CPP 36: Complex Fluids and Colloids V (joint session BP/CPP/DY, organized by DY)

Time: Wednesday 10:00–13:00 Location: H47

CPP 36.1 Wed 10:00 H47

Self-assembly in binary mixtures of liquid-crystalline rods and dipolar spheres: A free-energy study — •Alice C. von der Heydt, Stavros D. Peroukidis, and Sabine H. L. Klapp — Inst. f. Theoretische Physik, Techn. Univ. Berlin, Hardenbergstr. 36, 10623 Berlin

Mixtures of differently shaped particles with hard-core repulsion only can exhibit a variety of spatially periodic phase-separation patterns combined with liquid-crystalline order [1]. Simulations have revealed an even more complex behavior with uni- or biaxial, smectic and lamellar structures in binary mixtures of rods and soft magnetic spheres of comparable diameter [2]. In this study, we aim at a theoretical description that will allow us to trace phase boundaries and to explain topologies of some of these structures for a model mixture of hard rods with nematic order and dipolar hard spheres. The semi-analytical route we propose starts from a free-energy functional which governs the single-particle component-density distribution functions of position and orientation. This functional is constructed using concepts of classical density functional theory and the modified mean-field approximation for the dipolar interaction [3].

[1] Z. Dogic, D. Frenkel, S. Fraden, Phys. Rev. E **62**, 3925 (2000)
[2] S. D. Peroukidis, K. Lichtner, S. H. L. Klapp, Soft Matter **11**, 5999 (2015)
[3] G. M. Range, S. H. L. Klapp, Phys. Rev. E **69**, 041201 (2004)

CPP 36.2 Wed 10:15 H47

Clogging in a microfluidic hourglass — •Alvaro Marin[1], Massimiliano Rossi[1], Henri Lhuissier[2], and Christian J. Kähler[1] — [1]Institut für Strömungsmechanik und Aerodynamik, Universität der Bundeswehr München — [2]IUSTI - Aix-Marseille Université & CNRS

Mass flows through geometric constrictions tend to clog under certain circumstances, it occurs no matter what type of object you consider: sand in an hourglass, particles in a fluid through a porous medium or people leaving a room (Zuriguel et al., Scientific reports 4, 2014). However, it is well-known that hourglasses work optimally when the particle-to-neck ratio is within certain ratio without interruption, while arching occurs for particle-to-neck ratios above. In the case of porous mediums, filters and membranes, these get easily clogged by particles in the fluid and therefore unfunctional after a certain amount of time. Being the only solution the replacement of the membrane/filter. Certainly the adherence of the particles to the walls and to each other is an important parameter, but even in the case without adherence, the clogging probability is far from negligible. To study these regimes, we study microfluidic devices with a bottleneck of squared cross-section through which we force dilute polystyrene particle solutions with diameters comparable to the bottleneck size and down to one tenth its size. The experimental results show that particles flowing through a geometrical constriction in these conditions (as it occurs with the flow in certain filters and membranes) reveals strong statistical similarities with an hourglass, which is explained with a simple statistical model.

CPP 36.3 Wed 10:30 H47

Viscoelastic properties of marginal networks in a solvent — •Matthew Dennison and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany

Elastic networks that are at the margins of mechanical stability are known to exhibit an anomalously large resistance to deformation which is highly sensitive to applied forces and fields. While many previous studies have examined the static properties of such networks, relatively little is known about their dynamical behavior. Using a hybrid molecular dynamics and multi-particle collision dynamics simulation technique, we have studied how hydrodynamic interactions affect the stiffening behavior of marginal networks.

We show how the properties of the filaments making up the network, as well as the properties of the solvent it is immersed in, can affect the response of marginal networks to shear. We find that the network is less stiff when hydrodynamic interactions are present than when they are not. The network shear modulus scales as $G' \sim \omega^{\alpha_c}$, with a critical stiffening exponent α_c that can be controlled by varying the network concentration relative to that of the solvent. Our results show that this behavior arises due to the solvent aiding the relaxation of the network and suppressing the network non-affinity, with the system deforming more affinely when hydrodynamic interactions are maximized. Finally, we show how thermal fluctuations can suppress this observed stiffening behavior.

