Symposium Anomalous Diffusion in Complex Environments (SYAD)

jointly organized by
the Biological Physics Division (BP),
the Dynamics and Statistical Physics Division (DY), and
the Chemical and Polymer Physics Division (CPP)

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Anomalous diffusion in complex environments has received much attention in recent years. Examples range from active Brownian motion of self-propelled particles, and subdiffusive dynamics in crowded environments, to collective motion and escape problems in anomalous random walks.

Living cells take advantage of the anomalous motion in many ways. While subdiffusion in crowded cytoplasm is beneficial for a variety of cellular functions which depend on the localization of the involved reactants, active motion of motor proteins along cytoskeletal filaments makes long-distance intracellular transport feasible. Cell crawling and migration exhibit other interesting aspects of anomalous motion. The motility of cells and their ability to recognize and react to environmental changes are crucial for an efficient immune response. The motion of self-motile colloidal particles, which use a chemical reaction catalyzed on their surface to swim, is an example of artificial active matter where the directed propulsion subject to fluctuations leads to anomalous diffusion.

Among other topics, collective motion of anomalous random walkers seems to become one of the fascinating directions of current research. Little is known about how the particles may coordinate their motion when they individually perform anomalous random walk. Anomalous motion also complicates the search strategies and escape problems. While first passage problems in confined geometries have been thoroughly investigated for ordinary random walks or combinations of a few simple walks, there is a need to revisit such problems under realistic conditions such as self- propelled motion of tracer particles in cells. The goal of this symposium is to bring together the experts in soft condensed matter and biological systems, and overview the recent advances, ideas and concepts of anomalous transport in theory and experiment.

Overview of Invited Talks and Sessions

(Lecture room H15)

Invited Talks

SYAD 1.1	Thu	15:00–15:30	H15	**Phenomenology of Collective Chemotaxis in Artificial and Living Active Matter** — •Ramin Golestanian
SYAD 1.2	Thu	15:30–16:00	H15	**First-passage times of Markovian and non Markovian random walks in confinement** — •raphael Voituriez
SYAD 1.3	Thu	16:00–16:30	H15	**Cytoskeleton organization as an optimized, spatially inhomogeneous intermittent search strategy** — •Heiko Rieger, Yannick Schröder, Karsten Schwarz
SYAD 1.4	Thu	16:45–17:15	H15	**Ergodicity violation and ageing in living biological cells** — •Ralf Metzler
SYAD 1.5	Thu	17:15–17:45	H15	**Anomalous diffusion within cells** — Sarah Klein, •Cecile Appert-Rolland, Ludger Santen

Sessions

SYAD 1.1–1.5	Thu	15:00–17:45	H15	**Anomalous Diffusion in Complex Environments**
SYAD 2.1–2.6	Tue	14:00–15:30	H47	**Anomalous Diffusion (Joint Session with DY)**
SYAD 3.1–3.6	Thu	11:30–13:00	H45	**BP Focus Session: Anomalous Diffusion in Complex Environments**

SYAD 1: Anomalous Diffusion in Complex Environments

Time: Thursday 15:00–17:45 Location: H15

Invited Talk SYAD 1.1 Thu 15:00 H15
Phenomenology of Collective Chemotaxis in Artificial and Living Active Matter — •Ramin Golestanian — University of Oxford

The non-equilibrium dynamics of active particles that send and receive chemical signals could lead to enhanced and/or anomalous diffusion, as well as spontaneous formation of interesting structures and patterns due to the long-range nature of the interactions. We examine theoretically the consequences of this interaction, and present some results that exemplify the type of emergent properties that could result from them, including: spontaneous formation of small stable clusters or "molecules" that can exhibit functionality that depends on geometry, collective chemotaxis in a solution of catalytically active colloids that could lead to cluster formation, aster condensation, and spontaneous oscillations, swarming - in the form of a comet - of light-induced thermally active colloids with negative Soret coefficient due to a shadowing interaction, and collective behaviour of a colony of cells that divide and interact chemotactically.

