CPP 20: Complex Fluids and Soft Matter 2 (joint session DY/CPP)

Time: Wednesday 11:00–13:00 Location: DYa

CPP 20.1 Wed 11:00 DYa

Thermally driven material transport in thin freestanding films — •Torsten Trittel, Kirsten Harth, Christoph Klopp, and Ralf Stannarius — Otto-von-Guericke Universität, 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.

CPP 20.2 Wed 11:20 DYa

Phase Field Crystal Model of patchy colloids in two dimensions — •Robert F. B. Weigel and Michael Schmiedeberg — Friedrich-Alexander-Universität Erlangen-Nürnberg, 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 20.3 Wed 11:40 DYa

Orientational order parameters for arbitrary classical and quantum liquid crystals — •Michael te Vrugt and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149, Münster, Germany

The orientational order of liquid crystals is measured using orientational order parameters such as the polarization vector and the nematic tensor. These are obtained from an angular or Cartesian multipole expansion of the one-body distribution function of the liquid crystal. In recent years, there has been an increase of interest in particles with general shapes, as well as in so-called "quantum liquid crystals" which are relevant, e.g., in superconductors. However, the standard methods for defining order parameters are not applicable to biaxial particles or quantum systems. In this talk, we discuss how the orientational expansion method can be generalized to particles with arbitrary shape [1] and to quantum soft matter [2]. This provides a unified framework for general classical and quantum liquid crystals.

[1] M. te Vrugt and R. Wittkowski, AIP Advances 10, 035106 (2020)

[2] M. te Vrugt and R. Wittkowski, Annalen der Physik 532, 2000266 (2020)

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CPP 20.4 Wed 12:00 DYa

Analytical classical density functionals from an equation learning network — •ShangChun Lin[1], Georg Martius[2], and Martin Oettel[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany — [2]Max Planck Institute for Intelligent Systems, 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 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.

[1]G. Martius and C. H. Lampert, arXiv:1610.02995 (2016).
[2]S.-C. Lin, G. Martius and M. Oettel, JCP 152.2 (2020): 021102.

CPP 20.5 Wed 12:20 DYa

Particle-resolved topological defects of smectic colloidal liquid crystals in extreme confinement — •René Wittmann[1], Louis Cortes[2], Hartmut Löwen[1], and Dirk Aarts[2] — [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 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 study 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.

Publication: R. Wittmann et al., Nat Commun 12, 623 (2021).

CPP 20.6 Wed 12:40 DYa

Full phase diagram of continuous-time self-propelled particle models with alignment interaction — •Yinong Zhao[1], Pawel Romanczuk[1], and Cristian Huepe[2,3] — [1]Institute of Theoretical Biology, Department of Biology, Humboldt Universität zu Berlin — [2]CHuepe Labs, 2713 West Haddon Ave #1, Chicago, IL 60622, USA — [3]Northwestern Institute on Complex Systems and ESAM, Northwestern University, Evanston, IL 60208, USA

Self-propelled particle (SPP) models are widely used for exploring emergence of collective motion in nature. Despite the significant advances over the past decades in understanding self-organized active matter, many questions remain open about the general phase space of Vicsek-like alignment models and the regions of validity of corresponding analytical theories. We investigate a set of different continuous-time SPP-models with alignment interactions. We find that all these models share qualitatively the same phase diagram. Focusing on one of them, we identify three homogeneous states with long-range orientational order, that can be distinguished using statistical approaches. We tested the predictions of the Toner-Tu theory on these states and show that they do not hold for all three of them. Furthermore, we also phenomenologically explore the role of positional repulsion on the emergent spatial structure. Our study provides a broad, over-arching perspective on continuous-time alignment-based SPP model.