CPP 18: SYMPOSIUM Driven Soft Matter III

Time: Tuesday 16:30–18:30 Location: C 130

Invited Talk CPP 18.1 Tue 16:30 C 130

Bifurcations in complex fluids — •Ingo Rehberg and DFG-Forschergruppe 608 — Universität Bayreuth

The dynamic behavior of complex fluids in the neighborhood of bifurcation points is considered as particularly interesting, because here small changes of the external field lead to a maximal response. Moreover, the reaction of the fluid if often accompanied by symmetry breaking processes, which can be experimentally detected with great precision. In particular, we will present measurements of the reorientation of liquid crystalline gels under electric fields [1], and of the dynamic response of magnetic fluids to the change of external magnetic fields [2,3].

[1] Freedricksz transition in a thermoreversible nematic liquid gel; Matthias Müller, Wolfgang Schöpf, Ingo Rehberg, Günter Lattermann, Andreas Timme (submitted).

[2] Reorientation of a hexagonal pattern under broken symmetry: The hexagon flip; Christopher Groh, Reinhard Richter, Ingo Rehberg, and F. H. Busse, Phys. Rev. E 76, 055301(R) (2007).

[3] Response of a ferrofluid to travelling stripe forcing; Achim Beetz, Christian Gollwitzer, Reinhard Richter, Ingo Rehberg (submitted).

CPP 18.2 Tue 17:00 C 130

Dynamics in inhomogeneous liquids and glasses via the test particle limit — •Matthias Schmidt[1,2], Paul Hopkins[1], and Andrew J. Archer[3] — [1]H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, United Kingdom — [2]Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany — [3]Department of Mathematical Sciences, Loughborough University, Loughborough, Leicestershire, LE11 3TU, United Kingdom

We show that one may view the self and the distinct part of the van Hove dynamic correlation function of a simple fluid as the one-body density distributions of a binary mixture that evolve in time according to dynamical density functional theory. For a test case of soft core Brownian particles the theory yields results for the van Hove function that agree quantitatively with those of our Brownian dynamics computer simulations. At sufficiently high densities the free energy landscape underlying the dynamics exhibits a barrier as a function of the mean particle displacement, shedding new light on the nature of glass formation. For hard spheres confined between parallel planar walls the barrier height oscillates in-phase with the local density, implying that the mobility is maximal between layers, which should be experimentally observable in confined colloidal dispersions.

CPP 18.3 Tue 17:15 C 130

Dynamic density functional theory of fluids of platelike colloidal particles — •Markus Bier and Rene van Roij — Institute for Theoretical Physics, Utrecht University, The Netherlands

Fluids of platelike colloidal particles, e.g., suspensions of clay, exhibit a large range of phenomena such as flocculation, glass transitions, gelation, aging, and even liquid crystal phase transitions because of the interplay between translational and orientational degrees of freedom.

In recent years dynamic density functional theories (DDFT) for simple fluids, i.e., for particles with only translational degrees of freedom, have been derived based on Langevin dynamics, which can be considered as a reasonable description of dilute colloidal dispersions. DDFT is a convenient formalism to describe nonequilibrium configurations of inhomogeneous fluids given one knows a sufficiently precise density functional to descibe the equilibrium behaviour.

We proposed a DDFT for fluids of platelike colloidal particles based on a density functional for platelike colloidal particles within the Zwanzig approximation in order to investigate the relaxation within an external field [M. Bier and R. van Roij, Phys. Rev. E 76, 021405 (2007)] as well as the formation of nonequilibrium steady states under the influence of reservoirs which are not in equilibrium with each other [M. Bier and R. van Roij, submitted (see preprint arxiv:0710.5439v1)]. In this contribution we will briefly motivate the formalism and afterwards report in detail on the numerical findings.

CPP 18.4 Tue 17:30 C 130

Hydrodynamical jet oscillations and band structures in the flow of nano-rods — •Sebastian Heidenreich, Siegfried Hess, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergst. 36, D-10623

The flow properties of nano-rods are strongly affected by the dynamical behavior of molecular alignment. A theoretical description can be made by an relaxation equation [1] of the order parameter tensor. For plane Couette flow geometry the model implies a rather complex orientational behavior [2] even in the case where the alignment is spatially homogeneous and the flow profile is linear. In the last years the dynamics of the inhomogeneous alignment and the effect on the velocity profile was investigated intensively [3]. In our contribution we model fluid-wall interactions by boundary conditions for the alignment tensor (strong anchoring). Our numerical analysis for the plane Couette flow yields oscillating local spurts of the velocity profile, referred to as hydrodynamical jets which are caused by the competition of elasticity and flow coupling. Moreover, we observe time-dependent shear bands in startup flows.