Invited Talk SYAD 1.2 Thu 15:30 H15
First-passage times of Markovian and non Markovian random walks in confinement — •raphael Voituriez — CNRS/ Université Pierre et Marie Curie, Paris, France

The first-passage time is a key quantity for evaluating the kinetics of various processes, and in particular chemical reactions involving "small" numbers of particles. A striking example is given by gene transcription, where specific proteins search for target sequences on DNA. I will present asymptotic results which enable the evaluation of the distribution of the first-passage time to a target site for a wide range of random processes in confined domains, and show how these results can be extended to non Markovian processes.

Invited Talk SYAD 1.3 Thu 16:00 H15
Cytoskeleton organization as an optimized, spatially inhomogeneous intermittent search strategy — •Heiko Rieger, Yannick Schröder, and Karsten Schwarz — Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany

The efficiency of intracellular transport of cargo from specific source to target locations is strongly dependent upon molecular motor assisted motion along cytoskeleton filaments, microtubules and actin. Radial transport along microtubules and lateral transport along the filaments of the actin cortex underneath the cell membrane are characteristic for cells with a centrosome. Here we show that this specific filament organization for ballistic transport in conjunction with intermittent diffusion realizes a spatially inhomogeneous intermittent search strategy that is in general optimal for small thicknesses oft he actin cortex. We prove optimality in terms of mean first passage times for three different, frequently encountered intracellular transport tasks: 1) the narrow escape problem (e.g. transport of cargo to a synapse or other specific region of the cell membrane), 2) reaction kinetics enhancement (e.g. binding of two mobile reaction partners within the cell), 3) the reaction-escape problem (e.g. release of cargo at a synapse after intracellular vesicle pairing). Since homogeneous search strategies could only be realized by completely filling the search volume with randomly oriented cytoskeleton filaments, our results indicate that living cells realize optimal search strategies for various intracellular transport problems *economically* through a spatial cytoskeleton organization that involves only small amounts of randomly oriented actin filaments.

15 min break

Invited Talk SYAD 1.4 Thu 16:45 H15
Ergodicity violation and ageing in living biological cells — •Ralf Metzler — Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany

In 1905 Einstein formulated the laws of diffusion, and in 1908 Perrin published his Nobel-prize winning studies determining Avogadro's number from diffusion measurements. With similar, more refined techniques the diffusion behaviour in complex systems such as the motion of tracer particles in living biological cells is nowadays measured with high precision. Often the diffusion turns out to deviate from Einstein's laws.

This talk will discuss the basic mechanisms leading to anomalous diffusion as well as point out the physical and biological consequences, for instance, in gene regulation or cargo transport in cells. In particular the unconventional behaviour of non-ergodic, ageing systems will be discussed. Concrete examples include the motion of submicron and nanoprobes in biological cells, uncrowded and crowded lipid membranes, as well as interacting many particle systems.

Invited Talk SYAD 1.5 Thu 17:15 H15
Anomalous diffusion within cells — Sarah Klein[1,2], •Cecile Appert-Rolland[1], and Ludger Santen[2] — [1]Laboratory of Theoretical Physics, CNRS, Univ. Paris-Sud, Bat 210, 91405 Orsay, France — [2]Fachrichtung Theoretische Physik, Univ. des Saarlandes D-66123 Saarbrücken, Germany

Within cells, various objects (vesicles, organelles,...) need to be transported. Some processive molecular motors get attached to these objects (or cargos) to form a complex that will have a stochastic motion along a network of microtubules. Intriguingly, there is some evidence that this motion results from a tug-of-war between teams of motors that pull in opposite directions.

A stochastic model for cargo-motors complex allows us to study the properties of the resulting motion along a single microtubule. We find some anomalous diffusion, both subdiffusive or superdiffusive depending on the timescale. Interestingly, such anomalous diffusion has indeed been observed experimentally. I will discuss the importance of fluctuations in the dynamics, and present some hypotheses why nature chose such a transport process to carry cargos through the crowded interior of cells.

