TT 25: Brownian Motion and Transport (jointly with DY, CPP)

Time: Monday 15:00–18:45 Location: BH-N 243

Invited Talk TT 25.1 Mon 15:00 BH-N 243

universal statistics of records in random sequences — •satya majumdar — cnrs, lptms, universite paris-sud, orsay, france

Records are rather common in everyday life: we are always talking of record rainfall, record temperature, records in sports and stock prices etc. When the random sequence consists of independent random variables, the record statistics is well known. In this talk, I'll discuss the record statistics in a strongly correlated random walk sequence and show that they are universal, i.e., independent of the noise (jump) distribution. Several applications and extensions will be discussed–such as the effect of a constant drift and the effect of measurement errors.

TT 25.2 Mon 15:30 BH-N 243

Three-dimensional Brownian motion of 3D-shaped particles — •Felix Höfling — Max Planck Institute for Intelligent Systems, Stuttgart, and Institute for Theoretical Physics IV, Universität Stuttgart, Germany

The three-dimensional (3D) Brownian motion of colloidal particles of general 3D-shape is considered in the overdamped limit. First for an ellipsoidal particle, the Smoluchowski equation for the joint distribution of position and orientation is solved exactly through an expansion in moments. The non-Gaussian parameter is shown to simultaneously quantify the anisotropic positional diffusion and the orientational diffusion. The results are applied further to the interpretation of scattering experiments (e.g., dynamic light scattering) on suspensions of active (self-propelled) and passive nanoparticles.

Second, a screw-like shape, paradigmatic for chiral particles, is studied which gives rise to a strong hydrodynamic coupling between rotation and translation. Coupled Langevin equations for the six degrees of freedom are used to calculate auto- and cross-correlation functions of first and second order exactly. A suitable displacement–orientation correlation is shown to display a maximum at intermediate times, from which the strength of the rotation–translation coupling can be inferred. Finally, the above findings are generalised for a hydrodynamic friction matrix of general form, which encodes an arbitrary particle shape. The analytical results are supported by numerical simulations of the corresponding stochastic equations.

TT 25.3 Mon 15:45 BH-N 243

Velocity fluctuations of Brownian particle in inhomogeneous media and driven by colored noise as a sourse of 1/f fluctuations — •Rytis Kazakevicius and Julius Ruseckas — Institute of Theoretical Physics and Astronomy, Vilnius University, A. Gostauto 12, LT-01108 Vilnius, Lithuania

Nonlinear stochastic differential equations generating signals with 1/f spectrum in a broad range of frequencies have been used so far to describe socio-economical systems [1]. We have derived such equation from Langevin equations that describe the motion of a Brownian particle in an inhomogeneous environment. The inhomogeneous environment can be a result of a linear potential affecting the Brownian particle together with the steady state heat transfer due to the difference of temperatures at the ends of the medium. The correlation of collisions between the Brownian particle and the surrounding molecules can lead to the situation where the finite correlation time becomes important, thus we have investigated the effect of colored noise in our model. Existence of colored noise leads to the additional restriction of the diffusion and exponential cut-off of the distribution of particle positions. Narrower power law part in the distribution of the particle positions results in the narrower range of frequencies where the spectrum has power law behavior.

[1] V. Gontis, J. Ruseckas and A. Kononovicius, Physica A, 389 100 (2010).

TT 25.4 Mon 16:00 BH-N 243

Hydrodynamically enforced entropic trapping of Brownian particles — •Steffen Martens[1], Arthur Straube[2], Gerhard Schmid[3], Lutz Schimansky-Geier[2], and Peter Hänggi[3] — [1]Technische Universität Berlin, Berlin, Germany — [2]Humboldt-Universität zu Berlin, Berlin, Germany — [3]Universität Augsburg, Augsburg, Germany

In small systems spatial confinement causes entropic forces that in turn implies spectacular consequences for the control for mass and charge transport. Therefore, recent efforts in theory triggered activities which allow for an approximate description that involves a reduction of dimensionality. Up to present days, the focus was on the role of conservative forces and its interplay with confinement. Within the presented work, we overcome this limitation and succeeded in considering also "magnetic field" like, so termed non-conservative forces that derive from a vector potential [S. Martens et al., *Phys. Rev. Lett.* **110**, 010601 (2013)]. A relevant application is the fluid flow across microfluidic structures where a solute of Brownian particles is subject to both, an external bias and a pressure-driven flow. Then a new phenomenon emerges; namely, the intriguing finding of identically vanishing average particle flow which is accompanied by a colossal suppression of diffusion [S. Martens et al., arXiv:1407.5673]. This entropy-induced phenomenon, which we termed *hydrodynamically enforced entropic trapping*, offers the unique opportunity to separate particles of the same size in a tunable manner [S. Martens et al.,*Eur. Phys. J. ST* **222**, 2453-2463 (2013)].