[1] S. Hess, Z. Naturforsch. **30a**, 728, 1224 (1975)
[2] G. Rienäcker, M. Kröger, and S. Hess, Phys. Rev. E **66**, 040702(R) (2002);
[3] B. Chakrabarti, M. Das, C. Dasgupta, S. Ramaswamy, and A. K. Sood, Phys. Rev. Lett. **92**, 055501 (2004); S. Heidenreich, P. Ilg and S. Hess, Phys. Rev. E 75, 066302 (2007)

CPP 18.5 Tue 17:45 C 130

Dynamical density functional theory for anisotropic colloidal particles — •Martin Rex, Henricus Herman Wensink, and Hartmut Löwen — Institut für Theoretische Physik II: Weiche Materie, Universität Düsseldorf, Germany

We generalize the formalism of dynamical density functional theory for translational Brownian dynamics towards that of anisotropic colloidal particles which perform both translational and rotational Brownian motion. Using a mean-field approximation for the density functional and a Gaussian-segment model for the rod interaction, the dynamical density functional theory is then applied to a concentrated rod suspension in a confined slab-geometry made by two parallel soft walls. The walls are either expanded or compressed and the relaxation behavior is investigated for an equilibrated starting configuration. We find distinctly different orientational ordering during expansion and compression. During expansion we observe preferential parallel ordering of the rods relative to the wall while during compression there is homeotropic ordering perpendicular to the wall. We find a nonexponential relaxation behavior in time. Furthermore an external field which aligns the rods perpendicular to the walls is turned on or switched off and similar differences in the relaxational dynamics are found. Comparing the theoretical predictions to Brownian dynamics computer simulation data, we find good agreement.

CPP 18.6 Tue 18:00 C 130

Novel estimators for the effective charge of polyelectrolytes during electrophoresis — •Kai Grass[1] and Holm Christian[1,2] — [1]Frankfurt Institut for Advanced Studies, Ruth-Moufang-Strasse 1, D-60438 Frankfurt am Main, Germany — [2]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz, Germany

In this contribution, we present two novel estimates for the effective charge (Q_{eff}) of strongly charged polyelectrolyte chains during free solution electrophoresis by means of coarse-grained molecular dynamics simulations.

First, we show that it is possible to calculate Q_{eff} from the electrophoretic mobility obtained from Langevin simulations. Second, we are able to directly obtain Q_{eff} from the number of comoving counter ions. Both estimators yield similar results and show that the effective charge of polyelectrolyte chains grows linear in the number of monomers as previously predicted.

The effective charge is used to evaluate the scaling behavior of the hydrodynamic friction of the polyelectrolyte-counterion-complex. We show the violation of the Nernst-Einstein equation during free solution electrophoresis by obtaining a linear dependence on chain length for the hydrodynamic friction which differs from the scaling of the hydrodynamic size.

CPP 18.7 Tue 18:15 C 130

Dynamical properties of magnetic nanoparticles in ferrofluids investigated by Brownian dynamics — Guillaume Meriguet[1],

•Marie Jardat[1], Emmanuelle Dubois[1], Vincent Dupuis[1], Bela Farago[2], Regine Perzynski[1], and Pierre Turq[1] — [1]Universite Pierre et Marie Curie-Paris6, Paris, France — [2]Institut Laue Langevin, Grenoble, France

The dynamical properties of real ferrofluids, charge-stabilized aqueous dispersions of magnetic particles bearing a permanent dipole, are investigated with and without an external magnetic field by Brownian dynamics simulations. On the one hand, since the magnetic particles have an anisotropic optical index, their rotational properties have been studied experimentally: an external magnetic field induces a macroscopic birefringence the relaxation of which is followed after the magnetic field is suppressed. A non-equilibrium simulation procedure is proposed that mimics the experimental operating mode: after equilibrium simulations under magnetic field, the birefringence decay is recorded once the field is suppressed. On the other hand, the translational dynamics of the nanoparticles is investigated. The diffusion coefficient of the particles has been experimentally determined at several wave-vectors using neutron spin echo spectroscopy, with and without an external magnetic field. The same quantities are computed from Brownian dynamics simulations. The comparison between experimental and theoretical results allow us to evaluate the influence of several factors on the dynamics, such as the volume fraction, the dipolar interactions or hydrodynamic interactions.