CPP 62: Complex Fluids and Soft Matter - Part II (joint session DY, CPP, BP)

Time: Thursday 9:30–11:45 Location: BH-N 334

Invited Talk CPP 62.1 Thu 9:30 BH-N 334

Ultrasoft particles under out-of-equilibrium conditions — •Gerhard Kahl — Institut für Theoretische Physik, TU Wien, Vienna, Austria

On a coarse-grained level, colloids often interact via so-called ultrasoft potentials, which assume at short interparticle distances values in the order of a few $k_{\rm B}T$; thus, these particles are able to overlap at the cost of a relatively small energy penalty. Under equilibrium conditions such ultrasoft particles are able to form aggregates (clusters) of overlapping particles which can then either form a disordered or an ordered cluster phase. In the latter case, these aggregates populate the positions of a regular fcc or bcc lattice. Cluster crystals display rather unconventional properties, such as a density-independent lattice constant [1]. Also under out-of-equilibrium conditions, ultrasoft systems show unexpected features. Exposing a cluster crystal to shear leads – with increasing shear rate $\dot{\gamma}$ – to the following novel response-scenario: for small $\dot{\gamma}$-values the crystal melts; then gradually strings parallel to the flow direction form which are arranged in a hexagonal grid in the gradient-vorticity plane. Upon further increasing $\dot{\gamma}$ this lattice eventually melts [2]. Exposing a cluster crystal to Poiseuille flow the emergence of a quantized flow pattern is observed where the height and the width of the fluid stream display well-defined plateaus, indicating a successive fluidization of crystal layers adjacent to the channel walls [3].

[1] B.M. Mladek *et al.*, Phys. Rev. Lett. **96**, 045701 (2006).
[2] A. Nikoubashman *et al.*, Phys. Rev. Lett. **107**, 068302 (2011).
[3] A. Nikoubashman *et al.*, Soft Matter **8**, 4121 (2012).

CPP 62.2 Thu 10:00 BH-N 334

Dynamics of density excitations in shear-driven, confined binary mixtures — •Sascha Gerloff, Tarlan A. Vezirov, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Understanding friction on the microscopic scale is of great interest both from a fundamental and an applicational point of view. An important topic in this context is the appearance of density heterogeneities [1].

Here we perform overdamped Brownian dynamics simulations of a thin film of charged colloidal particles with two different sizes in planar shear flow. The particles interact via a combined Yukawa- and softsphere-potential. The parameters are set to suit experimental data for ludox silica particles, which where previously studied. The one-component system is known to form shear-induced multi-layer configurations in confinement and to show different intra-layer structures which depend on the applied shear rate. [2]

The corresponding two-component system under shear displays density excitations, provided that mixing of the two species is prohibited. We investigate the distribution and motion of these density excitations using voronoi tessellation. The density excitations are then identified as clusters of high local density in the spirit of the Hoshen-Kopelman algorithm.

[1] T. Bohlein, J. Mikhael and C. Bechinger, Nat. Mater. 11, 126-130 (2012).
[2] T. A. Vezirov and S. H. L. Klapp, Phys. Rev. 88, 052307 (2013).

CPP 62.3 Thu 10:15 BH-N 334

Analytical solutions for immiscible two-phase-flow in porous media — •Christoph Wolber and Rudolf Hilfer — Institut für Computerphysik, Universität Stuttgart, Allmandring 3, 70569 Stuttgart

A macroscopic theory for two-phase-flow in porous media that distinguishes between percolating (free-flowing) and non-percolating (trapped, disconnected) fluid parts has been studied. The theory naturally predicts hysteresis and spatiotemporal variations of residual and irreducible saturations. The computational advantage of the generalization over the traditional theory is the strict locality in time of all processes including hysteretic processes with simultaneous drainage and imbibition. Initial and boundary value problems on semi-infinite domains with constant total flux (generalized Buckley Leverett problems) have been solved semi-analytically with and without flow reversal. Complex combinations of shock fronts and rarefaction waves have been observed as the result.

