CPP 23: Complex Fluids and Soft Matter 1 (joint session DY/CPP)

Time: Wednesday 9:30–12:00 Location: H18

CPP 23.1 Wed 9:30 H18

Writing in Water — •Thomas Palberg and Nadir Möller — Institut für Physik, Johannes Gutenberg Universität Mainz

Writing is an ancient cultural technique, typically performed by leaving some trace in or on a solid surface. We here explore the possibilities of leaving the trace in a liquid medium close to a surface and obtain lines or letters with high contrast and durability. Ion exchange (IEX) resin beads are used as mobile proton or hydroxyl ion sources. Moving them across the substrate in low-salt water, leaves a pH trace. Added autonomously swimming particles are able to follow this trace, mimicking hunter and prey dynamics or mate tracing, but without leaving a visible testimony. Written lines are realized by adding larger amounts of micron-sized passive particles, which settle to the like-charged substrate. Being phoretically drawn to or repelled from the pH traces, they form a well-visible trail behind the source. Trails of cationic IEX are white on black, those of anionic IEX are black on white. Their diffusive fading is slowed by continued phoretic flows and trails are stable up to hours. Sources moving autonomously just scribble. Sources propelled straight by gravity leave high-contrast lines. Deliberate tilting sequences for the substrate, then, facilitate writing.

CPP 23.2 Wed 9:45 H18

Composition Dependent Instabilities in Mixtures With Many Components — •Filipe Thewes, Matthias Krüger, and Peter Sollich — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany

Understanding the phase behavior of mixtures with many components is a key step towards a physics-based description of intracellular compartmentalization. We study the instabilities of a model where the interactions as quantified by the second virial coefficients are taken as random Gaussian variables. Using tools from free probability theory we obtain the spinodal curve and the nature of instabilities for an arbitrary distribution of components, thus lifting the drastic simplification of uniform composition that has been made in earlier work. We illustrate our results with examples and show that, by controlling the density of only a few components, one can systematically change the nature of instabilities and achieve demixing for realistic scenarios, which appeared to be ruled out by previous studies. Inspired by these results, we introduce an additive model taking into account also deterministic interactions. We show how this systematic interaction leads to a competition between different forms of instabilities that can be tuned by controlling the model parameters. Since most experimental protocols for complex mixtures rely on tuning either the composition or systematic interactions, we expect our results to significantly extend the range of mixtures that can be treated within the mean-field model.

CPP 23.3 Wed 10:00 H18

Phase behaviour of mixtures of hard spheres and hard rods — •Poshika Gandhi[1], Joeri Opdam[2], Anja Kuhnhold[1], Tanja Schilling[1], and Remco Tuinier[2] — [1]Institute of Physics, Albert-Ludwigs-University Freiburg, Germany — [2]Institute for Complex Molecular Systems, Eindhoven University of Technology, The Netherlands

Phase behaviours of complex mixtures are challenging to predict. A binary mixture of hard spherocylinders (HSC) and hard spheres (HS) is one such system. As rod-like particles have large excluded volume, a free volume theory (FVT) can be used to gain insights into demixing phenomenon and phase stability.

Vliegenthart *et al*[1] modified an existing FVT for binary mixtures of HS to accommodate HSC. This FVT works well for the needle limit, i.e., weak excluded volume interactions between HSC. It, however, predicts the phase boundaries at too low HSC concentrations. Opdam *et al*[2] showed that by incorporating excluded volume interactions between the depletants even in the reservoir improves the FVT significantly.

We used the new FVT to predict phase boundaries of colloidal mixtures and compared them to MC simulations. The results show that accounting for all the excluded volumes of all the components may be pivotal in understanding phase behaviour of colloidal mixtures [3].

[1] G. A. Vliegenthart et al., J. Chem. Phys., **111**, 4153 (1999).
[2] J. Opdam, et al., J. Chem. Phys., **154**, 204906 (2021)
[3] J. Opdam, et al., Phys. Chem. Chem. Phys., **24**, 11820 (2022)

CPP 23.4 Wed 10:15 H18

Markov State Modelling of Self Assembling Colloidal Systems — •Salman Fariz Navas and Sabine H.L. Klapp — ITP, Technische Universität Berlin, Germany

Many colloidal particle systems display self-assembly phenomena yielding, e.g., clusters or gel-like materials. The current project focuses on the use of phase space discretization techniques towards developing a coarse-grained description of self-assembly processes in colloidal systems.