CPP 36.4 Wed 10:45 H47

Rheology of weakly attractive systems: the role of energy dissipation — •Ehsan Irani[1], Pinaki Chaudhuri[2], and Claus Heussinger[1] — [1]Institute for Theoretical Physics, Georg-August University of Göttingen, Göttingen, Germany — [2]Institute of Mathematical Sciences, Tamil Nadu, India

The rheological response of a particulate system with attractive interactions is studied using different models for the dissipation of energy. In systems with the damping force directed normally to the contact point, attractive interactions result in a finite yield stress, and an isostatic structure emerges below the jamming point with shear bands forming as a consequence of non-monotonic flow curves. On the other hand, tangential damping gives rise to the monotonic flow curves and a viscous flow develops in the overdamped regime. However in that case, decreasing the damping factor introduces the inertial time-scale, leading again to non-monotonic flow curves and inertia-induced shear-banding is observed in the underdamped regime. In both cases, the rheology of the system is expressed in terms of relevant damping time-scales and the ratio of dissipative to elastic forces.

CPP 36.5 Wed 11:00 H47

Transport properties of correlated fluids in confinement — •Christian Rohwer[1,2] and Matthias Krueger[1,2] — [1]Max Planck Institute for Intelligent Systems, 70569 Stuttgart, Germany — [2]4th Institute for Theoretical Physics, University of Stuttgart, 70569 Stuttgart, Germany

Correlations in confined fluids give rise to a wealth of remarkable phenomena. Several equilibrium phenomena, e.g. the critical (thermal) Casimir forces, have been described theoretically and observed experimentally. However, although certain non-equilibrium aspects of such systems can be probed experimentally or through computer simulations, a clear theoretical understanding for confined, correlated fluids out of equilibrium is still lacking.

In this work we consider a dynamical theoretical model for confined fluids with correlations (e.g. oil-water mixtures near / at the critical point), thereby extending known results for bulk systems. In particular, we investigate the steady state velocity profiles in a sheared near-critical fluid film, in dependence on various parameters (e.g. separation of the plates, bulk correlation length, external fields...). Our approach is based on linear response theory for small shearing velocities, and leads to a self-consistent formulation for the shear rate in the film.

We also address the dependence on the choice of dynamical model, since conservation laws strongly affect dynamical time-scales. Lastly we discuss potential experimental realisations of our model.

15 min. break

CPP 36.6 Wed 11:30 H47

The Gyroid phase in a System of Pear-shaped Particles — Philipp Schönhöfer[1], Matthieu Marechal[1], Klaus Mecke[1], Gerd Schröder-Turk[2], and •Douglas Cleaver[3] — [1]Theoretische Physik I, FAU Erlangen, Germany — [2]School of Engineering and IT, Murdoch University, Australia — [3]Materials and Engineering Research Institute, Sheffield Hallam University, UK

It is established that elongated or flattened mesogens like spherocylinders and oblate discs form liquid crystal phases – like the nematic or smectic phase – in addition to the isotropic fluid and crystalline solid states.

A highly complex liquid crystal phase which can be generated by amphiphiles or block co-polymers is the double gyroid Ia3d cubic phase. A promising system which forms this structure consists of hard pear-shaped particles with suitable aspect ratio and degree of tapering.

Using Molecular Dynamics and Monte Carlo simulations with a generalized Gay-Berne potential, the spontaneous formation of the gyroid phase was reproduced. Additionally a defect-free gyroid with the same number of particles per unit cell as the spontaneously formed phase was generated. We calculate the scattering functions and use Voronoi tesselation to study the geometrical properties of both systems.

The next step is to introduce hard spheres which will take up the role of solvent to model mixtures such as the lipid-water system. With an explicit solvent the system should be complex enough to model most common phenomena in cubic phases yet simple enough to allow us to simulate large systems.

CPP 36.7 Wed 11:45 H47

Critical three-body Casimir interaction — •Hendrik Hobrecht and Alfred Hucht — Fakultät für Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg

It was shown by Burkhardt and Eisenriegler that the critical Casimir interaction between two colloids at $T = T_c$ can be calculated exactly by a conformal mapping in arbitrary dimension d [1]. For the two-dimensional case $d = 2$ Bimonte et al. extended this calculation to arbitrary shaped objects [2], where the form of the interaction potential between two disks is known exactly. Utilizing those concepts we present a calculation which maps the case of two separated two-dimensional disks onto a limiting case of a three-body system, where two particles are in contact and one is free to move. We compare the results of this calculation to Monte Carlo simulations, using a highly efficient cluster algorithm [3].

[1] T. W. Burkhardt and E. Eisenriegler, Phys. Rev. Lett. 74, 3189 (1995).

[2] G. Bimonte et al., Europhys. Lett. 104, 21001 (2013).