TT 25.5 Mon 16:15 BH-N 243

On the Applicability of the Caldeira-Leggett Model to Condensed Phase Vibrational Spectroscopy — •Fabian Gottwald, Sergei Ivanov, and Oliver Kühn — Institut für Physik University of Rostock, Rostock, Germany

Formulating a rigorous system-bath partitioning approach remains an open issue. In this context the famous Caldeira-Leggett (CL) model that enables quantum and classical treatment on equal footing has enjoyed popularity. Although this model is by any means useful as a theoretical tool, its validity for describing anharmonic dynamics of real systems is often taken for granted. We investigate the applicability of the model by comparing the spectra resulting from the Generalized Langevin dynamics that is based on the CL model, with their counterparts from explicit classical molecular dynamics. It is shown that the model is not able to describe real systems unless the system part of the potential is effectively harmonic. We demonstrate that it is this anharmonicity, that is at the core of all deficiencies of the model and also point out the mathematical origin of its breakdown.

15 min. break

TT 25.6 Mon 16:45 BH-N 243

Dynamics of stochatic resisitive switching — •Paul Radtke[1], Arthur Straube[1], Andrew Hazel[2], and Lutz Schimanksy-Geier[1] — [1]Department of Physics, Humboldt-Universität zu Berlin, Berlin, Germany — [2]School of Mathematics, University of Manchester, Manchester, UK

Classes of dielectrics such as TiO_2 alter their resistance under the influence of an electric field or a current flowing through the system, an effect called resistive switching (RS). Thereby the resistance depends also on the past states of the system, it has a memory.

We will show how a particular one-dimensional lattice model for a bipolar device. In it, oxygen vacancies hop in between consequetive sites and thereby alter local resistances. Their dynamics governed by a Master equation with jumping rates modulated by an external electric field. We discuss the system properties and show that dynamics of the vacancies can be formulated in terms of a Burgers like equation. With its help the underlying motion of the oxygen vacancies is interpreted as nonlinear traveling waves.

TT 25.7 Mon 17:00 BH-N 243

Simulation of colloidal particles in channel geometries — •Ullrich Siems and Peter Nielaba — University of Konstanz, Germany

This talk will present the results of Brownian Dynamics Simulations of colloidal particles in external fields confined in channels. Colloidal particles are well suited model-systems for a variety of problems on different length scales, ranging from gravitational collapses over the description of pedestrians to models for atomic sized problems. In such systems confinement into channels can have a great influence on the diffusion and transport properties.

TT 25.8 Mon 17:15 BH-N 243

Nonlinear Microrheological response to a step force —

•Thomas Franosch — Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Innsbruck, Austria

In a microrheological experiment the thermal or forced motion of a colloidal particle is monitored to obtain information on mechanical properties of the surroundings. While the linear response is well-characterized in terms of the fluctuation-dissipation theorem, few exact results are available for strong driving.

Here we consider the time-dependent velocity of a colloidal particle immersed in a dilute suspension of hard spheres in response to switching on a finite constant force. The dimensionless number quantifying the strength of the driving is the Péclet number $\mathrm{Pe} = F\sigma/k_BT$. We present an analytical solution exact to first order in the packing fraction. In particular, we show that at *finite times* the response is an analytic function of the Péclet number, but displays singular behavior for infinite times. Our solution technique extends the stationary state calculation [1] to the time-dependent case. The non-commutitavity of the limits $\mathrm{Pe} \to 0$ and time $t \to \infty$ is traced back to the long-time tail in the velocity-autocorrelation function due to repeated encounters with the same colloid. The scenario is strongly reminiscent of a driven particle in a lattice Lorentz model with frozen obstacles [2], and corroborates that linear response becomes qualitatively wrong at long times for arbitrarily small driving.

[1] T.M Squires and J.F. Brady, Phys. Fluids 17, 073101 (2005)

[2] S. Leitmann, T. Franosch, Phys. Rev. Lett. 111, 190603 (2013)

TT 25.9 Mon 17:30 BH-N 243

Enhancement of mobility in a feedback controlled 1D colloidal system with repulsive interactions — •Robert Gernert and Sabine H. L. Klapp — Institut für theoretische Physik, Technische Universität Berlin

Feedback control schemes are a promising way to design static and dynamic properties of colloidal suspensions [1]. In the collective transport of colloids through 1D tilted washboard potentials clusters of attractive particles are known to overcome the hindering influence of the potential barriers [2]. Here we consider a corresponding system with repulsive interactions. To enhance the mobility we propose a feedback control scheme and demonstrate its function theoretically. The control is modelled by a symmetrically confining potential, like an optical tweezer, and it is always centered around the mean particle position. For the theoretical demonstration we use Dynamical Density Functional Theory (DDFT) with ultra-soft as well as hard-core particle interactions. For either type of interaction the influence of the hindering washboard potential can be suppressed completely – corresponding to an enhancement of the mobility by several orders of magnitude. Further, in the regime of moderate amplification velocity oscillations are induced.

