CPP 5: Anomalous Diffusion (joint session DY, CPP)

Time: Monday 9:30–12:00 Location: BH-N 334

CPP 5.1 Mon 9:30 BH-N 334

Anomalous diffusion in corrugated potentials with spatial correlations: faster than normal, and other surprises — •Igor Goychuk — Institute for Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam-Golm, Germany

Normal diffusion in corrugated potentials with spatially uncorrelated Gaussian energy disorder famously explains the origin of non-Arrhenius $\exp[-\sigma^2/(k_BT)^2]$ temperature-dependence in disordered systems. We show [1] that unbiased diffusion remains asymptotically normal also in the presence of spatial correlations decaying to zero. However, due to a temporal lack of self-averaging transient subdiffusion emerges on mesoscale, and it can readily reach macroscale even for moderately strong disorder fluctuations of $\sigma \sim 4-5\,k_BT$. Due to its nonergodic origin such subdiffusion exhibits a large scatter in single trajectory averages. However, at odds with intuition, it occurs essentially faster than one expects from the normal diffusion in the absence of correlations. We apply these results to diffusion of regulatory proteins on DNA molecules and predict that such diffusion should be anomalous, but much faster than earlier expected on a typical length of genes for a realistic energy disorder of several room k_BT, or merely $0.05-0.075$ eV.

[1] I. Goychuk and V. Kharchenko, Phys. Rev. Lett. **113**, 100601 (2014).

CPP 5.2 Mon 9:45 BH-N 334

Path Probabilities of Continuous Time Random Walks — •Stephan Eule — MPI fuer Dynamik und Selbstorganisation

Employing the path integral formulation of a broad class of anomalous diffusion processes, we derive exact relations for path probability densities of these processes. In particular, we obtain a closed analytical solution for the path probability distribution of a Continuous Time Random Walk (CTRW) process. This solution is given in terms of its waiting time distribution and short time propagator of the corresponding random walk as a solution of a Dyson equation. Applying our analytical solution we derive generalized Feynman-Kac formulae.

CPP 5.3 Mon 10:00 BH-N 334

Nonergodicity in scaled Brownian motion — •Felix Thiel and Igor M. Sokolov — Institut für Physik der Humboldt Universität zu Berlin: Newtonstraße 15, 12489 Berlin, Deutschland

Scaled Brownian motion (sBm) is a random process described by a diffusion equation with explicitly time-dependent diffusion coefficient (Batchelor's equation), which is often used for fitting experimental data for subdiffusion of unclear genesis. We show that it describes the rescaled mean position of a cloud of independent continuous time random walkers. Like the latter, sBm is neither stationary nor ergodic. Unlike continuous time random walks, the nonergodicity of sBm is not accompanied by a strong difference between its different realizations: its heterogeneity ("ergodicity breaking") parameter tends to zero for long trajectories.

CPP 5.4 Mon 10:15 BH-N 334

Understanding and Controlling Regime Switching in Molecular Diffusion — •Sarah Hallerberg[1] and Astrid S. de Wijn[2] — [1]Network Dynamics, Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen — [2]Department of Physics, Stockholm University

Diffusion can be strongly affected by ballistic flights (long jumps) as well as long-lived sticking trajectories (long sticks). Using statistical inference techniques in the spirit of Granger causality, we investigate the appearance of long jumps and sticks in molecular-dynamics simulations of diffusion in a prototype system, a benzene molecule on a graphite substrate. We find that specific fluctuations in certain, but not all, internal degrees of freedom of the molecule can be linked to either long jumps or sticks. Furthermore, by changing the prevalence of these predictors with an outside influence, the diffusion of the molecule can be controlled. The approach presented in this proof of concept study is very generic, and can be applied to larger and more complex molecules. Additionally, the predictor variables can be chosen in a general way so as to be accessible in experiments, making the method feasible for control of diffusion in applications. Our results also demonstrate that data-mining techniques can be used to investigate the phase-space structure of high-dimensional nonlinear dynamical systems.

Phys. Rev. E 90, 062901, 2014

CPP 5.5 Mon 10:30 BH-N 334

Optimisation of search efficiency by combination of Levy flights and Brownian motion — •Vladimir V. Palyulin — Physics Department, Technical University of Munich, D-85747 Garching, Germany

Problems of target search occur in a wide range of applications ranging from animals looking for prey to diffusion control of molecular processes. For a long time the field was dominated before by a notion, that Lévy flights with a critical exponent $\alpha = 1$ are optimal. Recently we proved that this statement is not always correct, and often Brownian motion presents a better alternative [1]. In this new study we show that intermittent search, which consists of Lévy flights and Brownian motion presents even better alternative. In order to show that we computed an average of inverse rate of target location, which works as a good measure of search efficiency. Analytical and numerical results are obtained from fractional Fokker-Planck equation and supported by Monte-Carlo simulations.

