DY 27: Transport and Anomalous Diffusion

Time: Thursday 14:30–17:15 Location: MA 004

Topical Talk DY 27.1 Thu 14:30 MA 004
Single particle trajectories and weak ergodicity breaking in ageing systems — •Ralf Metzler — Inst for Physics & Astronomy, University of Potsdam, Germany — Physics Dept, Tampere University of Technology, Finland

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 such anomalous diffusion as well as point out its consequences. In particular the unconventional behaviour of non-ergodic, ageing systems will be discussed within the framework of continuous time random walks. Indeed, non-ergodic diffusion in the cytoplasm of living cells as well as in membranes has recently been demonstrated experimentally.

DY 27.2 Thu 15:00 MA 004
Fluctuations of time averages for Langevin dynamics in a binding force field — •Andreas Dechant[1], Eric Lutz[2], David A. Kessler[3], and Eli Barkai[3] — [1]Department of Physics, Universität Augsburg, D-86356 Augsburg, Germany — [2]Department of Physics, Freie Universität Berlin, D-14195 Berlin, Germany — [3]Department of Physics, Institute of Nanotechnology and Advanced Materials, Bar Ilan University, Ramat Gan 52900, Israel

We derive a simple formula for the fluctuations of the time average around the thermal mean for overdamped Brownian motion in a binding potential. Using a backward Fokker-Planck equation, introduced by Szabo et al. in the context of reaction kinetics, we show that for ergodic processes these finite measurement time fluctuations are determined by the Boltzmann measure. For the widely applicable logarithmic potential, ergodicity is broken. We quantify the large non-ergodic fluctuations and show how they are related to a super-aging correlation function.

DY 27.3 Thu 15:15 MA 004
Fractional Brownian ratchets — •Igor Goychuk[1] and Vasyl Kharchenko[1,2] — [1]Institute of Physics, University of Augsburg, Universitätstr. 1, D-86135 Augsburg, Germany — [2]Institute of Applied Physics, 58 Petropavlovskaya str., 40030 Sumy, Ukraine

We study fluctuating tilt Brownian ratchets based on fractional subdiffusion in sticky viscoelastic media characterized by a power law memory kernel [1]. Unlike the normal diffusion case the rectification effect vanishes in the adiabatically slow modulation limit and optimizes in a driving frequency range [2]. It is also shown [3] that anomalous rectification effect is maximal (stochastic resonance effect) at optimal temperature and can exhibit a surprisingly good quality. Moreover, subdiffusive current can flow in the counter-intuitive direction upon a change of temperature or driving frequency. The dependence of anomalous transport on load exhibits a remarkably simple universality.

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[1] I. Goychuk, Phys. Rev. E **80**, 046125 (2009); Adv. Chem. Phys. **150**, 187–253 (2012); [2] I. Goychuk, Chem. Phys. **375**, 450 (2010); [3] I. Goychuk and V. Kharchenko, arXiv:1111.4833[cond-mat.stat-mech] (2011).

DY 27.4 Thu 15:30 MA 004
The resolution of the entropy production paradox of fractional diffusion equations — •Janett Prehl[1], Karl Heinz Hoffmann[1], and Chris Essex[2] — [1]TU Chemnitz, Institut für Physik, D-09107 Chemnitz, Germany — [2]University of Western Ontario, Departement of Applied Mathematics, London, ON, Canada N6A 5B7

Both, time- and space-fractional diffusion equations can be defined as a one parameter bridging regime going from diffusion equation to wave- or half wave equation. The solutions of these fractional diffusion equations represent superdiffusion processes. Contrary to intuition, the corresponding entropy production rates grow moving from irreversible diffusive to reversible wave-like behavior. This paradox was discovered for the time- and space-fractional diffusion equation and not only for the Shannon entropy but also for its generalized entropy definitions, the Tsallis and the Rényi entropy. For the first time we show a generalized method to resolve this paradoxical behavior for both fractional equations and all introduced entropy definitions.

[1] C. Essex, C. Schulzky, A. Franz, K. H. Hoffmann, *Phys,A* (2000) **284**: 299–309
[2] J. Prehl, C. Essex, K. H. Hoffmann, *Phys.A* (2010) **389**: 215–224

DY 27.5 Thu 15:45 MA 004
Convex Hulls of Levy Walks — •Mirko Lukovic, Stephan Eule, and Theo Geisel — MPI for Dynamics and Self-Organization, Goettingen, Germany

Recently there has been much debate in the scientific community as to whether the observed walk patterns of foraging animals are Lévy-like or not. This is mainly due to the poor accuracy of the statistical methods employed to indentify Lévy behaviour from collected data samples of animal trajectories. There are cases where strong evidence was found for Lévy walks by using an extremely large data set of animal movement (Humphries *et al.* Nature 2010). We propose the use of convex hulls (minimum convex polygon enclosing the recorded points (Majumdar *et al.* 2009)) of the home range of animals as a robust and accurate method to discriminate between different types of foraging animal motions. The method is simple and robust even in the case where data available is sparse and it should be able to determine the degree of how Lévy-like a recorded trajectory is. In addition, we do not need to know in which order the animal visited the registered points.

DY 27.6 Thu 16:00 MA 004
Efficient simulation of Fractional Brownian Motion for several values of the Hurst exponent — •Alexander K. Hartmann[1], Satya N. Majumdar[2], and Alberto Rosso[2] — [1]Institute of Physics, University of Oldenburg, Germany — [2]LPTMS, Université Paris-Sud, France

We study Fractional Brownian Motion (FBM), i.e., Gaussian processes with zero mean and a correlator of the form $C(t,t') = t^{2H} + (t')^{2H} - |t-t'|^{2H}$, in the presence of an absorbing boundary. The strength of the correlation is described by the *Hurst exponent* H, whereas $H = 0.5$ corresponds to the uncorrelated random walk (diffusion), $H > 0.5$ to positive correlations (superdiffusion) and $H < 0.5$ to anticorrelations (subdiffusion) of the movement. FBM is, e.g., believed to describe the translocation of polymers through pores.