CPP 62.4 Thu 10:30 BH-N 334

Saturation overshoot and hysteresis for twophase flow in porous media — •Rouven Steinle and Rudolf Hilfer — Institute for Computational Physics, University of Stuttgart, Germany

Observations of non-monotone saturation profiles (saturation overshoot) during twophase infiltration processes have recently attracted much attention because such profiles are mathematically excluded within the Richards approximation to the traditional Darcy theory. Here it is shown that a traditional Darcy theory combined with a simple hysteresis model yields non-monotone saturation profiles in the Buckley-Leverett limit. Analytical arguments and numerical simulations are reported. They agree quantitatively in predicting saturation overshoot. A simple jump-type hysteresis in the relative permeabilities suffices to yield a saturation overshoot, while hysteresis in the capillary pressure is not needed [1]. Extensive numerical simulations of the mathematical model reveal a strong dependence of the overshoot phenomenon on the initial and boundary conditions.

[1] Hilfer, R. and Steinle, R., *Saturation overshoot and hysteresis for twophase flow in porous media*, Eur.Phys.J.ST, vol. 223, pp. 2323 (2014)

CPP 62.5 Thu 10:45 BH-N 334

Free energy cost of forming a solid-liquid interface — •Ronald Benjamin[1] and Jürgen Horbach[2] — [1]Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität, 40225 Düsseldorf — [2]Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität, 40225 Düsseldorf

Knowledge of the solid-liquid interfacial free energy is crucial to an understanding of nucleation, crystallization, and wetting phenomena. In this talk, we present a novel simulation technique to compute this quantity directly for an interface between a crystal and its melt [1]. Our approach solves an important problem arising out of hysteresis effects which led to uncontrolled errors in previous studies. We apply our method to different interaction potentials [1, 2] and do a careful finite-size scaling analysis in each case to obtain reliable estimates of the solid-liquid interfacial free energies.

Reference:-
1.) Crystal-liquid interfacial free energy via thermodynamic integration.-R. Benjamin and J. Horbach, J. Chem. Phys. 141, 044715 (2014).
2.) Crystal-liquid interfacial free energy of hard spheres via a novel thermodynamic integration scheme.- R. Benjamin and J. Horbach, arXiv 1410.8798 (2014).

CPP 62.6 Thu 11:00 BH-N 334

Transient microrheology of viscoelastic fluids — •Juan Ruben Gomez Solano[1,2] and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universitaet Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max-Planck-Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany

Viscoelasticity is ubiquitous in soft matter ranging from biological fluids to new synthetised materials, whose mechanical response deviate from Newtonian behavior under applied stress or strain. Microrheology has proved successfully in recent years as an alternative to bulk rheology in investigating linear and steady-state flow properties of microlitre samples of such materials. More complex transient behavior, e.g. creep and strain recovery after flow startup and cessation, is far less well understood within the context of microrheology. In this work we experimentally study the transient motion of a colloidal particle actively dragged by an optical trap through different viscoelastic fluids (wormlike micelles, polymer solutions, and entangled lambda-phage DNA). We observe that, after sudden removal of the moving trap, the particle recoils due to the relaxation of the deformed fluid microstructure until its complete strain recovery. We find that the relaxational dynamics of the particle proceeds via a double exponential decay, whose relaxation times remain independent of the initial particle velocity whereas their amplitudes strongly depend on it. We show that this transient information, which has no counterpart for colloids moving in Newtonian fluids, can be exploited to determine linear and non-linear flow properties of the embedding fluid.

CPP 62.7 Thu 11:15 BH-N 334

Flow properties of anisotropic fluids — •Sebastian Heidenreich[1], Sabine H. L. Klapp[2], and Markus Bär[1] — [1]Physikalisch Technische Bundesanstalt, Berlin, Germany — [2]Technische Universität Berlin, Germany

From liquid crystal polymers to suspensions of bacteria anisotropic fluids are ubiquitous in nature and technology. The flow exhibits intriguing phenomena like flow alignment, shear banding, tumbling, shear thickening/thinning, large-scale correlation and mesoscale turbulence. The emergence of such fascinating aspects is often related to the anisotropy and to the out-of equilibrium character of the considered system. In the first part of our presentation we review selected flow phenomena of passive fluids with anisotropy. We discuss the role of the order parameter like the alignment tensor for the description of the flow properties. In particular, we introduce the relaxation equation for the alignment tensor coupled to the hydrodynamic flow and discuss the orientational dynamics in the shear flow. In the second part of the talk we focus on active fluids like dense bacterial suspensions and we introduce the governing hydrodynamic equations for self-sustained individuals that are swimming in a Newtonian fluid. We discuss the relationship to the passive counterpart and finally present recent work on mesoscale bacterial turbulence.

15 min. break