[1] B. Qian, D. Montiel, A. Bregull, F. Cichos, and H. Yang, Chem. Sci. 4, 1420 (2013)

[2] M. Evstigneev, S. von Gehlen, and P. Reimann, PRE 79, 011116 (2009)

TT 25.10 Mon 17:45 BH-N 243

Surface interactions of active Janus particles on a hexagonal close-packed colloidal crystal surface — •Udit Choudhury[1], John G. Gibbs[1,2], and Peer Fischer[1,3] — [1]Max Planck Institute for Intelligent Systems, Heisenbergstr. 3, 70569 Stuttgart, Germany — [2]Dept. of Physics & Astronomy, Northern Arizona University, Flagstaff, AZ 86011, USA — [3]Institute for Physical Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany

Autonomous, self-driven colloidal particles are being given greater attention in recent years due to the interesting dynamics associated with out-of-equilibrium systems. Although particle-particle interactions of active colloids, e.g. self-assembly and clustering, are beginning to be regularly studied, particle-surface interactions are less well investigated. Herein, we empirically study the surface interactions of spherical Janus-particles half-coated with Pt in the presence of hydrogen peroxide. The surface consists of close-packed 2D monolayer of hard spheres (beads). This non-planar surface thus corresponds to a periodic potential akin to a fcc (111) lattice face. In this way, the system is an analogue of surface diffusion of adatoms that possess kinetic energy. We find that as the concentration of hydrogen peroxide is increased, the effective translational diffusion also increases which is comparable to enhanced diffusion of adatoms on surfaces at higher temperatures. Rotational diffusion dictates fluctuations in the orientation of the driven bead that lead to jumps form one potential well to its nearest neighbor.

TT 25.11 Mon 18:00 BH-N 243

Charged transfer in a dynamical Landau-Zener Model: Application in QCA — •Alejandro Santana-Bonilla[1], Mirna Kramar[1], Rafael Gutierrez[1,2], and Giovanni Cuniberti[1,2] — [1]Technische Universität Dresden Faculty of Mechanical Science and Engineering Institute for Materials Sciences — [2]Max Bergmann Center of Biomaterials

The development of molecular based quantum cellular automata (mQCA) would open the possibility to low-dissipation information processing. One key parameter in the mQCA paradigm is the stability of intra-molecular charge transfer, which guarantees the association of *1* and *0* to two different charge configurations in the mQCA building cell. Especifically, a given charge configuration needs to be stable against thermal fluctuations. Also important is how the mQCA charge state reacts to an external driver with a given time-dependence. In this study we present a theoretical study based on the solution of the time-dependent Schrödinger equation to describe intra-molecular charge transfer in an effective model of an mQCA cell under the action of a time-dependent driver field and including thermal fluctuations. The model is parametrized via first-principle calculations in a toy molecular system able to catch the minimal requirements of a m-QCA cell

TT 25.12 Mon 18:15 BH-N 243

Calibration free 3D tracking of confined nanoparticles in a tunable nanofluidic slit — •Stefan Fringes, Michael Skaug, Heiko Wolf, Urs T. Dürig, and Armin W. Knoll — IBM Research, 8803 Rüschlikon, Switzerland

We investigate the behavior of nanoparticles in a nanofluidic slit with tunable confinement and spatial and temporal resolution of 10nm and 2ms, respectively. The high speed detection of the particles' X, Y and Z coordinates allows us to obtain the spatiotemporal probability distribution of individual particles and thus to study their confining potential-landscape both in lateral and vertical direction. To obtain the 3D trajectory of a nanometer-sized particle we use interferometric scattering detection (iSCAT). The method exploits the interference between the scattered wave from the particles and the highly reflective reference surface for a precise localization in vertical direction [1]. Evaluating the particle contrast for varying slit distances enables us to measure the scattering phase, amplitude, and consequently the z-position of individual particles without prior calibration of the particle contrast [2]. Precise knowledge of the nanoparticles' paths and surrounding potentials allows us to study confinement effects on Brownian motion and charge regulation at the participating interfaces. It further enables us to precisely trap and immobilize nanoparticles at a specific location on the substrate.

[1] P. Kukura et al., Nature Methods 6, 923-927 (2009).

[2] N. Mojarad et al., Optics Express 21, 8, 9377-9389 (2013).

TT 25.13 Mon 18:30 BH-N 243

Towards single molecule trapping and manipulation with dynamic temperature gradients — Marco Braun, Andreas Bregulla, and •Frank Cichos — Molecular Nanophotonics Group, Universität Leipzig, Linnéstraße 5, 04103 Leipzig

Single nano-objects in solution are driven by Brownian motion which is fueled by thermal energy. These Brownian fluctuations increase in strength with increasing temperature. Therefore, it is at first glance counter intuitive to confine Brownian fluctuations with the help of elevated temperatures. In thermal nonequilibrium, however, temperature gradients induce thermo-phoretic and thermo-osmotic drifts which provide the means for single particle manipulation in solution. Here we describe experiments which use optically heated metal nanostructures to create dynamical temperature profiles in solution. These temperature profiles induce well defined thermo-phoretic drift fields and act as effective potentials for objects suspended in liquid. Combined with optical feedback mechanisms, such effective potentials can be shaped to store and manipulate single or even multiple objects in a small observation volume. The developed thermophoretic trapping system therefore paves the way for extended single molecule studies in solution or even well-controlled bi- or multi molecular interaction studies.