[Klein, Appert-Rolland, Santen, EPL 107 (2014) 18004,
Eur. Phys. J. Special Topics 223 (2014) 3215,
EPL 111 (2015) 68005]

SYAD 2: Anomalous Diffusion (Joint Session with DY)

Time: Tuesday 14:00–15:30 Location: H47

SYAD 2.1 Tue 14:00 H47
Diffusion and subdiffusion of interacting particles on comblike structures — •Pierre Illien[1], Olivier Bénichou[2], Gleb Oshanin[2], Alessandro Sarracino[2], and Raphaël Voituriez[2] — [1]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, UK — [2]Laboratoire de Physique Théorique de la Matière Condensée, Université Pierre-et-Marie-Curie, Paris, France

The subdiffusive motion of tracers in crowded media, e.g., biological cells, is widespread, and has motivated a large amount of theoretical work related to diffusion in complex media. Comblike structures have received a particular interest as they constitute minimal models of systems with geometrical constraints. Here, we investigate the effect of excluded-volume interactions on tracer diffusion on such lattices.

We study the dynamics of a tracer particle (TP) on a comb lattice populated by randomly moving hardcore particles. When the TP is constrained to move on the backbone of the comb and in the limit of high density of the particles, we present exact analytical results for the cumulants of the TP position, showing a subdiffusive behavior $t^{3/4}$. At longer times, a second regime is observed where standard diffusion is recovered, with a surprising nonanalytical dependence of the diffusion coefficient on the particle density. When the TP is allowed to visit the teeth of the comb, we unveil a rich and complex scenario with several successive subdiffusive regimes, resulting from the coupling between the geometrical constraints of the lattice and particle interactions. In this case, remarkably, the presence of hard-core interactions asymptotically speeds up the TP motion along the backbone of the structure.

SYAD 2.2 Tue 14:15 H47

Anomalous transport of circular swimmers in disordered structures: classical edge-state percolation — •Thomas Franosch[1], Walter Schirmacher[2], Benedikt Fuchs[3], and Felix Höfling[4] — [1]UIBK Innsbruck — [2]Universität Mainz — [3]Med.-Uni Wien — [4]FU Berlin

Recently micron-sized self-propelled particles have been realized as model systems [1] for complex living organisms such as bacteria. If the agent is asymmetric a natural circular motion [2] emerges which yields characteristic skipping orbits when interacting with boundaries.

Here, we investigate by molecular dynamics simulations the dynamics of circular swimmers in a two-dimensional model with randomly distributed scatterers. For small radii of the swimming motion the agents orbit only around isolated clusters of scatterers, while at large radii diffusive behavior emerges. A de-localization transition occurs which is generated by percolating skipping orbits along the edges of obstacle clusters. Directly at the transition the mean-square displacements displays subdiffusive transport. The dynamic exponents differ from those of the conventional transport problem on percolating systems, thus establishing a new dynamic universality class [3]. Last, we draw an analogy to the field-induced localization transition in magnetotransport in 2D electron gases in a disordered array of antidots.

[1] F. Kümmel, et al., Phys. Rev. Lett. **110**, 198302 (2013).

[2] S. van Teeffelen and H. Löwen, Phys. Rev. E **78**, 020101(R) (2008).

[3] W. Schirmacher, B. Fuchs, F. Höfling, and T. Franosch, Phys. Rev. Lett. (2015, in print).

SYAD 2.3 Tue 14:30 H47

Scales of Function Spaces for Weyl Fractional Calculus — •Tillmann Kleiner and Rudolf Hilfer — Institute for Computational Physics, University of Stuttgart, Germany

Anomalous diffusion models are frequently based on fractional differential equations [1]. Analytical investigations of these mathematical models require suitable function spaces on which the fractional derivatives operate as continuous operators. This contribution introduces function spaces suitable for Weyl fractional calculus. Scales of locally convex spaces with topology generating seminorms are constructed using weighted maximal functions. These scales are sets of spaces partially ordered by inclusion. Minimal and maximal spaces with respect to this ordering are determined such that Weyl fractional derivatives operate on them continuously or isomorphically. Such spaces can also be determined for sets of linear combinations of these operators with orders restricted to some fixed subset of $\mathbb{C}$. Inclusions of spaces within the scale correspond to continuous injections with dense range. As a result the investigated operators and their inverses are continuous extensions from the subspace of test functions for all suitable spaces.

