DY 54: Statistical Physics: General II

Time: Thursday 15:00–17:45 Location: ZEU/0114

DY 54.1 Thu 15:00 ZEU/0114

Fluctuating hydrodynamics of non-equilibrium interacting many-body systems — •Felipe Pereira-Alves and Aljaž Godec — Mathematical Physics and Stochastic Dynamics, Institute of Physics, University of Freiburg (GER)

Extending fluctuating hydrodynamics to non-equilibrium systems remains a significant theoretical challenge. In this work we investigate, on the level of distribution-valued fluctuating hydrodynamics, general short-range interacting systems as well as the long-range interacting Dyson process evolving from deterministic non-equilibrium initial conditions. We characterize the probability measure of the distribution-valued fluctuation field during the relaxation to equilibrium and illustrate the results on the example of discretely (in space) observed fluctuation field and compare the results to particle-resolved simulations.

DY 54.2 Thu 15:15 ZEU/0114

Non-ergodicity and breakdown of hydrodynamics in a one-dimensional cold gas — Taras Holovatch[1,2], Yuri Kozitsky[3], Krzysztof Pilorz[3], and •Yurij Holovatch[1,2,4,5] — [1]Yukhnovskii Institute for Condensed Matter Physics of the NAS of Ukraine, Lviv, Ukraine — [2]L4 Collaboration and Doctoral College for the Statistical Physics of Complex Systems, Lviv-Leipzig-Lorraine-Coventry, Europe — [3]Institute of Informatics and Mathematics, Maria Curie-Skłodowska University, Lublin, Poland — [4]Centre for Fluid and Complex Systems, Coventry University, Coventry, UK — [5]Complexity Science Hub, Vienna, Austria

We study dynamics of a 1D chain of elastically interacting particles with masses alternating between two different values, M,m,M,m,.. . Its dynamics is initiated by giving unit velocity in the positive direction to the particle located at the origin. For random particle positions, the resulting long-time behavior was found (S. Chakraborti et al., SciPost Phys. 2022, 13, 074) to posses rather remarkable features: (i) a shock front develops in the bulk of the gas and is governed by Euler hydrodynamics, (ii) the recoiled particles in the splatter move ballistically. In our study we have found (T. Holovatch et al., Phys. Rev. E 2025, 112, L052101) that for equidistant particle positions there exist mass ratios M/m for which (i) the splatter is absent; (ii) the number of simultaneously moving particles is at most three; (iii) the blast front moves in the ballistic way. We support our explicit calculations by MD simulations.

DY 54.3 Thu 15:30 ZEU/0114

Geometry-induced timescales in viscoelastic fluids — •Rupayan Saha[1], Niloyendu Roy[2], Debankur Das[1], Clemens Bechinger[2], and Matthias Krüger[1] — [1]Institute for Theoretical Physics, Georg-August-Universität Göttingen, Göttingen 37073, Germany — [2]Fachbereich Physik, Universität Konstanz, Konstanz 78457, Germany

Recoil experiments provide a powerful window into the non-Markovian properties of complex fluids, revealing memory effects that are usually obscured in conventional rheological measurements. While translational recoil of colloidal probes in viscoelastic media has been successfully modelled with **few distinct timescales**, orientational recoil exhibits an **unbounded** relaxation spectrum, manifested in the divergence of the recoil amplitude with increasing shear-time (t_{sh}) or system size (L). To resolve its physical origin, we design a **first-principles theoretical framework** rooted in the *geometric constraints of torsional flow*. Our model, based on concentric spherical shells, demonstrates that the orthogonality between angular momentum propagation and torsional stress storage generates **a radial scaling law for relaxation modes**. The theory thus establishes **geometry**—not material-complexity—as the primary candidate for engineering complex memory in soft matter. We finally elucidate why such *long relaxation times* have not been previously discovered through conventional rheology.