Specifically, we develop a corresponding Markov State Model from particle-resolved Brownian Dynamics simulations, wherein the Markov states are the various local structural configurations present in the system and the Markovian process describing the stochastic transition of particles from one structure to the other.

The specific self-assembly problem studied here involves the aggregation of colloidal particles with field-induced multipolar interactions [1]. We use bond orientational order parameters and the coordination number as parameters to define the discrete states. The number of particles in the largest cluster in the system (n) is used as a parameter to quantify the progress of the overall aggregation. Transition probability matrices (TPM) between the different states are then computed for each value of n. Information regarding relaxation times and pathways relevant to the aggregation process are extracted by analyzing changes in the TPM elements.

[1] Florian Kogler, Orlin D. Velev, Carol K. Hall and Sabine H. L. Klapp, Soft Matter 11, 7356 (2015)

CPP 23.5 Wed 10:30 H18

Repulsion of topological defects in quasi-2D liquid crystal films — •Kirsten Harth[1,2] and Ralf Stannarius[3] — [1]Fachbereich Technik, TH Brandenburg, Brandenburg an der Havel, Deutschland — [2]MARS und MRTM, Otto von Guericke Universität Magdeburg, Deutschland — [3]Institut für Physik und MARS, Otto von Guericke Universität Magdeburg, Deutschland

The dynamics of topological defects is of interest, e.g., in phase transitions, cosmology or structural organization of colloids and active matter. Liquid crystals are a straightforward system allowing optical characterization of defect motion. As anisotropic fluids, they are characterized by orientational order, introducing long-range elastic forces, in addition to liquid-like fluidity with viscosity coefficients related to, e.g., the local shear flow directions respective to the local orientational field. This causes intriguing effects and must not be neglected.

The comparison of recent exeriments [1,2] in free-standing smectic C films to theoretical and numerical predictions [2,3] leaves a number of questions unanswered. A proper consideration of flow coupling and / or of an anistropy of the elastic constants in a simulation with realistic boundary conditions may solve the issues. We explain why elastic anisotropy is particularly important here. Experimental and numerical data are compared to elucidate the effect of elastic constants and flow on the repeulsion dynamics.

[1] A. Missaoui, et al., PR Research 2 013080 (2020). [2] R. Stannarius, K. Harth, PRL 117 157801 (2016). [3] e.g. X. Tang, J. V. Selinger, Soft Matter 13 5481 (2017) ; Soft Matter, 15 587 (2019)

15 min. break

CPP 23.6 Wed 11:00 H18

Incipient motion for 3d geometries — •Dominik Geyer, Paolo Malgaretti, Othmane Aouane, and Jens Harting — Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11), Cauerstr. 1, 91058 Erlangen, Germany

The incipient motion describes the threshold conditions between erosion and sedimentation. This natural process is relevant for a broad field of natural and industrial processes, for example, cell detachment, cleaning of surfaces, and transportation in pipelines. Our interest is in the incipient motion of a single particle on non-trivial geometries. The crucial parameter for describing incipient motion is the so-called Shields number which is the ratio between viscous forces and buoyancy. Interestingly, the incipient motion has been reported at values of the Shields number much smaller than unity ($\theta \simeq 10^{-2}$) hence questioning whether the proposed Shields number is indeed capturing the relevant physical phenomena. In order to critically discuss this aspect, we per-

form lattice Boltzmann simulations of a solid particle on a substrate consisting of solid spheres taking into account the local fluid velocity and the particle size. Our numerical data will allow us to calculate the effective viscous force acting on the particle and hence to propose possible corrections to the Shields number which can better account for the experimental and numerical data.