[1] *Applications of Fractional Calculus in Physics*, edited by R. Hilfer (World Scientific, Singapore, 2000).

SYAD 2.4 Tue 14:45 H47

A simple non-chaotic map generating subdiffusive, diffusive, and superdiffusive dynamics — Lucia Salari[1], Lamberto Rondoni[1,2], Claudio Giberti[3], and •Rainer Klages[4,5] — [1]Dipartimento di Scienze Matematiche, Politecnico di Torino — [2]GraphenePoliTO Lab, Politecnico di Torino and INFN Sezione di Torino — [3]Dipartimento di Scienze e Metodi dell' Ingegneria, Universita di Modena e Reggio E. — [4]Max Planck Institute for the Physics of Complex Systems, Dresden — [5]School of Mathematical Sciences, Queen Mary University of London

Consider equations of motion that generate dispersion of an ensemble of particles in the long time limit. An interesting problem is to predict the diffusive properties of such a dynamical system starting from first principles. Motivated by numerical results on diffusion in polygonal billiards, we introduce an interval exchange transformation lifted onto the whole real line that mimicks deterministic diffusion in these billiards. By definition our simple map model is not chaotic, in the sense of exhibiting a vanishing Lyapunov exponent. We show analytically that it nevertheless displays a whole range of normal and anomalous diffusion under variation of a single control parameter [1].

[1] L. Salari et al., Chaos **25**, 073113 (2015)

SYAD 2.5 Tue 15:00 H47

Localisation of ballistic tracers in the two-dimensional Lorentz model interpreted as a renormalisation group flow — •Felix Höfling — Fachbereich Mathematik und Informatik, Freie Universität Berlin — Max-Planck-Institut für Intelligente Systeme, Stuttgart, und IV. Institut für Theoretische Physik, Universität Stuttgart

The Lorentz model serves as a minimal model to explain many facets of the rich phenomenology of anomalous transport, as frequently observed in porous materials and cellular transport [1]. Here, I will discuss the localisation transition of "ballistic" tracers (subject to Newton's equations of motion) in the two-dimensional, overlapping Lorentz model. Extensive simulations provide evidence for the universality of the dynamic critical exponent, which has been crucial in the interpretation of recent studies [2,3]. The long-time asymptotes, however, are obscured by non-universal corrections to scaling, explaining the contradicting values for the diffusivity exponent in the literature. A spectral analysis of the obtained correlation functions allows for an interpretation of the dynamics as an renormalisation flow of the transport at long times and gives insight into the fixed point structure of the RG flow.

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

[2] S. K. Schnyder, M. Spanner, F. Höfling, T. Franosch, and J. Horbach, Soft Matter **11**, 701 (2015).

[3] W. Schirmacher, B. Fuchs, F. Höfling, and T. Franosch, arXiv:1511.05218, Phys. Rev. Lett. in print (2015).

SYAD 2.6 Tue 15:15 H47

Non-adiabatic quantum pumping by a randomly moving quantum dot [1] — •Daniel Waltner[1] and Stanislav Derevyanko[2] — [1]Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Department of Physics of Complex Systems, Weizmann Institute of Science, Rehovot 76100, Israel

We look at time dependent fluctuations of the electrical charge in an open 1D quantum system represented by a quantum dot experiencing random lateral motion. In essentially non-adiabatic settings we study both diffusive and ballistic (Levy) regimes of the barrier motion where the electric current as well as the net pumped electric charge experience random fluctuations over the static background. We show that in the large-time limit, the wavefunction is naturally separated into the Berry-phase (BP) component (resulting from the singular part of the wave amplitude in the co-moving frame) and the non-adiabatic correction (arising from fast oscillating, slow decaying tails of the same amplitude). Based on this separation we report two key results: firstly, the disorder averaged wave function and current are asymptotically mainly determined by the same BP contribution that applies in the case of adiabatic motion. Secondly, after a short transition period the pumped electric charge exhibits fluctuations that grow much faster than predicted by the adiabatic theory. We also derive the exact expressions for the average propagator (in the co-moving basis representation) for the diffusive and ballistic types of motion considered.