[3] H. Hobrecht and A. Hucht, Phys. Rev. E 92, 042315 (2015)

CPP 36.8 Wed 12:00 H47

Defect-mediated melting of two-dimensional colloidal quasicrystals — Miriam Martinsons and •Michael Schmiedeberg — Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Quasicrystals are structures that possess long range order but no translational symmetry. Due to additional degrees of freedom in quasicrystals there are properties and phenomena that for quasicrystalline structures significantly differ from their counterpart in periodic crystals.

We study how thermally excited excitations or defects develop in two-dimensional colloidal quasicrystals close to the melting transition. According to an extension of the KTHNY theory [1], the formation and dissociation of pairs of dislocation and disclinations is expected to cause the melting of the quasicrystal. Melting should occur via an intermediate phase termed pentahedratic phase [1].

We use Monte-Carlo and Brownian dynamics simulations to study the melting process of decagonal colloidal quasicrystals. By analyzing the positional and bond-orientational correlation functions during the melting process we reveal an intermediate state with quasi-long ranged orientational order but only short ranged positional order as in the predicted pentahedratic phase. Furthermore, we observe network-like structures composed of defects spanning through defect-free areas as well as a coexistence between the intermediate phase and the fluid.

[1] P. De, R.A. Pelcovits, J. Phys. A 22, 1167 (1989); Phys. Rev. B 38, 5042 (1988).

CPP 36.9 Wed 12:15 H47

Protein phase separation controlled by phosphorylation — •David Zwicker[1,2], Oliver Wüseke[3], Jeffrey B. Woodruff[3], Markus Decker[3], Steffen Jaensch[3], Anne Schwager[3], Anthony A. Hyman[3], and Frank Jülicher[2] — [1]School of Engineering and Applied Sciences, Harvard University — [2]Max Planck Institute for the Physics of Complex Systems, Dresden — [3]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden

Biological cells have to organize their proteins in space and time. Membrane-enclosed compartments, like the nucleus, are one solution to this problem. Recent discoveries show that liquid-like droplets are an alternative organization principle. To understand how phase separation can help cells to organize their proteins in space and time, we investigated the formation of the pericentriolar material (PCM), an integral part of the cell scaffold. We combine the theory of phase separation in the presence of chemical reactions with in vivo and in vitro experiments. Our work suggests that the protein responsible for forming the PCM occurs in two different states: one in which it is soluble in the cytosol and one in which it phase separates. The transition between these two states is regulated by chemical reactions that maintain the system away from thermodynamic equilibrium. This allows the cell to control the nucleation process and the growth dynamics, and thus also the droplet count and size. I will discuss the physical principles of this spatial organization, which are likely important for other cellular compartments and might also be used in technological applications.

CPP 36.10 Wed 12:30 H47

Two and three dimensional shapes of simple three and four junction comb polymers — Marvin Bishop[1], Adam J. Barillas[1], Tylor Borgeson[1], •Robin de Regt[2], and Christian von Ferber[2] — [1]Departments of Computer Science and Mathematics, Manhattan College, NY, USA — [2]Applied Mathematics Research Centre, Coventry University, UK

We redesign and apply a scheme originally proposed by G. Wei [Physica A **222**, 155 (1995)] to produce numerical shape parameters with high precision for arbitrary tree-branched polymers based on their Kirchhoff matrix eigenvalue spectrum. This algorithm and a Monte Carlo growth method on square and triangular lattices are employed to investigate the shapes of ideal three and four junction two dimensional comb polymers. We find that the extrapolated values obtained by all of these methods are in excellent agreement with each other and the available theory. We confirm that polymers with a complete set of interior branches display a more circular (resp. spherical) shape.

CPP 36.11 Wed 12:45 H47

How (classical) density functional theory describes structure in electric double layers — •Andreas Härtel[1], Sela Samin[2], and Rene van Roij[2] — [1]Institute of Physics, Johannes Gutenberg-University Mainz, Germany — [2]Institute for Theoretical Physics, Center for Extreme Matter and Emergent Phenomena, Utrecht University, The Netherlands

Ongoing scientific interest is aimed on the properties and structure of electric double layers (EDLs), which are crucial for capacitive water treatment and energy harvesting technologies like desalination devices, blue engines, and thermocapacitive heat-to-current converters. A promising tool for their microscopic description is (classical) density functional theory, which we have applied in order to analyze pair correlations and charge ordering in the primitive model of charged hard spheres. Interestingly, this simple model already describes structural in-plane transitions of EDLs, which occur while their corresponding electrodes are charged. Furthermore, our results demonstrate the impact of screening by solvents on the ability of EDLs to adsorb charges. In conclusion, our work points up issues in the theoretical description of EDLs, which finally might lead to a more sophisticated theory for ionic systems.