DY 71: Poster: Noneq. Stat. Phys., Stoch. Thermo, Brownian Dyn.

Time: Thursday 15:30–18:00 Location: Poster A

DY 71.1 Thu 15:30 Poster A

Non-stationary Generalized Langevin Equation for the Crystallization Process — •Philipp Pelagejcev[1], Thomas Voigtmann[3,4], Hugues Meyer[1,2], and Tanja Schilling[1] — [1]Physikalisches Institut, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [2]Research Unit in Engineering Science, Université du Luxembourg, L-4364 Esch-sur-Alzette, Luxembourg — [3]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [4]Department of Physics, Heinrich Heine University, Universitätsstraße 1, 40225 Düsseldorf, Germany

We study crystallization from an undercooled melt in the context of non-equilibrium statistical physics. We have recently derived an equation of motion for an averaged observable over a bundle of system trajectories by means of time-dependent projection operator techniques. Here we apply this technique to the analysis of simulation trajectories.

We observed the crystallization process of an undercooled fluid of Lennard Jones particles in a Molecular Dynamics Simulation under constant temperature (where the heat bath is realised with a Nosé-Hoover thermostat). From the sampled size of the largest crystalline cluster in the system, we construct the memory kernel of the Generalized Langevin Equation. We observe significant memory effects, i.e. the process is not described well by a Markovian approximation.

DY 71.2 Thu 15:30 Poster A

Effect of hidden slow degrees of freedom on fluctuation theorems: An analytically solvable model — •Marcel Kahlen and Jannik Ehrich — Institut für Physik, Carl von Ossietzky Universität, 26111 Oldenburg, Germany

Systems with hidden degrees of freedom are a common occurrence within the field of stochastic thermodynamics. Because the full dynamics are not accessible in these setups, the total entropy production cannot be measured. Nevertheless, coarse-graining allows one to define an apparent entropy production. Usually this quantity does not fulfill fluctuation theorems of the usual type [1].

We present a simple model for which we can analytically calculate the fluctuation theorems involving the apparent entropy production. For this model we discuss the role of the strength of the coupling between the hidden and observed degrees of freedom and the limit of time-scale separation between them. Our model also serves as a case study on thermodynamic inference.

[1] J. Mehl, B. Lander, C. Bechinger, V. Blickle, and U. Seifert, Phys. Rev. Lett. **108**, 220601 (2012)

DY 71.3 Thu 15:30 Poster A

A minimal model of an autonomous thermal motor — Hans Fogedby and •Alberto Imparato — Department of Physics and Astronomy, Aarhus University, Ny Munkegade, Building 1520 DK-8000 Aarhus C, Denmark

We consider a model of a Brownian motor composed of two coupled overdamped degrees of freedom moving in periodic potentials and driven by two heat reservoirs. This model exhibits a spontaneous breaking of symmetry and gives rise to directed transport in the case of a non-vanishing interparticle interaction strength. For strong coupling between the particles we derive an expression for the propagation velocity valid for arbitrary periodic potentials. In the limit of strong coupling the model is equivalent to the Büttiker-Landauer model for a single particle diffusing in an environment with position dependent temperature. By using numerical calculations of the Fokker-Planck equation and simulations of the Langevin equations we study the model for arbitrary coupling, retrieving many features of the strong coupling limit. In particular, directed transport emerges even for symmetric potentials. For distinct heat reservoirs the heat currents are well-defined quantities allowing a study of the motor efficiency. We show that the optimal working regime occurs for moderate coupling. Finally, we introduce a model with discrete phase space which captures the essential features of the continuous model, can be solved in the limit of weak coupling, and exhibits a larger efficiency than the continuous counterpart.

DY 71.4 Thu 15:30 Poster A

Transitions between superstatistical regimes: validity, breakdown and applications — Petr Jizba[1,2], •Jan Korbel[3,1], Hynek Lavicka[4,5], Martin Proks[1], Vaclav Svoboda[1], and Christian Beck[6] — [1]Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Czech Republic — [2]Institute of Theoretical Physics, Freie Universitaet Berlin, Germany — [3]Department of Physics, Zhejiang University, Hangzhou, P. R. China — [4]Alten Belgium N.V., Brussels, Belgium — [5]Department of Institutional, Environmental and Experimental Economics, University of Economics in Prague, Czech Republic — [6]School of Mathematical Sciences, Queen Mary, University of London, United Kingdom