[1] S. Derevyanko, D. Waltner, J. Phys. A **48** (2015) 305302

SYAD 3: BP Focus Session: Anomalous Diffusion in Complex Environments

Joint session with DY, organized by Reza Shaebani and Ludger Santen, Saarland University, for BP.

Time: Thursday 11:30–13:00 Location: H45

SYAD 3.1 Thu 11:30 H45

Apparent Super-Diffusion Induced by Trail-Mediated Self-Interaction of Microorganisms — •Till Kranz, Anatolij Gelimson, and Ramin Golestanian — Rudolf-Peierls Centre for Theoretical Physics, University of Oxford

Many microorganisms, namely surface bound bacteria [1] and amoeboid slime moulds [2], leave trails of sticky substances. We will present a simple model of a self-propelled microorganism whose propulsion force depends on the concentration of trail material [3]. The trail-mediated self-interactions of a single microorganism and its own trail profoundly alter the dynamics. Above a critical interaction strength with the trail a discontinuous localisation transition emerges. Close to the transition, the orientational dynamics becomes super-diffusive and, in fact, super-ballistic, on a diverging timescale. Interestingly, no such super-diffusive regime appears for the translational dynamics. We will discuss the implications for real biological systems and the interplay of their finite timescales with the emergent diverging timescale.

[1] K. Zhao *et al.*, Nature **497**, 388 (2013)
[2] B. Rodiek and M. J. B. Hauser, EPJ ST **224**, 1199 (2015)
[3] W. T. Kranz, A. Gelimson, and R. Golestanian, arXiv:1504.06814

SYAD 3.2 Thu 11:45 H45

Transport of active Brownian particles in complex environments — •Maria Zeitz and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany

From the perspective of physics, biological microswimmers such as bacteria can be viewed as active particles. Since bacteria often inhabit porous or crowded environments, we examine the dynamics and transport of active particles in a complex environment. We focus on active Brownian particles (APB), which provide a simple model for microswimmers. ABPs have an intrinsic speed and perform rotational as well as translational diffusion.

We study the transport of ABPs moving in a two-dimensional environment of randomly placed and fixed obstacles of a given area fraction ϕ_o. For increasing ϕ_o we observe a transition from diffusive transport to trapping on long time scales, which happens close to the percolation threshold of the void space $1 - \phi_0 \approx 0.67$. The behavior on long time scales is universal and depends only on the obstacle density and not on the intrinsic dynamics of the particle. However, on time scales much shorter than the rotational diffusion time, we find ballistic transport and on intermediate timescales we find subdiffusive transport. The crossover times between the three regimes depend not only on ϕ_o but also on the details of particle propulsion, e.g. Peclét number.

In a second step we study how obstacles can serve as nucleation seeds for clustering in collective motion of ABPs and therefore promote clogging.

SYAD 3.3 Thu 12:00 H45

Impact of detachment frequency on transport dynamics of cytoskeletal motor proteins — •Anne E Hafner, M Reza Shaebani, Ludger Santen, and Heiko Rieger — Department of Theoretical Physics, Saarland University, Saarbrücken, Germany

Cytoskeletal motor proteins are involved in key intracellular transport processes which are vital for maintaining appropriate cellular function. The motors exhibit distinct states of motility: active motion along filaments, and inactive state in which the motor detaches from the filament and remains effectively stationary by performing passive diffusion in the vicinity of the detachment point due to cytoplasmic crowding until it attaches again to the cytoskeleton. The rates of transitions between motion and pause states are considerably affected by changes in environmental conditions which influences the efficiency of cargo delivery to specific targets. By considering the motion of molecular motor on a single filament as well as a dynamic filamentous network, we present an analytical model for the dynamics of self-propelled particles which undergo frequent pause phases, and validate the theoretical predictions by performing extensive Monte Carlo simulations. The transition rates between the two states drastically change the dynamics: multiple transitions between different types of anomalous diffusive dynamics may occur and the crossover time to the asymptotic diffusive or ballistic motion varies by several orders of magnitude. We map out the phase diagrams in the space of transition rates, and address the role of initial conditions of motion on the resulting dynamics.