Recently, analytical predictions [1,2] were obtained for the distribution $P(x)$ of walk endpoints x. Standard numerical simulations study FBM via generating (discrete-time) random walks directly. They are, in particular for $H < 0.5$, very demanding, since the success probability of generating a non-absorbed trajectory is very small. Hence, such simulations were restricted to a small number L of discrete steps. Here, using a special Monte Carlo Simulation, long walks up to $L = 10^7$ could be generated for values $H = 1/4$, $4/9$, $1/2$ and $2/3$. The results are compared with the analytical predictions.

[1] A. Zoia, A. Rosso, S. N. Majumdar, Phys. Rev. Lett. **102**, 120602 (2009)
[2] K. J. Wiese, S. N. Majumdar, A. Rosso, arXiv:1011.4807

DY 27.7 Thu 16:15 MA 004
Simulation of colloids in microchannels: channel width effects on diffusion — •Ullrich Siems and Peter Nielaba — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

The results of a Brownian dynamics simulations (BD) of colloidal particles in a two-dimensional microchannel are presented. The particles pair potential is modeled by a repulsive $1/r^3$ potential and a hard core interaction. The diffusion along the channel direction is investigated for various channel widths at a constant interaction strength. For channels, where the mutual passing of particles is forbidden due to the hard core interaction, single-file diffusion has been observed in agreement with former simulations and experiments.
For wider channels a three regime diffusion behavior can be observed: the diffusion is normal in the short-time limit and long-time limit, but sub-diffusive on intermediate time scales. The time evolution of the mean square displacement can be completely characterized by the two transition times and the diffusion coefficients for the short-time and the long-time limit. These parameters were obtained by a fit of a Fermi

distribution to the logarithmic coordinates of the time-dependent diffusion coefficient $D(t) = < \Delta x^2 > /2t$. The transition times and the long-time diffusion coefficient have an oscillating dependency on the channel width, which can be explained by layering effects.

DY 27.8 Thu 16:30 MA 004

Effective diffusion and subdiffusion in inhomogeneous lattice models — •Federico Camboni — Humboldt University Berlin Germany

We discuss the problem of the evaluation of an effective diffusion coefficient for a particle in a disordered medium with energetic disorder (homogeneous and isotropic in the statistical sense) in arbitrary dimension. We present a formal, general expression for such a diffusion coefficient based on the reduction of the system to an effective resistor-capacitor network, with site-dependent activities playing a role of electric potential. We discuss the effective medium approximation for the diffusivity and its upper and lower Hashin-Shtrikman bounds. We moreover investigate situations under which anomalous diffusion in a random potential model can apprear, and show that there are two and only two corresponding situations, namely the ones corresponding to a generalized trap model and to the percolation case.

DY 27.9 Thu 16:45 MA 004

Space-resolved Dynamics in a Simple Porous Media Model — •Markus Spanner[1], Simon Schnyder[2], Thomas Voigtmann[3], and Thomas Franosch[1] — [1]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany — [3]Institut für Materialphysik im Weltraum, DLR, 51170 Köln, Germany and Zukunftskolleg, Universität Konstanz, 78457 Konstanz, Germany

The Lorentz model is a simple model for transport in porous materials, where a point-like tracer explores the space between an array of quenched spherical obstacles. It was shown in previous computer simulations, that in the vicinity of the localization transition, the remaining void space becomes fractal, thus transport is drastically hindered and anomalous dynamics emerges. When considering only trajectories on the infinite cluster, sub-diffusive motion $\delta r^2_\infty \sim t^{2/d_\mathrm{w}}$ is found to follow an exponent of $d_\mathrm{w} = 4.81$, known as the walk dimension.

Employing further extensive molecular dynamics simulation, both for ballistic and Brownian motion, we investigate the spatio-temporal dynamics of tracer particles in the Lorentz model in terms of the intermediate scattering functions. Covering different time and length scales simultaneously, these functions are sensitive to both the underlying spatial fractal and the anomalous transport.

We compare our simulation results close to the critical density to a mode-coupling approach, and find that certain aspects are surprisingly well predicted.

DY 27.10 Thu 17:00 MA 004

Minimal mean first passage time in a piecewise linear potential landscape — •Vladimir V. Palyulin[1] and Ralf Metzler[2] — [1]Physik Department (T30g), Technical University of Munich, James Franck Strasse, 85747 Garching, Germany — [2]Chair for Theoretical Physics, Inst for Physics & Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany

How can we minimize the mean first passage time between two points x_1 and x_2, whose energies are E_1 and E_2 ($E_1 > E_2$)? Naively, one might suppose that the solution is a linear potential drop between the two points. However, in our analysis we show that for an energy landscape consisting of two linear parts, a potential barrier with height $E_b > E_1$ leads to a decrease of the mean first passage time. Similar results hold for subdiffusive conditions.

Our a priori surprising findings are obtained analytically and supported by numerical analysis. Several approaches were used, namely, direct numerical solution of fractional Fokker-Planck equation with Gruenwald-Letnikov representation of the fractional derivative, numerical inverse Laplace transform of first passage time density obtained by solution of equation in Laplace space, and Monte Carlo simulation approach.