DY 45: Brownian Motion and Transport

Time: Wednesday 16:30–17:45 Location: H46

DY 45.1 Wed 16:30 H46

Velocity and displacement statistics under nonlinear friction showing bounded particle speed — •Andreas M. Menzel — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

Often, models on the stochastic motion of colloidal particles in a surrounding fluid assume linear "viscous" friction. This case can be solved analytically for free Brownian motion of non-interacting particles.

A prominent example of nonlinear friction is given by "dry" friction of the Coulomb type. In this case, the friction always shows the same magnitude as soon as the particle is in motion. Stochastic models using this type of friction were broadly analyzed over the past few years using different technical tools.

In the present contribution, we introduce a different type of nonlinear friction. It increases linearly with the velocity at low particle speed; it increases more than linearly at higher speeds; finally, it diverges at a certain maximum particle speed. Both, velocity and displacement statistics, are evaluated under stochastic motion in one dimension using the Fokker-Planck approach. For a specific value of the maximum particle speed, significant analytical progress can be made, revealing a formal connection to the Schrödinger equation for an infinite square-well potential. The mean-squared displacement is found to still increase linearly in time, while higher-order moments signal non-Gaussian displacement statistics. Using elements from quantum-mechanical perturbation theory, the influence of an additional drift force is included. Our description should apply for the stochastic motion in shear-thickening environments, possibly starch suspensions.

DY 45.2 Wed 16:45 H46

Friction dynamics of colloidal crystal layers in shear flow — •Sascha Gerloff and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Friction at the nanoscale is characterized by complex non-equilibrium dynamics, whose understanding is relevant for various different systems. An important example is the frictional dynamics of two atomically flat crystalline surfaces in contact, which currently attract strong attention from both, the theoretical and experimental point of view. Here we present results from overdamped Brownian dynamic simulations to investigate the non-equilibrium dynamics of confined colloidal suspensions in shear flow. We focus on slit-pore confinement where the colloids form colloidal crystal layers. We first revisit the shear-induced dynamics of a one-component bilayer system, displaying a pronounced de-pinning transition related to shear induced melting. Using a one-particle model we estimate the critical shear rate for this transition. As a second step we investigate the frictional dynamics of layers with different crystalline structure. To this end, we introduce an additional layer of small colloids to the system and stabilize it via a constant force. For this system, the dynamics at small shear rates is dominated by a local transport mechanism related to density excitations. Investigating the properties and dynamics of these density excitations is key to understand the overall dynamics of the layer. For small shear rates, we find the relative velocity of the layer to be proportional to the number and velocity of the density excitations.

DY 45.3 Wed 17:00 H46

Quantum-state diffusion approach to the dissipative dynamics of a 1-d double-well system — •Chiara Liverani[1], Michael Finnis[1,2], and Eva-Maria Graefe[3] — [1]Department of Physics, Imperial College London — [2]Department of Materials, Imperial College London — [3]Department of Mathematics, Imperial College London

The generalisation of classical transition rate theory to quantum mechanics is a long-standing problem. A common approach is to interpret Feynman's isomorphism between a quantum-mechanical particle and a periodic ensemble of harmonically interacting classical particles in a dynamical sense, leading for example to the so-called ring-polymer molecular dynamics (RPMD) method.

Here we investigate a toy model to shed further light on the connection between this type of semiclassical description for the open quantum dynamics and the results based on the quantum master equation. We study the time evolution of a particle in a double-well potential governed by a Lindblad equation, as a quantum analogue of a classical Langevin equation. We use the quantum state diffusion approach, where the evolution of the density operator is modelled by an ensemble average over stochastic Schrödinger equations. We investigate the effects of quantum-mechanical tunnelling and coherence in comparison to the classical dynamics and to that yielded by the RPMD method.

DY 45.4 Wed 17:15 H46

Large deviations in Taylor dispersion — •Marcel Kahlen[1], Andreas Engel[1], and Christian Van den Broeck[2] — [1]Institut für Physik, C. v. Ossietzky Universität, 26111 Oldenburg, Germany — [2]Faculty of Sciences, Hasselt University, B-3590 Diepenbeek, Belgium

Taylor dispersion plays an important role in our daily life. Addressing the dispersion of particles in shear flow, it is important for problems reaching from environmental pollution to the construction of water pipes.

A useful approach to analyze Taylor dispersion is to discretize the flow into N layers with different advection velocities. In this way it has been shown, that for sufficiently large time the distribution of particles is to leading order Gaussian. The theory of large deviations goes beyond this Gaussian approximation by quantifying the probability of exponentially rare realizations of particle distributions. The Gaussian result can be regained by a Taylor expansion of the large deviation function. Since the dispersion of particles is directly related to the sojourn times of the particles in the respective layers, the large deviation properties of the particle separations may be deduced from the large deviation behaviour of the empirical density.

In the talk, we apply the theory of large deviations to particle dispersion in an N-layer model. For $N = 2$ we check our results against the exact analytic solution that exists for this case. Results for $N > 2$ are compared to extensive numerical simulations. For $N \to \infty$, we show that our approach is in agreement with the Donsker-Varadhan result for the empirical density.

DY 45.5 Wed 17:30 H46

Brownian Nanoparticle Racetracks — •Stefan Fringes, Michael J. Skaug, and Armin W. Knoll — IBM Research - Zurich, Rüschlikon, Switzerland

Inspired by the transport principle of molecular motors in cells, artificial Brownian motors have been studied theoretically and experimentally to achieve directed motion and sorting of particles in a fluidic environment. Ingredients of such Brownian motors are a spatially asymmetric potential landscape and unbiased external inputs driving the system out of equilibrium. In our implementation we exploit the interaction potential of charged 60 nm gold-nanospheres to like charged confining surfaces in a nanofluidic slit. We shape the asymmetric potential by patterning a 3D ratchet topography in one of the two confining surfaces using thermal scanning probe lithography. The system is driven out of equilibrium by applying a zero-mean AC-electric field. We observe a net drift of several microns per second along a direction dictated by the ratchet geometry. All relevant physical quantities can be measured *in-situ* enabling a parameter free comparison to theory. Our concept works on highly scaled ratchet tracks having a track width of < 500 nm and a curvature down to 1 μm radius. We demonstrate the directed motion of nanoparticles in a complex racetrack and on demand transport along orthogonal racetrack directions.