DY 54.4 Thu 15:45 ZEU/0114

Ion and Water Density Profiles in Nano-Confinement — •Haoyuan Quan, Maximilian Becker, Hanne Antila, and Roland Netz — Freie Universität Berlin, Berlin, Germany

Confined salt solutions are important in biology and in technical applications, such as environmentally friendly energy conversion, yet even basic trends of how ion and water densities change in confinement remain unclear. Using molecular dynamics simulations of graphene slits in equilibrium with bulk aqueous salt solutions, we determine concentration profiles of a variety of alkali-halide ion pairs as a function of slit width and bulk concentration. Using ion and water depletion lengths, which clearly reflect ion-specific effects, we construct a robust and thermodynamically consistent theory to describe water and ion concentrations in confined systems for varying slit widths and bulk salt concentrations.

DY 54.5 Thu 16:00 ZEU/0114

The electron transfer process at the electrode/electrolyte solution interface: A stochastic model and its Monte Carlo implementation — •Diego Veloza-Diaz[1], Friederike Schmid[1], Robinson Cortes-Huerto[2], Pietro Ballone[2], and Nancy C. Forero-Martinez[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — [2]Max Planck Institute for Polymer Research, Germany

A kinetic model of the electron transfer at the electrode/electrolyte interface is developed, implemented in a Monte Carlo framework, and applied to simulate this process in idealised systems consisting of the primitive model of electrolyte limited by an impenetrable conducting surface. A charged, spherical interface surrounding an equally spherical sample of electrolyte is introduced to model a single-electrode system, providing a computational analogue to the conceptual half-cell picture widely used in electrochemistry. The electron transfer itself is described as a simple surface-hopping process underlying a first-order reaction corresponding to one of the coupled M/M+ and X*/X half-reactions. Then, electron transfer at the interface is combined with the self-diffusion of ions in the electrolyte, which supply reagents and disperse products, allowing the system to settle into a stationary non-equilibrium state. Simulations of the primitive model of an electrolyte in contact with a charged, impenetrable surface show that, after a brief transient, the system sustains a steady current through the half-cell. Since the simulated interface is very idealised, strategies to overcome the limitations of the present model are outlined and briefly discussed.

DY 54.6 Thu 16:15 ZEU/0114

Fermion as a non-local particle-hole excitation — •Girish Setlur — Department of Physics, Indian Institute of Technology Guwahati

We show that the fermion, in the context of a system that comprises many such entities, which, by virtue of the Pauli exclusion principle, possesses a Fermi surface at zero temperature, may itself be thought of as a collection of non-local particle-hole excitations across this Fermi surface. This result is purely kinematical and completely general, not restricted to any specific dimension, and is applicable to both continuum and lattice systems. There is also no implication that it is applicable only to low-energy phenomena close to the Fermi surface. We are able to derive the full single-particle dynamical Green function of this fermion at finite temperature by viewing it as a collection of these non-local particle-hole excitations. The Green function of the fermion then manifests itself as a solution to a first-order differential equation in a parameter that controls the number of particle-hole pairs across the Fermi surface, and this equation itself reveals variable coefficients that may be identified with a Bose-Einstein distribution, implying that there is a sense in which the non-local particle-hole excitations have bosonic qualities while not being exact bosons at the level of operators. We also recall the definition of the non-local particle-hole operator that may be used to diagonalize the kinetic energy of free fermions of the sort mentioned above. Number-conserving products of creation and annihilation operators of fermions are expressible as a (rather complicated) combination of these non-local particle-hole operators.

