CPP 36: Complex Fluids and Soft Matter 2 (joint session DY/CPP)

Time: Thursday 10:00–11:30 Location: H18

CPP 36.1 Thu 10:00 H18

Underscreening in the Restricted Primitive Model — •Andreas Härtel — Institute of Physics, University of Freiburg, Germany

Electric double layers occur where charges are screened by other charges, for instance, when charged surfaces of electrodes, colloids, or cells are exposed to electrolytes (mobile ions in a solvent). Increasing the concentration of mobile ions leads to more efficient screening, if concentrations are sufficiently low. At high concentrations, however, the screening by finite-sized ions becomes less efficient than those of point-like ions due to packing, an effect called underscreening. Some experiments report underscreening as a strong effect that follows some universal scaling [1], but the observation could not been explained by theoretical models yet. Conversely, independent theoretical studies actually ruled out the most important model for electrolytes of finite-sized ions as a candidate able to explain underscreening, namely the restricted primitive model [2]. In this talk I will discuss in which sense underscreening can and cannot be found in the restricted primitive model and in which sense the effect follows some universal scaling. I will support the discussion by recent theoretical results obtained from simulations and liquid state theories.

[1] Lee et al., Underscreening in concentrated electrolytes, Faraday Dicuss. 199, 239 (2017).

[2] Cats et al., Primitive Model Electrolytes in the Near and Far Field: Decay Lengths from DFT and Simulations, J. Chem. Phys. 154, 124504 (2021).

CPP 36.2 Thu 10:15 H18

Reciprocal and nonreciprocal eigenmodes of viscoelastic fluids — •Juliana Caspers[1], Clemens Bechinger[2], Nikolas Ditz[2], Matthias Fuchs[2], Felix Ginot[2], Karthika Krishna Kumar[2], Luis Frieder Reinalter[2], and Matthias Krüger[1] — [1]Institute for Theoretical Physics, Georg-August Universität Göttingen, 37073 Göttingen, Germany — [2]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

Complex fluids such as wormlike micellar solutions are in general non-Markovian. In equilibrium, their behavior is often well approximated by a simple Maxwell model with one characteristic timescale [1]. Recoil experiments, after a colloidal probe has been sheared through the solvent, however, displayed a double-exponential relaxation [2]. We found excellent agreement of our measurements with a linear two-bath particle model. Depending on whether the optical trap which confines the probe is turned on or off, we find two sets of eigenmodes in our model, corresponding to either nonreciprocal (trap on) or reciprocal (trap off) forces. Using different recoil protocols as well as equilibrium mean square displacement measurements we confirmed the existence of these two different sets of timescales with experiments. Finally, for linear systems, we find a Volterra relation between two memory kernels, characterizing reciprocal and nonreciprocal forcing.

[1] F. Ginot, J. Caspers, M. Krüger, C. Bechinger. *Phys. Rev. Lett.* **128**, 028001 (2022)

[2] F. Ginot, J. Caspers, L. F. Reinalter, K. Krishna Kumar, M. Krüger, C. Bechinger. *arXiv:2204.02369* (2022)

CPP 36.3 Thu 10:30 H18

Elastic Turbulence in von Kármán geometry — •Reinier van Buel and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Elastic turbulence, occurring in viscoelastic fluid flow at vanishing Reynolds numbers, is an interesting flow state [1-4] and has been experimentally studied in the von Kármán geometry [1]. Elastic turbulence is especially appealing for the mixing of fluids on the micron scale, which is extremely challenging in Newtonian fluids where transport relies on diffusion. Here, we present a fully three-dimensional numerical investigation of the von Kármán flow using the Oldroy-B model [4]. We observe a non-axisymmetric mode with four-fold symmetry that drives the flow instability towards elastic turbulence and compare it to results obtained from a linear stability analysis. By analyzing the velocity fluctuations and defining an order parameter, we identify a bistable flow state above a sub-critical transition, which switches between a weakly chaotic flow state and elastic turbulence and exhibits hysteretic behavior. Furthermore, we reveal a sharp increase in the flow resistance at the transition to elastic turbulence, which we attribute to the elastic contribution of the work performed at the open side surface of the flow. Finally, an analysis of the spatial and temporal velocity power spectra confirms the turbulent nature of the flow.

[1] A. Groisman and V. Steinberg, Nature **405**, 53 (2000).

[2] R. Buel, C. Schaaf, H. Stark, Europhys. Lett. **124**, 14001 (2018).

