DY 80: Brownian Motion and Transport

Time: Friday 10:00–11:15 Location: BH-N 128

DY 80.1 Fri 10:00 BH-N 128

Analyzing Transport Properties of Nanoparticles in Magnetic Ratchets — •Daniel Kappe[1,2] and Andreas Hütten[1] — [1]Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany — [2]Bielefeld Institute for Applied Materials Research, Bielefeld University of Applied Sciences, Germany

Magnetic nanoparticles have a broad range of possible applications, ranging from cancer treatment to drug delivery and diagnostics. When detecting biomolecules, nanoparticles are superior to micrometer sized particles, because their surface can only bind to a couple of molecules instead of a thousands. But directed, controlled transport is tricky, because of their high diffusivity. A magnetic ratchet utilizes this property and an asymmetric potential to drive the particles. We introduce a scheme to evaluate the transport efficiency of magnetic ratchets.

In order to calculate the efficiency of such setups, a Monte Carlo based numerical integration of the Langevin equation was implemented [1]. The algorithm considers viscous forces, Brownian motion and forces arising from magnetic field gradients, but no particle-particle interactions. Particles subject to a time and space dependent force field, governed by the setup in use. The efficiency of a setup is analyzed reviewing the mean displacement of all particles.

We aim to improve understanding of different setups and tune their parameters, like switching frequencies and external fields, to find and extend the range of particles working in a particular setup.

[1] D. Ermak, H. Buckholz, J. comp. Phys., 35, 169-182 (1980)

DY 80.2 Fri 10:15 BH-N 128

Quantum motion of ions in a molecular junction during current flow — •Lev Kantorovich — Physics, King's College London, London, WC2R 2LS

We consider a combined system of electrons and nuclei of a molecular junction. Initially the whole system is in thermal equilibrium at some temperature, no partitioning approximation is made. Then, a bias is applied causing a current to flow. Using path integrals and non-equilibrium Green*s Functions formalisms, an expression for the density matrix of ions (reduced with respect to electrons) is derived and hence the corresponding effective Liouville equation. It is assumed that atomic displacements with respect to average (and time dependent) atomic positions are small (the harmonisation approximation). Then a hierarchy of equations of motion for average ionic positions is obtained without any additional approximations. This work generalises the method of Ref. [Jing-Tao Lü et al, PRB 85, 245444 (2012)] in two main aspects: (i) going beyond the partitioned approximation and (ii) the stochastic equations of motion for quantum ions are rigorously derived.

DY 80.3 Fri 10:30 BH-N 128

Anomalies, Rare Events, and Brownian Motion — Jose M. Miotto[1], Simone Pigolotti[2], Aleksei V. Chechkin[3,4], and •Sandalo Roldan-Vargas[5] — [1]Leiden Institute of Advanced Computer Science, Leiden University, Netherlands — [2]Okinawa Institute for Science and Technology, Japan — [3]Institute for Physics and Astronomy, University of Potsdam, Germany — [4]Akhiezer Institute for Theoretical Physics, Kharkov, Ukraine — [5]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

In one of his celebrated 1905 papers, Albert Einstein proposed for the first time a statistical interpretation of Robert Brown innocent observation based on the corpuscular constitution of matter. His theory suggested that the long time motion of a Brownian particle is diffusive whereas the probability distribution of the particle displacements is Gaussian. For more than one hundred years these predictions were systematically validated in real systems and the coexistence between Diffusivity and Gaussianity became a paradigm. However, recent experiments on mesoscopic particle systems have claimed the existence of a time regime where diffusion is not accompanied by a purely Gaussian distribution of displacements. By molecular dynamics simulations of 2- and 3-D glass and gel forming-liquids we show the emergence of a non-Gaussian exponential tail in the probability distribution of particle displacements whose exponential rate is dimension dependent. We further show that the diffusive regime accompanying the non-Gaussian distribution of displacements is the result of a mixture of anomalous diffusivities.

DY 80.4 Fri 10:45 BH-N 128

Large deviation function for a driven underdamped particle in a periodic potential — •Lukas P. Fischer, Patrick Pietzonka, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, Germany

Large deviation theory is a versatile tool that proved useful for establishing connections between current fluctuations and thermodynamic steady state properties, e.g. the thermodynamic uncertainty relation [1]. Previous studies, however, were limited to systems which are diffusive in all variables, i.e. overdamped Brownian motion or Markov jump processes. We extend the work to underdamped Brownian motion of a single, driven particle in a periodic potential [2]. To this end, we derive an explicit expression for the large deviation functional of the empirical phase space density, which replaces the level 2.5 functional used for overdamped dynamics. Using this approach, we obtain several bounds on the large deviation function of the particle current. We compare them to bounds for overdamped dynamics that have recently been derived. Furthermore, we assess the tightness of the bounds in a numerical case study for a cosine potential.

[1] A.C. Barato, U.S., Phys. Rev. Lett. **114**, 158101 (2015)
[2] L.P.F., P.P., U.S., submitted to Phys. Rev. E

DY 80.5 Fri 11:00 BH-N 128

Dynamic mode locking in a driven colloidal system — Michael Juniper[1], Urs Zimmermann[2], •Arthur Straube[3], Rut Besseling[4], Dirk Aarts[1], Hartmut Löwen[2], and Roel Dullens[1] — [1]Department of Chemistry, University of Oxford, UK — [2]Institute of Theoretical Physics, Heinrich-Heine-Universität Düsseldorf, Germany — [3]Freie Universität Berlin, Institute of Mathematics, Berlin, Germany — [4]InProcess-LSP, Oss, The Netherlands

We examine both experimentally and theoretically the microscopic dynamics underlying mode locking in a colloidal system [1,2]. We first look at a colloidal particle driven by a modulated force over a sinusoidal optical potential energy landscape. Coupling between the competing frequencies of the modulated drive and that of particle motion over the periodic landscape leads to synchronization of particle motion into discrete modes, manifesting as Shapiro steps in the average particle velocity. State diagrams from experiment, simulation, and theory agree well. Further, we use this approach to examine the enhancement of mode locking in a flexible chain of magnetically coupled particles, which we ascribe to breathing modes caused by mode-locked density waves. Finally, we demonstrate that an emergent density wave in a static colloidal chain mode locks as a quasi-particle, with microscopic dynamics analogous to those seen for a single particle.

[1] M. Juniper, A. Straube, R. Besseling, D. Aarts, R. Dullens, Nat. Commun. 6, 7187 (2015)
[2] M. Juniper, U. Zimmermann, A. Straube, R. Besseling, D. Aarts, H. Löwen, R. Dullens, New J. Phys. 19, 013010 (2017)