SYAD 3.4 Thu 12:15 H45

The Power Spectrum of Ionic Nanopore Currents: The Role of Ion Correlations — •mira zorkot, Ramin Golestanian, and Douwe Jan Bonthuis — Rudolf Peierls Centre for Theoretical Physics, Oxford University, Oxford, OX13NP, United Kingdom

Measuring the ionic current passing through a nanometer-scale membrane pore has emerged over the past decades as a versatile technique to study molecular transport. These measurements su*er from high noise levels that typically exhibit a power law dependence on the frequency. A thorough theoretical understanding of the power spectrum is essential for the optimisation of experimental setups and for the use of measurement noise as a novel probe of the nanopores microscopic properties.

We calculate the power spectrum of electric-*field-driven ion transport through nanopores using both linearized mean-fi*eld theory and Langevin dynamics simulations. With only one *tting parameter, the linearized mean-*field theory accurately captures the dependence of the simulated power spectrum on the pore radius and the applied electric *field. Remarkably, the linearized mean-*field theory predicts a plateau in the power spectrum at low frequency f, which is con*rmed by the simulations at low ion concentration. At high ion concentration, however, the power spectrum follows a power law that is reminiscent of the 1/f dependence found experimentally at low frequency. Based on simulations with and without ion-ion interactions, we attribute the low-frequency power law dependdence to ion-ion correlations.

SYAD 3.5 Thu 12:30 H45

Fluctuation relations for anomalous dynamics generated by time fractional Fokker-Planck equations — Peter Dieterich[1], •Rainer Klages[2,3], and Aleksei V. Chechkin[2,4,5] — [1]Institut fuer Physiologie, Technische Universitaet Dresden — [2]Max Planck Institute for the Physics of Complex Systems, Dresden — [3]Queen Mary University of London, School of Mathematical Sciences — [4]Institute for Theoretical Physics NSC KIPT, Kharkov, Ukraine — [5]Institute of Physics and Astronomy, University of Potsdam

Anomalous dynamics characterized by non-Gaussian probability distributions (PDFs) and/or temporal long-range correlations can cause subtle modifications of conventional fluctuation relations (FRs). As prototypes we study three variants of a generic time-fractional Fokker-Planck equation with constant force. Type A generates superdiffusion, type B subdiffusion and type C both super- and subdiffusion depending on parameter variation. Furthermore type C obeys a fluctuation-dissipation relation whereas A and B do not.We calculate analytically the position PDFs for all three cases and explore numerically their strongly non-Gaussian shapes. While for type C we obtain the conventional transient work FR, type A and type B both yield deviations by featuring a coefficient that depends on time and by a nonlinear dependence on the work.We discuss possible applications of these types of dynamics and FRs to experiments.

P. Dieterich et al., New J. Phys. **17**, 075004 (2015)

SYAD 3.6 Thu 12:45 H45

Induced anomalous diffusion nearby cell membranes — •Abdallah Daddi-Moussa-Ider, Achim Guckenberger, and Stephan Gekle — Biofluid Simulation and Modeling, University of Bayreuth, 95440 Bayreuth, Germany

The approach of a small particle to the cell membrane represents the crucial step before active internalization and is governed by thermal diffusion. Using a fully analytical theory, we show that the membrane induces a long-lived subdiffusive behavior on the nearby particle, during which the residence time is increased by up to 50 % for a typical scenario. The corresponding scaling exponent is found to be as low as 0.87 in the perpendicular direction, and as low as 0.92 in the parallel direction. Such behavior is qualitatively different from the normal diffusion near a hard wall or in a bulk fluid. A good agreement is found for the frequency dependent mobility between the analytical predictions and the numerical simulations that we performed using a boundary integral method.