DY 23: Statistical Physics: General II

Time: Tuesday 14:00–15:15 Location: ZEU 250

DY 23.1 Tue 14:00 ZEU 250

Microscopic theory for the shear-induced structure distortion in concentrated suspensions of spherical colloids — •Carmine Anzivino[1], Francesco Leone[1], Luca Banetta[2], Michael S. Murillo[3], and Alessio Zaccone[1] — [1]Department of Physics "A. Pontremoli", University of Milan, via Celoria 16, 20133 Milan, Italy — [2]Department of Applied Science and Technology, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129, Turin, Italy — [3]Department of Computational Mathematics, Science and Engineering, Michigan State University, East Lansing, Michigan 48824, USA

We combine an analytical solution of the Smoluchowski convection-diffusion equation that fully takes into account the boundary-layer structure, with generalized integral equations of the liquid state. We investigate the shear-induced structural distortion in suspensions of spherical colloids, in concentrated regimes of packing fraction so far explored only by means of numerical simulations [1].

For hard spheres, our findings are in very good parameter-free agreement with numerical data from literature [2]. In addition, our scheme predicts (for the first time) a consistent enhancement of the structure factor S(k) at vanishing k, upon increasing the shear rate, which we argue may signal the onset of a shear-induced phase transition from the isotropic phase to a non-uniform one.

[1] L. Banetta, F. Leone, C. Anzivino, M.S. Murillo and A. Zaccone, Phys. Rev. E 106, 044610 (2022). [2] J.F. Morris and B. Katyal, Physics of Fludis 14, 1920 (2002).

DY 23.2 Tue 14:15 ZEU 250

Coupling of a particle-based solver to a fluctuating hydrodynamic reservoir through an adaptive resolution simulation approach — •Abbas Gholami[2], Rupert Klein[1], and Luigi Delle Site[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany

Adaptive Resolution Simulation (AdResS) is a multi-resolution approach for coupling different particle-based regions. In AdResS, a fully atomistic subregion (open system) is in contact with reservoirs of non-interacting particles through a small buffer region. In this approach, a thermostat and an external (thermodynamic) force are applied in the reservoir and buffer regions to ensure the same behaviour as the reference simulation. Coupling a particle-based domain with a continuum reservoir will significantly reduce computational costs while preserving satisfactory precision in different regions.

This work uses a novel algorithm to couple the AdResS particle-based simulator to a Navier-Stokes Landau-Lifshitz solver. The coupling algorithm suggests that the proper thermodynamic force for the AdResS simulation will be interpolated among a set of pre-calculated thermodynamic forces based on the resulting continuum state at the interface region. On the other hand, to pass the information from the particle side to the continuum reservoir, the result of the AdResS simulation will apply to the corresponding continuum cells with proper interface values. The accuracy of this coupling algorithm is demonstrated through various numerical scenarios with different initial conditions.

DY 23.3 Tue 14:30 ZEU 250

The orientation field generated by a moving defect: multivalued solutions of the diffusion equation — •Jacopo Romano, Benoit Mahault, and Ramin Golestanian — Max Planck Institute for Dynamics and Self-Organization

Point-like topological defects are singular configurations that occur in a variety of in and out of equilibrium systems with two-dimensional orientational order. As they are associated with a nonzero circuitation condition, the presence of defects induces a long-range perturbation of the orientation landscape around them. Their effective dynamics is thus generally described in terms of quasi-particles interacting through the orientation field they produce, which in the simplest setting is described by the diffusion equation. Due to the multivaluedness of the orientation field, its expression for a defect moving with an arbitrary trajectory cannot be obtained via simple techniques and is often approximated by that of a static defect. Here, we propose a solution to this problem that relies on particular gauge invariance properties of the proper multivalued field derivatives. Our approach allows to derive the exact expression for the orientation created by multiple moving defects, which we find to depend on their past trajectories and thus to be nonlocal in time. Performing various expansions in relevant regimes, we show how improved approximations with respect to the static defect solution can be obtained. Moreover, our results lead to so far unnoticed structures in the orientation field of moving defects which we discuss in light of existing experimental results.

DY 23.4 Tue 14:45 ZEU 250

Perturbative and Semiclassical Expansions in Quantum Thermodynamics Using a Modified Keldysh Contour — •Sadeq S. Kadijani, Vasco Cavina, Massimiliano Esposito, and Thomas L. Schmidt — Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg

Modified Keldysh contours are a versatile tool for calculating moment generating functions (MGFs) in the context of quantum thermodynamics and quantum transport theory, and are the backbone of both Green's functions (GFs) and path integral approaches to open quantum systems. By using a different modification of the Keldysh contour, we will construct a perturbation expansion of the MGFs and discuss its semi-classical expansion. Using the symmetry property of the modified contour, we prove that the perturbative expansion obtained in this way satisfies the fluctuation theorem (FT) in every order of perturbation theory. We show that the contribution of the different diagrams can be added to obtain a general expression of the work statistics in terms of a sum of independent Poisson processes.

To further investigate the work MGF we apply the Feynman path integral techniques to the modified contour. In this way, the MGF can be written in terms of the action, which depends on the fields running on the modified contour. The action can be used to obtain a semiclassical expansion of the MGF, which is then used to compute explicitly the zeroth (classical) and the first quantum correction to the work MGF.

DY 23.5 Tue 15:00 ZEU 250

Effect of Frequency-Dependent Viscosity on Molecular Friction in Liquids — •Henrik Kiefer[1], Domenico Vitali[2], Benjamin Dalton[3], Laura Scalfi[4], and Roland Netz[5] — [1]Freie Universität Berlin, Department of Physics, Berlin, Germany — [2]Freie Universität Berlin, Department of Physics, Berlin, Germany — [3]Freie Universität Berlin, Department of Physics, Berlin, Germany — [4]Freie Universität Berlin, Department of Physics, Berlin, Germany — [5]Freie Universität Berlin, Department of Physics, Berlin, Germany

A fundamental problem in molecular dynamics is the relation between the frequency-dependent friction of a molecule in a liquid and the hydrodynamic properties of the liquid. We investigate this connection in the case of a water molecule moving in liquid water using all-atomistic molecular dynamics simulations and linear hydrodynamic theory. For this, we analytically calculate the frequency-dependent friction of a sphere with finite surface slip moving in a non-Newtonian compressible fluid by solving the linear transient Stokes equation, including frequency-dependent shear and volume viscosities, which are both determined from MD simulations of bulk liquid water. By fitting the effective sphere radius and the slip length, the frequency-dependent friction and velocity autocorrelation function from the transient Stokes equation and simulations quantitatively agree with the frequency-dependent friction of a single water molecule moving in liquid water, as defined by the generalized Langevin equation from MD simulation trajectories, provided accurate frequency-dependent viscosities are used.