CPP 23.7 Wed 11:15 H18

Phase behaviour in a mono-layer colloidal membrane — •Léa Beaules, Anja Kuhnhold, and Tanja Schilling — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

Kosterlitz-Thouless-Halperin-Nelson and Young (KTHNY) theory predicted that the melting of a purely 2D hard disk system would be defect-mediated and occur via two continuous transitions: from the solid to the intermediate hexatic phase and, from the hexatic to the fluid phase. Since then phase behaviour of this system as well as closely related systems have been extensively investigated and debated, showing that the hexatic-liquid transition is of first order for purely hard system [1]. Additionally, upon increasing interaction range or adding dispersity in the system the transition can become continuous or the hexatic phase can vanish [2].

However a large number of real systems can be more accurately approximated as a quasi-2D system that exhibits out of plane interactions, e.g. biological membranes; therefore understanding their role in the phase behaviour is important. Thus to extend our understanding of these systems, we use Monte-Carlo simulations to study an infinite mono-layer membrane of hard rod-like particles. We investigate how the orientational degree of freedom of the rods, and the range of their out of plane interactions affect the phase behaviour of the system.

[1] E. P. Bernard and W. Krauth, Phys. Rev. Lett. **107**, p. 155704 (2011).

[2] Y.-W. Li and M. P. Ciamarra, Phys. Rev. E **102**, p. 062101 (2020).

CPP 23.8 Wed 11:30 H18

Particle-resolved topological defects of smectic colloidal liquid crystals in 2d confinement — •René Wittmann[1], Paul A. Monderkamp[1], Louis B. G. Cortes[2,3], Dirk G. A. L. Aarts[3], Frank Smallenburg[4], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine Universität Düsseldorf, Germany — [2]School of Applied and Engineering Physics, Cornell University, USA — [3]Department of Chemistry, Physical and Theoretical Chemistry Laboratory, University of Oxford, UK — [4]Laboratoire de Physique des Solides, CNRS, Université Paris-Saclay, France

We present a general classification scheme [1] of the intrinsic structure of smectic colloidal liquid crystals in two spatial dimensions, dictated by the interplay between the intrinsic layering and the externally imposed boundary structure. Thereby, we demonstrate that topological defects emerge in the form of spatially extended grain-boundaries, which are characterized by coexisting nematic and tetratic orientational order. We examine these intriguing topological properties on the particle scale by means of Monte-Carlo simulations, fundamental-measure-based density functional theory and real-space microscopy of colloidal rods. The structural details agree on a quantitative level. In particular, we analyze the typical shape of grain-boundary networks in a large range of polygonal confinements [1] and the stability of different competing topological states in nontrivial domains with additional interior boundaries [2].

[1] P. A. Monderkamp et al., Phys. Rev. Lett. 127, 198001 (2021).

[2] R. Wittmann et al., Nat. Commun. 12, 623 (2021).

CPP 23.9 Wed 11:45 H18

Structure of nematic hard rod tactoids — •Anja Kuhnhold[1] and Paul van der Schoot[2] — [1]University of Freiburg, Freiburg, Germany — [2]Eindhoven University of Technology, Eindhoven, The Netherlands

Droplets of ordered phases of anisotropic particles take on specific shapes and internal structures. Compared to droplets of spherical particles, tactoids are elongated with cusp-like tips. Several parameters dictate the overall shape and structure: density of the system, elastic constants of the particles, anchoring strength, interfacial tension, and volume of the tactoid. [1]

We compare Monte Carlo simulation results of hard rod tactoids in a bath of spherical ghost particles to predictions from a scaling theory. We focus on small tactoids where the macroscopic scaling description might break down. We find that smaller tactoids have a more uniform director field than larger tactoids. Also, the segment density increases towards the tactoid tips in agreement with the theory. In addition, we find further density modulations when the average density increases.

Besides, we test the effect of an aligning field on the shape and structure of the tactoids and find that the director field becomes more uniform and the aspect ratio increases, but not to a vast extent. [2]

[1] P. Prinsen, P. van der Schoot, EPJ E **13**, 35 (2004).

[2] A. Kuhnhold, P. van der Schoot, JCP **156**, 104501 (2022).