Superstatistics is a widely employed tool of non-equilibrium statistical physics which plays an important role in analysis of hierarchical complex dynamical systems. Yet, its "canonical" formulation in terms of a single parameter is often too restrictive when applied to complex empirical data. Here we show that a multi-scale generalization of the superstatistics paradigm is more versatile, allowing to address such pertinent issues as transmutation of statistics or inter-scale stochastic behavior [1]. To put some flesh on the bare bones, we provide a numerical evidence for a transition between two superstatistics regimes, by analyzing high-frequency (minute-tick) data for share-price returns of seven selected companies. Salient issues, such as breakdown of superstatistics in fractional diffusion processes or connection with Brownian subordination are also briefly discussed. [1] P.Jizba, J. Korbel, H. Lavicka, M. Proks, V. Svoboda, and C. Beck, Physica A 493, 29-46 (2018)

DY 71.5 Thu 15:30 Poster A

Extreme values of entropy production in an electronic double dot — •Shilpi Singh[1], Edgar Roldan[2], Izaak Neri[2], Ivan Khaymovich[2], Dmitry Golubev[1], Ville Maisi[1], Joonas Peltonen[1], Frank Julicher[2], and Jukka Pekola[1] — [1]Department of Applied Physics, Aalto University, 00076 Aalto, Finland — [2]Max Planck Institute for the Physics of Complex Systems, Nothnitzer Strasse 38, 01187 Dresden, Germany

The second law of thermodynamics implies that in mesoscopic systems entropy increases on average but leaves open the possibility for these systems to transiently absorb heat from their environment when driven out of equilibrium. Fluctuation relations relate the probability to dissipate a certain amount of heat and to absorb the same amount of heat during a fixed time interval and have been confirmed in experiments. Extreme-value statistics of thermodynamic fluxes characterize the most extreme deviations from the average behaviors. Here we report on the experimental measurement of stochastic entropy production and of records of negative entropy in a metallic double dot under a constant external bias to realize nonequilibrium steady state. We find that the cumulative distribution of entropy production's negative record and the mean value at all times obey the infimum law presented in [PRX 7, 011019]. Our work provides general bounds and equalities for the extreme-value statistics of correlated random variables about which not much is known. This may help to understand the statistics of overheating events in single-electronic devices which are relevant for the design of reversible computers near Landauer's limit.

DY 71.6 Thu 15:30 Poster A

Collective power: Minimal model for thermodynamics of nonequilibrium phase transitions — •Tim Herpich, Juzar Thingna, and Massimiliano Esposito — Complex Systems and Statistical Mechanics, Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg, Luxembourg

We establish a direct connection between the linear stochastic dynamics, the nonlinear mean-field dynamics, and the thermodynamic description of a minimal model of driven and interacting discrete oscillators. These exhibit at the mean-field level two bifurcations separating three phases: a single stable fixed point, a stable limit cycle indicative of synchronization, and multiple stable fixed points. The apparent contradiction with the underlying linear Markovian dynamics which ensures convergence to a unique steady state is resolved via metastability, i.e. the appearance of gaps in the upper real part of the spectrum of the Markov generator. The dissipated work of the stochastic dynamics exhibit signatures of nonequilibrium phase transitions over long metastable times which disappear in the infinite-time limit. Remarkably, it is also reduced by attractive interactions between oscillators. When operating as a work-to-work converter we study the power output and efficiency of our device in the presence of nonequilibrium phase transitions. We find that the maximum power output is achieved far-from-equilibrium in the synchronization regime and that the efficiency at maximum power is surprisingly close to the universal linear regime prediction. Our work builds bridges between thermodynamics of nonequilibrium phase transitions and bifurcation theory.

DY 71.7 Thu 15:30 Poster A

Quantum heat engines and laser cooling: Floquet theory beyond the Born-Markov approximation — •Sebastian Restrepo[1], Javier Cerrillo[1], Philipp Strasberg[2], and Gernot Schaller[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Complex Systems and Statistical Mechanics, University of Luxembourg, Luxembourg

We combine the formalism of Floquet theory, full counting statistics and a collective coordinate mapping to access the dynamics and thermodynamics of a periodically driven thermal machine beyond the conventional Born-Markov approximation. We identify a collective degree of freedom in the reservoir that is included as part of the original system and that is responsible for the strong coupling and non-Markovian effects. The periodicity of our model is exploited using Floquet theory to obtain a master equation for the newly defined supersystem with full counting statistics methods permitting a thermodynamic analysis. The formalism is applied to a thermal machine consisting of a driven two-level system coupled to two reservoirs at different temperatures with one of the couplings considered time-dependent. In the weak coupling non-Markovian regime the thermal machine can act either as a heat engine or a refrigerator. As the coupling is increased, we identify four different operation regimes and see the eventual disappearing of the refrigerator. We observe that the efficiency and coefficient of performance decrease for stronger couplings. Taking the limit of a single reservoir, our model is able to replicate the setup of state preparation in laser cooling of trapped ions.