[3] R. Buel and H. Stark, Sci. Rep. **10**, 1-9 (2020).

[4] R. Buel and H. Stark, Phys. Fluids **34**, 4 (2022).

CPP 36.4 Thu 10:45 H18

Coarsening dynamics of quasi 2D emulsions in free-standing smectic films — •Christoph Klopp, Torsten Trittel, and Ralf Stannarius — Institute for Physics, Otto von Guericke University Magdeburg, Germany

Hydrodynamic phenomena in thin films play a crucial role in biological systems, in nature and modern technology. Various experimental and theoretical studies explored, e.g., the motion of objects in quasi two-dimensional films [1], the merging of inclusions [2-4] and the structural change of emulsions during long-term observations. Here, we demonstrate and describe the coarsening dynamics of emulsions formed by smectic islands (flat circular regions) on liquid crystal bubbles in microgravity at the International Space Station (ISS). The smectic islands form polydisperse, disordered arrangements representing quasi 2D emulsions. We analyze the time evolution of these ensembles that proceed through direct island coalescence or the exchange of material through the background film (Ostwald ripening). Coarsening is ubiquitous in liquid emulsions and foams, and important for their stability. We compare our results with such systems and analyze the dominant process for the 2D coarsening dynamics.

Acknowledgements: This study was supported by NASA, DFG and DLR within the OASIS and OASIS-Co projects.

References: [1] A. Eremin et al., Phys. Rev. Lett., 107, 268301 (2011) [2] N. S. Shuravin et al., Phys. Rev. E, 99, 062702 (2019) [3] Z. H. Nguyen et al., Phys. Rev. Research, 3, 033143 (2021) [4] C. Klopp et al., Soft Matter 16 4607 (2020)

CPP 36.5 Thu 11:00 H18

Phase transitions in the generalised chiral Lebwohl-Lasher model — •Philipp Elsässer and Anja Kuhnhold — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

The behaviour of liquid crystals can be described by using the Lebwohl-Lasher (LL) model, where unit vectors that resemble nematic directors are positioned on a simple cubic lattice. Due to the interaction potential, which favours parallel orientations, this model is well suited to analyse isotropic-nematic (IN) phase transitions.

There exist several extensions to this model with which its applicability can get further enhanced. We use two combined extensions to obtain the generalised chiral Lebwohl-Lasher model: We apply a generalisation to tune the sharpness of the potential, as in the work of Fish and Vink [1] and add a chiral term which is based on the work of Memmer et al. [2]. In this system we study the phase transition properties with the help of Monte Carlo simulations. To identify characteristic properties of the transitions, we apply finite-size scaling. This allows us to determine chirality-sharpness parameter pairs with which we can manipulate the nature of the transition between ordered and disordered states [3].

[1] J. M. Fish, R. L. C. Vink, PRE **81**, 021705 (2010).

[2] R. Memmer, O. Fliegans, PCCP **5**, 558 (2003).

[3] P. Elsässer, A. Kuhnhold, PRE **105**, 054704 (2022).

CPP 36.6 Thu 11:15 H18

Systematic parametrization of non-Markovian dissipative thermostats for coarse-grained molecular simulations with accurate dynamics — •Viktor Klippenstein and Nico F. A. Van Der Vegt — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, Technische Universität Darmstadt, 64287 Darmstadt, Germany

The Mori-Zwanzig theory, in principle, allows to derive an exact equation of motion for coarse-grained degrees of freedom based on the dynamics of an underlying fine-grained reference system.[1] Still, in practice the simultaneous representation of structural and dynamic properties in particle-based models poses a complicated problem, e.g. due

to the non-linearity of the exact coarse-grained equation of motion.

A viable approximate approach is to start from a conservative coarse-grained force-field and to extend the standard Newtonian equation of motion used in molecular simulation with a linear generalized Langevin thermostat. We demonstrate how such a thermostat can be parametrized to correctly represent dynamic properties, both in a purely bottom-up approach[2,3] or by applying iterative optimization.[3] We consider the Asakura-Oosawa model as a test case.[3]

[1] V. Klippenstein, M. Tripathy, G. Jung, F. Schmid, and N. F. A. van der Vegt, The Journal of Physical Chemistry B 125, 4931 (2021).
[2] V. Klippenstein and N. F. A. van der Vegt, The Journal of Chemical Physics 154, 191102 (2021).
[3] V. Klippenstein and N. F. A. Van Der Vegt, The Journal of Chemical Physics under review (2022).