# CPP 46: Complex Fluids and Soft Matter (joint session DY/CPP)

Time: Tuesday 9:30–13:00 Location: ZEU 160

CPP 46.1 Tue 9:30 ZEU 160

**Topological states of hard rods in extreme annular confinement** — •René Wittmann[1], Louis Cortes[2], Dirk Aarts[2], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Department of Chemistry, University of Oxford, UK

Hard particles are a standard model for colloidal systems and can be effectively studied within classical density functional theory (DFT). Fundamental mixed measure theory (FMMT) allows to predict the phase behavior of a hard-body fluid solely from the shape of individual particles. Recent experimental advances allow for the synthesis of colloids with a nearly hard interaction that can be analyzed on the single-particle level. Slices of a system of such silica rods confined in a three-dimensional chamber under gravity can be considered a quasi-two-dimensional fluid that exhibits typical liquid-crystal behavior in confinement.

Applying FMMT to hard discorectangles in two dimensions, we map out a full phase diagram. Then we focus on a smectic fluid in extreme complex confinement, where the optimal bulk layer spacing competes with the extrinsic geometric and topological constraints. As a result, we characterize a variety of topologically different states in an annular geometry, also observed in particle-resolved experiments with silica rods. By further comparing the free energy of the different states, naturally provided by our DFT, we map out a topological phase diagram, indicating the stable topology depending on the details of the annular geometry.

CPP 46.2 Tue 9:45 ZEU 160

**Phase Field Crystal Model of patchy colloids in two dimensions** — Robert Weigel and •Michael Schmiedeberg — Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Motivated by our recent simulation studies of quasicrystals that occur in systems of patchy colloids [1,2], we develop a Phase Field Crystal Model for such particles. We consider two-dimensional patchy colloids with symmetrically placed attractive sites on their surface, such that they interact with preferred binding angles. We construct a free energy functional that is similar to the free energy used for liquid crystals [3], but obeys the symmetry of the patchy colloids. The functional depends on both a density field and an orientation field. Free numerical minimization of the free energy yields a rich phase behavior of complex structures.

[1] Gemeinhardt et al., Eur. Phys. J. E 41, 126 (2018).
[2] Gemeinhardt et al., EPL 126, 38001 (2019).
[3] Achim et al., Phys. Rev. E 83, 061712 (2011).

CPP 46.3 Tue 10:00 ZEU 160

**Relations between angular and Cartesian orientational expansions*** — •Michael te Vrugt and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

Orientational expansions, which are widely used in the natural sciences, exist in angular and Cartesian form. Although these expansions are orderwise equivalent, it is difficult to relate them in practice. Moreover, the standard expansion has to be modified for particles with asymmetric shape, where a description in terms of spherical harmonics or symmetric traceless tensors is not sufficient. We discuss various methods for orientational expansions and their application for the definition of orientational order parameters in liquid crystal physics. In particular, we explain how conversion tables between angular and Cartesian expansions can be constructed, which we have done up to third order. This is important, e.g., for the comparison of theoretical and experimental results in liquid crystal physics.

**Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1*

CPP 46.4 Tue 10:15 ZEU 160

**Dynamic wrinkling of thin liquid crystal films** — •Dominik Mnich, Torsten Trittel, Kirsten Harth, Christoph Klopp, and Ralf Stannarius — Otto von Guericke University, Institute for Physics, 39106 Magdeburg, Germany

We demonstrate spontaneous wrinkling as a dynamical pattern in freely floating liquid-crystalline films. These films behave liquid-like with respect to flow within the film plane. The adjustment of the film shape to quick changes often requires the formation of additional layers. Centimeter-sized freely floating smectic bubbles are studied during the excitation with acoustic waves. We show that such films develop an undulation instability under acoustic excitation. The results of parabolic flight and ground lab experiments are presented. The observed "wrinkles" show charactistic wavelengths in the submillimeter range. We introduce a basic model of the wavelength selection mechanism.