DY 71.8 Thu 15:30 Poster A

Application of a Jump-Diffusion Model to Solid-Liquid Interfaces in Ionic Liquids — •Mario Udo Gaimann[1], Andreas Baer[1], Nataša Vučemilović-Alagić[1,2], Ana-Sunčana Smith[1,2], and David Matthew Smith[2,3] — [1]PULS Group at the Institute for Theoretical Physics I and EAM, FAU Erlangen-Nürnberg, Germany — [2]Division of Physical Chemistry, Institute Ruđer Boščović Zagreb, Croatia — [3]Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

Ionic liquids possess a range of tunable properties, such as conductivity and low melting points [1]. These properties are desirable for a broad range of applications, most prominently catalysis at solid-liquid interfaces. Ions in vicinity of these interfaces show patterned or layered adsorption. To understand particle movements in and across layers found in these systems, we employ molecular dynamics to study a confined, periodic sample system consisting of hydroxylated sapphire as well as $[C_2Mim]^+$ cations and $[NTf_2]^-$ anions. Common mean-square displacement approaches inherently predict ions' diffusion tensors as a function of location within the pattern incorrectly, as the diffusive limit can not be reached for small displacements. To resolve this problem, we apply a jump-diffusion model as proposed by Liu *et al.* [2], based on introducing virtual boundaries and solving the Smoluchowski equation within these virtual slabs. We then determine the transport coefficients as a function of the distance from the sapphire.

[1] Rogers R D and Seddon K R 2003 *Science* **302** 5646
[2] Liu P, Harder E and Berne B J 2004 *J. Phys. Chem.* B **108** 21

DY 71.9 Thu 15:30 Poster A

Hot Brownian Motion on Short Time Scales — •Alexander Fischer and Frank Cichos — Molecular Nanophotonics, Peter-Debye-Institute, Universität Leipzig

Hot Brownian motion describes the motion of a heated microsphere in a liquid. It is a fundamental issue for thermal non-equilibrium. A temperature field is created around the heated particle decaying with 1/r and a stationary temperature and viscosity field is moving with the particle through the liquid. The non-equilibrium dynamics of the particle now differs from the unheated particles and an effective temperature and viscosity is introduced to describe the system. Here we report on a study of the fluctuations of a heated particle in an optical trap with nanosecond and nanometer resolution. We achieved to measure the accelerated motion and from that the temperature increase of our particles. The first evidence of the changing characteristic time constants on short time scales was detected.

DY 71.10 Thu 15:30 Poster A

Thermophoresis of Charged Colloids in Electrolyte Solutions — •Martin Fränzl and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Germany

In the last decades thermophoresis of colloids was mainly discussed in terms of thermoosmotic pressure. However, in the recent years it has become clear that, for charged systems in an electrolyte solution the thermoelectric or Seebeck effect may provide an additional non-local driving force. In a non-uniform temperature, positive and negative ions, dissolved in water, have the tendency to migrate towards colder regions. However, in general one of the ion species is moving more rapidly, resulting in a thermoelectric field between the hot and the cold boundary. This field can drive charged colloids to the hot or to the cold, depending on the sign of the electrolyte Seebeck coefficient. The present work investigates the thermoelectric effects by locally heating a gold film with a focused laser beam within a colloidal suspension and discusses the resulting colloidal transport.

DY 71.11 Thu 15:30 Poster A

The Lattice Model of Crowding and Trapping in Line with Experiments in Model Membranes — •Mislav Cvitković[1], Marius Glogger[2], Markus Engstler[2], Susanne Fenz[2], and Ana-Sunčana Smith[3] — [1]Ruđer Bošković Institute, Division of Physical Chemistry, CLS Group, Zagreb, Croatia — [2]Universität Würzburg, Biocenter: Department of Cell and Developmental Biology, Germany — [3]FAU Erlangen–Nürnberg, Institute for Theoretical Physics, PULS Group, Germany

Lateral diffusion of proteins in biological membranes is a fundamental process that is, in living cells, affected both by protein crowding and intermolecular interactions. To account for these effects, we use a 2D lattice gas of hard particles that interact with ensemble of randomly localized traps. We characterize the behaviour of the system on all time scales, and provide an explicit expression for the long time diffusion coefficient as a function of relevant system parameters. Furthermore, we analyse traces from single–molecule experiments on GPI–anchored Variant Surface Glycoproteins (VSGs) that were purified from *Trypanosoma brucei* and reconstituted into supported lipid bilayers. VSGs are found to occur in two conformations [Bartossek *et al.*, *Nature Microbiology* 2:1523 (2017)] and their obstructed diffusion in experiment is found to have similar features to those predicted by the lattice gas model in a broad range of concentrations of VSG.