15 min. break

DY 54.7 Thu 16:45 ZEU/0114

Emergence of generic first-passage time distributions for large Markovian networks — •Julian B. Voits[1] and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, University of Heidelberg, Germany — [2]BioQuant-Center for Quantitative Biology, University of Heidelberg, Germany

In many situations of practical interest, for example for decision-making in biological systems, it is sufficient to characterize a stochastic process by the time at which a final, absorbing state is reached (first-passage time). A prominent example is kinetic proofreading, where cells achieve remarkably accurate decisions through non-equilibrium reaction cycles. Earlier work studying corresponding models observed that as the system size grows, the first-passage time distributions converged to one of two universal forms on the time scale of its mean: either quasi-deterministic (delta-like) or quasi-memoryless (exponential). Building on the graph-theoretical interpretation of first-passage processes, here we provide a unifying explanation for these universal limits based on the distribution of the eigenvalues of the generator matrix. Then, we derive general conditions under which the distribution converges to either the deterministic or exponential limit. We demonstrate the theory by applying it to a generic birth-death process and conclude by discussing illustrative cases where the simple limiting behavior does not hold, which contradicts the naive expectation that a forward bias is sufficient to lead to a deterministic outcome.

DY 54.8 Thu 17:00 ZEU/0114

Derivation of a multi-dimensional non-equilibrium generalized Langevin equation — •Benjamin Hery — Department of Physics, Freie Universität Berlin, 14195 Berlin, Germany

The Mori-Zwanzig formalism is a powerful theoretical framework for deriving generalized Langevin equations (GLEs) for observables of interest using evolution and projection operators. Using a multi-dimensional Mori projection operator, we derive a non-equilibrium Mori GLE for a multi-dimensional observable of interest $\vec{A}$ that consists in a Markovian force, a running integral over time of a non-Markovian friction force, and a orthogonal force that is often interpreted as a random force. We study the structure of the derived GLE in three limiting cases: when the components of $\vec{A}$ are uncorrelated, when the system is at equilibrium, and when both conditions happen at the same time. In particular, we highlight the presence of a contribution to the Markovian force that takes the form of an instantaneous friction force which only vanishes when the components of $\vec{A}$ are uncorrelated.

DY 54.9 Thu 17:15 ZEU/0114

Predicting Friction Modifications under Harmonic Confinement via Perturbative Mori Projections — •Felix Riesterer and Roland Netz — Department of Physics, Freie Universität Berlin, Germany

Previous studies have shown that external potentials can alter friction, yet a comprehensive theoretical explanation for this effect is still lacking. This issue is particularly relevant for enhanced sampling techniques, such as umbrella sampling, where applied biases can distort dynamical observables.

We present a theoretical framework based on perturbative projections within the Mori Generalized Langevin Equation (GLE). The approach provides an explicit first-order prediction of the friction correction due to an external potential using only unbiased simulations. Furthermore, it clarifies the conditions under which such corrections arise.

To validate the theory, we perform molecular dynamics simulations of a Lennard-Jones fluid (argon) confined in a harmonic potential of varying strength. The theoretical predictions capture the friction enhancement to first order in the potential stiffness. These results demonstrate how harmonic umbrella sampling can modify friction, highlighting the potential impact on the interpretation of dynamical quantities obtained from biased simulations.

DY 54.10 Thu 17:30 ZEU/0114

Perturbative projection of many-body systems with applications in enhanced sampling of biomolecules — •Joan Salas-Llabrés — Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

Using a modification of the well-known Mori-Zwanzig projection operator formalism, a Generalized Langevin Equation (GLE) is derived for a general observable of interest that only depends on the phase space positions, from a many-body Hamiltonian in the presence of a constant linear external potential. In particular, the friction memory kernel is analytically computed, and via an operator perturbative expansion, it is expanded in terms of the external potential up to first order in the potential strength. We name this approach "perturbative projection", and it allows to see the effects that this bias can have on the effective dynamics of a reaction coordinate, in particular on its friction. To test the obtained analytical expression and thus compare to some order of approximation the change in friction with direct results, we choose the conformational dynamics of alanine nonapeptide in water, obtained via molecular dynamics simulations. The results show agreement over a range of bias strengths. This provides new insight into the effects of an external bias on the dynamics of a system of interest, pointing to its fundamental nature in the level of its Hamiltonian, and which in particular has important consequences for the analysis of results coming from enhanced sampling techniques.