CPP 46.5 Tue 10:30 ZEU 160

**Thermally driven material transport in thin freestanding films** — •Torsten Trittel, Christoph Klopp, Kirsten Harth, and Ralf Stannarius — Otto von Guericke University, Institute for Physics, 39106 Magdeburg, Germany

In addition to their important role in display applications, liquid crystals are attractive in the field of fundamental physics. Smectics can form thin free-standing films with aspect ratios exceeding one million to one (width/thickness). These homogeneously thin films serve as an ideal model system for the study of two-dimensional hydrodynamics. We investigate thermally driven material transport within the film plane under microgravity conditions. Temperature differences in the film lead to thermocapillary (Marangoni) flow. In materials with a normal (negative) temperature coefficient of the surface tension $d\sigma/dT < 0$, temperature inhomogeneities lead to material transport from the warm to the cold film edge. In materials with $d\sigma/dT > 0$, flow is reversed. We present a quantitative model, which predicts that the temperature difference between the hot and cold film edge is the relevant parameter, not the gradient as in conventional thermoconvection.

[1] Trittel et al., Marangoni Flow in Freely Suspended Liquid Films, Phys. Rev. Lett., 122 (2019)

CPP 46.6 Tue 10:45 ZEU 160

**Defect annihilation 2D using free-standing smetic films** — •Kirsten Harth[1], Amine Missaoui[1], Peter Salamon[2], and Ralf Stannarius[1] — [1]Institut für Physik, Otto-von-Guericke Universität Magdeburg — [2]Department of Complex Fluids, Wigner Research Center, Budapest, Hungary

Interacting defects in quasi-2D geometries occur in manifold systems, from strings in cosmology over spin systems in Bose-Einstein condensates or thin magnetic films to liquid crystals. Free-standing smecti C films (smC FSF) represent a quite simple sytem for studying fluid mechanics and pattern formation in 2D. They are particularly easy to handle and orientational patterns are directly observable using polarizing microscopy, but few experiments exist so far. Theory is either fully numerical or focuses on very simplified situations. Orientational problems among the defects and with the far director field were only recently noticed.

With a special method, we are able to prepare isolated pairs of +1 and -1 defects in homogeneous smC FSF, and we study their annihilation. Aligned defect pairs qualitatively follow expectations from theory and approach on straight paths. Misoriented defects pairs display curved trajectories, and their dynamics quantitatively disagrees with theoretical predictions[1]. We discuss experimental findings and possible explanations for the discrepancies.

[1] X. Tang and J. V. Selinger, Soft Matter 13, 5481 (2017)
[2] A. Missaoui, K. Harth, P. Salamon, R. Stannarius, arXiv:1911.05224

**15 min. break.**

CPP 46.7 Tue 11:15 ZEU 160

**Static properties of modulated hard-spheres liquid.** — •Michele Caraglio, Charlotte F. Petersen, and Thomas Franosch — Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Technikerstraße 21A, A-6020 Innsbruck, Austria

The structure of a liquid can be manipulated with externally applied fields. This can be achieved experimentally with interfering lasers and has been implemented with colloidal particles [1, 2]. This possibil-

ity also paves the way to a better understanding of confined liquids [3], which are prevalent in nature and necessary in many industrial applications.

We investigate static properties in a hard-sphere liquid with modulated density profile obtained by applying an external periodic field. In this system we will control three dimensionless parameters: the packing fraction, the amplitude of the potential relative to temperature and its wavelength relative to particle diameter. For this purpose, the Ornstein-Zernike integral equation using Percus-Yevick closure relation is solved numerically. The theory requires the density profile as input, which can be obtained from density functional theory. Similar to a liquid confined in a slit, a non-monotonic evolution of the static structure factor peak and the pressure is observed upon variation of the potential wavelength.

[1] C. Bechinger, M. Brunner and P, Leiderer, PRL 86, 2001. [2] F. Evers, et al., PRE 88, 2013. [3] S. Saw and C. Dasgupta, J. Chem. Phys. 145, 2016.