DY 71.12 Thu 15:30 Poster A

Apparent superdiffusion in subdiffusive d-dimensional generalized Lévy walks — •Tony Albers and Günter Radons — Institut für Physik, Technische Universität Chemnitz, Germany

We investigate a generalized Lévy walk [1] type of motion in a d-dimensional space, where the velocities of the flights depend on the durations of the flights in a nonlinear, deterministic way. This model of anomalous diffusion is essentially characterized by two exponents determining the asymptotic decay of the distribution of flight durations and the nonlinear dependence of the flight velocities on the flight durations. We provide analytical results for the asymptotic time dependence of the ensemble-averaged and time-averaged squared displacement and the randomness of the latter characterized by the ergodicity breaking parameter. In this contribution, we focus on a certain region of the two-dimensional parameter space, where the ensemble-averaged squared displacement increases slower than linear (subdiffusion) whereas the time-averaged squared displacement increases faster than linear (superdiffusion). This new kind of ergodicity breaking is studied in detail.

[1] M. F. Shlesinger, B. J. West, and J. Klafter, Phys. Rev. Lett. **58** 1100 (1987)

DY 71.13 Thu 15:30 Poster A

Heterogeneous diffusion in comb-like structures — •Trifce Sandev[1,2,3], Alexander Schulz[4], Holger Kantz[4], and Alexander Iomin[5] — [1]Ss. Cyril and Methodius University in Skopje, Macedonia — [2]RSD, Skopje, Macedonia — [3]MANU, Skopje, Macedonia — [4]MPIPKS Dresden, Germany — [5]Technion, Haifa, Israel

We consider diffusion with a position dependent diffusion coefficient along a backbone in different comb and fractal grid structures. The comb structures consist of main channel (backbone) and trapping fingers. Diffusion along the backbone, which is chosen to be the x-direction, occurs only at $y = 0$, and the fingers play the role of traps. This is a particular example of geometrical traps, where a particle, moving along the backbone, can get trapped inside a finger of the comb, where it diffuses in the y-direction, until it returns by chance to the backbone. Such behaviour of the particle can be described in the framework of the continuous time random walk theory, where the returning probability scales similarly to $t^{-1/2}$, and the waiting times are distributed according $t^{-3/2}$. We present analytical results for the mean squared displacement for the power-law position dependent diffusion coefficient along the backbone. We observe various diffusion regimes, such as subdiffusion, superdiffusion, hyperdiffusion, as well as stochastic localization. Our analytical results are in a good agreement with the numerical analysis of this heterogeneous transport, obtained in the framework of the Langevin equations description [1].

[1] T. Sandev, A. Schulz, H. Kantz, and A. Iomin, Chaos Solitons & Fractals, DOI: 10.1016/j.chaos.2017.04.041 (2017).

DY 71.14 Thu 15:30 Poster A

Time- and ensemble-averages in evolving systems: Brownian particles exposed to random potentials — Jörg Bewerunge, •Florian Platten, Christoph Zunke, and Stefan U. Egelhaaf — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

Anomalous diffusion is a ubiquitous phenomenon in complex systems. It is often quantified using timeand ensemble-averages to improve statistics, although time averages represent a non-local measure in time and hence can be difficult to interpret. We present a detailed analysis of the influence of time- and ensemble-averages on dynamical quantities by investigating Brownian particles in a rough potential energy landscape (PEL). Initially, the particle ensemble is randomly distributed, but the occupancy of energy values evolves towards the equilibrium distribution. This relaxation manifests itself in the time evolution of time- and ensemble-averaged dynamical measures. Individual colloidal particles are exposed to a laser speckle pattern inducing a non-Gaussian roughness and are followed by optical microscopy. The relaxation depends on the degree of roughness of the PEL. It can be followed and quantified by the time- and ensemble-averaged mean squared displacement. Moreover, the heterogeneity of the dynamics is characterized using single-trajectory analysis. The results of this work are relevant for the correct interpretation of single-particle tracking experiments in general.

DY 71.15 Thu 15:30 Poster A

Statistical Distribution of the Area Inside Random Walks Which Return to Their Origin — •Vincent Sacksteder — Royal Holloway University of London

We study 2-D random walks, Levy flights, and Levy walks, using both analytical calculations and extensive Monte Carlo simulations. Counting only loops (walks which return to the origin), and examining the area A of these loops, we calculate the probability distribution of A. We find that the loop area distribution is proportional to the inverse of A for ordinary random walks and decreases more rapidly for Levy flights. The loop area distribution calculated here determines the quantum corrections to electrical conductivity in 2-D disordered systems, which are known as weak localization corrections.