percolate and hence form finite voids that confine the tracers. Thus the tracer motion becomes localized. However, often the obstacles are mobile, e.g., proteins in biological membranes or organelles in cells. We developed a colloidal model system which permits to tune the particle dynamics through the application of a laser light field. It allows us to study the effect of obstacle mobility. If the obstacles are sufficiently mobile, localization of the tracers is avoided and transient subdiffusion is observed.

DY 60.10 Thu 12:30 BH-N 334

Scaled Brownian motion with resetting — •Anna Bodrova[1], Alexei Chechkin[2,3], and Igor Sokolov[1] — [1]Humboldt University, Department of Physics, Newtonstrasse 15, 12489 Berlin, Germany — [2]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [3]Akhiezer Institute for Theoretical Physics, Kharkov Institute of Physics and Technology, Kharkov 61108, Ukraine

In the intermittent stochastic processes the dynamics of the system may be interrupted and recommenced at random times from the initial condition. Examples of such processes are found in many fields such as chemistry, biology, ecology and computer science. The time between resetting events may be distributed according to the exponential law or according to the power law. It may be shown that random resetting fundamentally changes the properties of the diffusion process. In the presence of resetting there is a competition between the tendency of diffusive spreading and confinement around the initial state. In our study during the resetting events the particle performs scaled Brownian motion: diffusive motion with time-dependent diffusion coefficient. We calculate mean-squared displacement and probability density function as main characteristics of this process.

DY 60.11 Thu 12:45 BH-N 334

Self-trapping self-repelling random walks — •Peter Grassberger — Juelich Research Center, Juelich, Germany

The model studied in this talk is a seemingly minor modification of the "true self-avoiding walk" (TSAW) model of Amit, Parisi, and Peliti in two dimensions. The walks in it are self-repelling up to a characteristic time T^* (which depends on various parameters), but spontaneously (i.e., without changing any control parameter) become self-trapping after that. For free walks, T^* is astronomically large, but on finite lattices the transition is easily observable. In the self-trapped regime, walks are subdiffusive and intermittent, spending longer and longer times in small areas until they escape and move rapidly to a new area. In spite of this, these walks are extremely efficient in covering finite lattices, as measured by average cover times.

Basically, the phenomenon is due to a delicate balance between two opposite effects of landscape gradients and roughnesses on random walks: While a gradient enhances diffusion, roughness slows it down. Initially, the walker creates a hill by depositing debris, and the hill gradient wins. But the hill surface is also rough. When roughness becomes too large, the walk becomes subdiffusive which increases further the roughness, leading finally to catastrophic trapping.

The phenomenon seems to be described by scaling laws, and some exponent and critical parameter values seem to be simple rationals. In addition, the deposited debris forms (on square lattices and for some parameter values) non-trivial patterns that suddenly re-arrange at sharp times.

DY 60.12 Thu 13:00 BH-N 334

Non-Gaussian Brownian and viscoelastic diffusion — •Ralf Metzler — Institute of Physics & Astronomy, U Potsdam, Potsdam

Brownian motion as well as viscoelastic anomalous diffusion are stochastic processes driven by Gaussian noise. A growing number of systems is reported in which the mean squared displacement is linear or anomalous, yet the associated probability densities are non-Gaussian. Examples include Brownian motion with exponential probability density for the motion of colloidal beads along tubular structures or in semiflexible polymer networks. Stretched Gaussian shapes along with Brownian motion are seen for the motion of cells on surfaces. Viscoelastic, anomalous motion is observed for submicron tracers in both bacteria and yeast cells. In many systems, at sufficiently long times a crossover to Gaussian behaviour is observed.

In this presentation I will introduce the various observations of non-Gaussian diffusion. In particular, I will report large scale simulations of lipid bilayer systems: in the dilute case viscoelastic and Gaussian diffusion is observed, while in protein-crowded situations stretched Gaussians are observed. This behaviour can, to a good extent, be explained due to geometric constrictions on the motion. I will then introduce a mathematical model for the description of non-Gaussian motion in terms of a stochastically varying diffusion coefficient. In the short time limit this approach is equivalent to the known approach of superstatistics, while at long times a crossover to Gaussian statistics with an effective diffusivity is found.