CPP 46.8 Tue 11:30 ZEU 160

**Analytical classical density functionals from an equation learning network** — •Shang-Chun Lin[1], Georg Martius[2], and Martin Oettel[1] — [1]Institut für Angewandte Physik, Eberhard Karls Universität Tübingen, 72076 Tübingen, Germany — [2]Max Planck Institute for Intelligent Systems Tübingen, 72076 Tübingen, Germany

We explore the feasibility of using machine learning methods to obtain an analytic form of the classical free energy functional for two model fluids, hard rods and Lennard*Jones, in one dimension. The Equation Learning Network proposed in Ref.[1] is suitably modified to construct free energy densities which are functions of a set of weighted densities and which are built from a small number of basis functions with flexible combination rules. This setup considerably enlarges the functional space used in the machine learning optimization. As a result in Ref [2], we find a good approximation for the exact hard rod functional. For the Lennard–Jones fluid, we let the network learn the full excess free energy functional and the excess free energy functional related to interparticle attractions. Both functionals show a good agreement with simulated density profiles inside and outside the training region. If time allow, we will show the result that forgo the idea gas contribution.

[1]G. Martius and C. H. Lampert, arXiv:1610.02995 (2016).
[2]S.-C. Lin, G. Martius and M. Oettel, arXiv:1910.12752 (2019).

CPP 46.9 Tue 11:45 ZEU 160

**First order phase transitions: From bifurcation diagrams to the thermodynamic limit** — •Uwe Thiele[1], Tobias Frohoff-Hülsmann[1], Sebastian Engelnkemper[1], Edgar Knobloch[2], and Andrew J. Archer[3] — [1]Institut für Theoretische Physik and Center of Nonlinear Science (CeNoS), Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Department of Physics, University of California, Berkeley, California 94720, USA — [3]Department of Mathematical Sciences, Loughborough University, Loughborough, LE11 3TU, UK

We consider simple mean field continuum models for first order liquid-liquid demixing and solid-liquid phase transitions and show how the Maxwell construction at phase coexistence emerges on going from finite-size closed systems to the thermodynamic limit [1]. The theories considered are the Cahn-Hilliard model of phase separation, which is also a model for the liquid-gas transition, and the phase field crystal model of the solid-liquid transition. Our results show that states comprising the Maxwell line depend strongly on the mean density with spatially localized structures playing a key role in the approach to the thermodynamic limit. [1] U. Thiele et al., New J. Phys., at press (2019), doi: 10.1088/1367-2630/ab5caf.

CPP 46.10 Tue 12:00 ZEU 160

**Controlling Elastic Turbulence** — •Reinier van Buel and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Controlling the flow patterns of viscoelastic fluids is extremely challenging due to their inherent non-linear and time-dependent properties. These complex fluids exhibit transitions from laminar to turbulent flows, which is useful for heat and mass transport in liquids at the micron scale [1], whereas in Newtonian fluids transport is dominated by diffusion. Turbulent viscoelastic flows show similar properties as their counterparts in Newtonian fluids[1,2] and consequently the observed flow pattern is called *elastic turbulence* [1]. It occurs in shear flow for increasing Weissenberg number Wi, the product of polymer relaxation time and shear rate.

Numerically solving the Oldroyd-B model in a two-dimensional Taylor-Couette geometry, we have identified and described the supercritical transition to turbulent flow at a critical Weissenberg number [2]. Here, we demonstrate that elastic turbulence can be controlled by a time-modulated shear rate. The order parameter measuring the strength of turbulence continuously goes to zero with increasing modulation frequency or Deborah number De. It ultimately vanishes via a supercritical transition, where flow then becomes laminar. Moving closer to the critical Weissenberg number, smaller modulation frequencies are sufficient to induce laminar flow.

[1] A. Groisman and V. Steinberg, Nature **405**, 53 (2000).
[2] R. Buel, C. Schaaf, H. Stark, Europhys. Lett. **124**, 14001 (2018).