[1] V.V. Palyulin, A.V. Chechkin and R. Metzler, Proc. Natl. Acad. Sci. USA, **111**, 2931 (2014).

15 min. break

CPP 5.6 Mon 11:00 BH-N 334

Single-file diffusion in a quenched energy landscape — •Henning Krüsemann[1] and Ralf Metzler[1,2] — [1]University of Potsdam, Potsdam, Germany — [2]Tampere University of Technology, Tampere, Finland

The diffusion of hardcore interacting particles in a narrow (1D) channel is called single-file diffusion. Examples in physics can be found especially in biophysics, e.g. the transport of molecules through a narrow pore.

The dynamical properties in a single file differ strongly from those of freely diffusing particles and different types of subdiffusion can be observed.

In this talk we discuss the msd of single-file diffusion with different particle interactions in a quenched energy landscape. We present simulation results and approach the problem theoretically.

CPP 5.7 Mon 11:15 BH-N 334

Dynamical consequences of oriented particles interacting with their fractal surrounding — •Janett Prehl[1], René Haber[1], Heiko Herrmann[1,2], and Karl Heinz Hoffmann[1] — [1]Institut für Physik, Technische Universiät Chemnitz, Chemnitz, Deutschland — [2]Centre for Nonlinear Studies, Tallinn University of Technology, Tallinn, Estland

In order to model diffusive particles in porous media, often random walks of point particles on fractals are utilized as model system. It exhibits subdiffusive behavior, where the anomalous diffusion exponent is smaller than one, and the corresponding random walk dimension is larger than two. This is due to the limited space available in fractal structures. Within this presentation we endow the particles with an orientation [1, 2] and analyze their dynamics on fractal structures. In particular, we focus on the dynamical consequences of the interactions between the local surrounding fractal structure and the particle orientation, which are modeled using an appropriate move class. These interactions can lead to particles becoming temporarily or permanently stuck in parts of the structure. A surprising finding is that the random walk dimension is not affected by the orientation while the diffusion constant shows a variety of interesting and surprising features.

[1] R. Haber, J. Prehl, K. H. Hoffmann, and Heiko Herrmann, *J. Phys. A: Math. Theor.* **47** (2014) 155001
[2] R. Haber, J. Prehl, H. Herrmann, and K. H. Hoffmann, *Phys. Lett. A* **377** (2013) 2840–2845

CPP 5.8 Mon 11:30 BH-N 334

Fractal grid comb model — •Trifce Sandev[1,2], Alexander Iomin[2,3], and Holger Kantz[2] — [1]Radiation Safety Directorate,

Partizanski odredi 143, P.O. Box 22, 1020 Skopje, Macedonia — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany — [3]Department of Physics, Technion, Haifa 32000, Israel

A grid comb model is a generalization of the well known comb model, and it consists of N backbones. For N=1 the system reduces to the comb model where subdiffusion takes place with the transport exponent 1/2. We present an exact analytical evaluation of the transport exponent of anomalous diffusion for finite and infinite number of backbones. We show that for an arbitrarily large but finite number of backbones the transport exponent does not change. Contrary to that, for an infinite number of backbones (fractal grid comb), the transport exponent depends on the fractal dimension of the backbone structure. Thus, the grid comb model, suggested here, establishes an exact relation between a complicated fractal geometry and the transport exponent. Such a product structure of backbones times comb is an idealization of more complex comb-like fractal networks, as they may appear e.g., in certain anisotropic porous media.

CPP 5.9 Mon 11:45 BH-N 334

On diffusivity landscapes in soft matter — •Felix Roosen-Runge[1] and Dominique J. Bicout[1,2] — [1]Institut Laue-Langevin, Grenoble, France — [2]UMR 5525, CNRS and Université Grenoble 1, France

The concept of energy landscapes has been successfully and extensively applied for the understanding of a broad range of phenomena in complex soft matter systems, such as the glass transition and protein folding. However, many experimental accounts – e.g. single-particle tracking, scattering methods and diffusion MRI – access dynamical properties, and not the free energy landscape directly. Thus, it is important to understand and exploit the effects of diffusivity landscapes, i.e. an inhomogeneous diffusivity and viscosity. First, we discuss applicability, implications and limitations of the concept of diffusivity landscapes. Second, we provide analytical approximate solutions for the diffusion equation in dynamically heterogeneous environments. Third, the results can be connected to experiments on e.g. water diffusion in hydration shells, or tracer diffusion through membranes or porous structures.