CPP 46.11 Tue 12:15 ZEU 160

**Universal properties of creep flow** — •Marko Popović[1], Tom de Geus[1], Wencheng Ji[1], Alberto Rosso[2], and Matthieu Wyart[1] — [1]Institue of Physics, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — [2]LPTMS, CNRS, Univ.Paris-Sud, Universite Paris-Saclay, 91405 Orsay, France

Amorphous solids, such as atomic glasses, colloidal suspensions, granular matter or foams, begin to deform plastically when exposed to external stress $\Sigma$. Steady state flow of these materials in absence of thermal fluctuations is usually described as $\dot{\epsilon} \sim (\Sigma - \Sigma_c)^\beta$ for stresses above critical stress $\Sigma_c$ and vanishes below it, while in presence of thermal fluctuations flow persists below $\Sigma_c$ but is exponentially suppressed. The transient plastic deformation, called creep flow, is much less understood despite its importance in practical applications. Creep flow often displays a power-law decay in time $\dot{\epsilon} \sim t^{-\mu}$ after which it can either arrest or eventually yield at fluidisation time $\tau_f$. In recent years various numerical values and/or laws have been suggested for the exponent $\mu$ and time $\tau_f$ in particular experimental or numerical studies. We propose that mechanism underlying creep flow is the same as that of the steady state flow, which allows us to predicts parameters $\mu$ and $\tau_f$ of creep flow in terms of the steady state flow parameters, both in athermal and thermally activated systems. We successfully tested all our predictions using different mesoscopic elasto-plastic models of amorphous solids and found them to be consistent with published experimental results.

CPP 46.12 Tue 12:30 ZEU 160

**Formation of networks from attractive particles under shear** — •Sebastian Bindgen[1], Dieter Diels[1], Pierre de Buyl[2], Joost de Graaf[3], and Erin Koos[1] — [1]Department of Chemical Engineering, KU Leuven, Celestijnenlaan 200f - box 2424, 3001 Leuven, Belgium — [2]Institute for Theoretical Physics, KU Leuven, Celestijnenlaan 200d - box 2415, 3001 Leuven, Belgium — [3]Institute for Theoretical Physics, Utrecht University, Princetonplein 5, 3584 CC Utrecht, The Netherlands

Simulations give access to physical quantities at the particle-level, which are not readily accessible via experimental techniques. Lees-Edwards boundary conditions replicate in-vitro conditions and have seen significant use in the polymer community. We have implemented and tested a version of this algorithm in the MD simulation package ESPResSo. The implementation, which is based on pair-wise thermostating using the dissipative particle dynamics technique, can also mimic non-linear effects such as shear banding. We demonstrate that our implementation captures the enhanced diffusion of particles coupled to the fluid. Furthermore, we use our implementation to study the dynamic properties of depletion gels including their formation and breakup under shear flow. Recent investigations have shown that hydrodynamics affects the time scales on which these gels form under quiescence, while leaving the final structure unaltered. We aim to show these processes under dynamic conditions. Our study is of clear interest for industrial systems such as ink or pastes as they can experience various complex flow fields during processing and application.

CPP 46.13 Tue 12:45 ZEU 160

**Tactoids, membranes and fribrils – finite assemblies of rod-like particles** — •Anja Kuhnhold, Nils Göth, Nadja Helmer, Victor Tänzel, and Tanja Schilling — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

Systems composed of rod-like particles and spherical depleting agents show a variety of self-assembled shapes and structures. We discuss a few of them and present corresponding Monte Carlo simulation results. The model system ingredients are hard spherocylinders as rod-

like component and implicit Asakura-Oosawa spheres as depletants. In addition we study the effect of a chiral pair interaction between the rods.

This work got inspired by experiments using viruses as rod-like particles and polymer coils as depleting agents, see e.g. [1,2]. The monodispersity of viruses makes them a nice model system to compare simulations to. Beyond the comparison simulation results can be used to direct the self-assembly for specific structure-function relationships, e.g. templating or sensing.

[1] T. Gibaud, J. Phys.: Condens. Matter **29**, 493003 (2017).
[2] B. Sung et al., Soft Matter **15**, 9520 (2019).