Density of states of colloidal glasses

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Experimental studies on the self-organization of colloidal inclusions in liquid crystal membranes

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Different kinds of colloidal particles dispersed in anisotropic liquids (i.e. liquid crystalline phases) have recently attracted increasing attention for their unique collective behavior. These particles can be embedded either into the bulk of a nematic liquid crystalline phase [1; 2] (3D system) or in a smectic free standing film [3] (2D system). In both cases, the particles alter the director field alignment in their vicinity. The resulting elastic deformations then drive elastic interactions between the particles which cluster into a great variety of aggregates.

In the case of 2D system, the colloidal particles consist of cholesteric, nematic inclusions or even hard spheres embedded in a tilted smectic free standing film. The elastic distortions induced around the inclusions coupled with the high in-plane anisotropy result in the creation of topological defects and thus elastic interactions.

In this work, we focus on the different possibilities to modify the inclusion interaction by changing the characteristics of the inclusions and of the liquid crystal medium. Transformation of the interaction can be achieved by changing the chirality (polarization value) of the liquid crystal [4,5]; external conditions e.g. temperature [5]; size and shape of the particles [6,7]. The positions of topological defects on the inclusion boundary and anchoring conditions can be tuned up, by changing the configuration of the liquid crystal near the inclusions, and by this way to a change of the interparticle interaction. The modification of the interparticle interaction leads to the rearrangement of superstructures formed by the inclusions (linear chains, ordered clusters, two-dimensional lattice structures).

The reported phenomena on the change of inclusion interaction open the way to a better control of the structures formed by inclusions.

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Defects structure and effective pair interactions in nematic colloids

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We use the Landau-de Gennes free energy formalism to study nematic-mediated effective interactions between spherical particles, assuming strong homeotripic anchoring at the surface of the particles. A single particle of large enough radius generates a dipolar director configuration with a small companion disclination ring. While small particles generate quadrupolar configurations with an equatorial disclination ring. In the dipolar configuration the disclination ring has a nontrivial orientation which locally breaks the polar symmetry of the far field director. Both configurations have a wide range of metastability (as a function of particle radius and temperature) which is responsible for a very complex effective pair-wise interaction. At short distances the corresponding force-distance curves exhibit jumps and hysteresis upon approach/separation due to the rearrangements of the corresponding disclination rings. At large distances the interaction potential behaves like dipole-dipole, dipole-quadrupole, or quadrupole-quadrupole depending on the nematic distortions around particles.

Islands in free standing smectic C films

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Colloidal dispersions in liquid crystals are different from the ordinary colloids due to the long-range orientational order of the liquid crystal molecules. In addition, colloidal particles present complex interactions that have a long-range dipolar or quadrupolar profile that are an important feature of the self-organisation into supermolecular structures specific from colloidal liquid crystals. The structures observed in experiments are stabilized by the presence of topological defects that induce complex short-range repulsions. The study of such interactions in films is important for a complete understanding of three dimensional colloidal dispersions in liquid crystal. We present some of the work done on dipolar and quadrupolar interactions of colloidal particles in smectic C films.

The Trouble with Critical Wetting

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A long-standing problem in condensed-matter physics concerns the nature of the critical wetting transition in three-dimensional systems with short-ranged forces. The controversy originally focused on the discrepancy between predictions of strongly non-universal critical effects, based on renormalization group analysis of an interfacial Hamiltonian, and Monte Carlo studies of wetting in the 3D Ising model, which are instead broadly consistent with mean-field expectations. This gulf between theory and simulation was widened further by subsequent refinements of the interfacial model which appeared to show that fluctuations should necessarily drive the transition first-order. This prediction is in qualitative disagreement with the simulation studies and would radically later the anticipated structure of the global surface phase diagram.

We review recent progress made towards overcoming these problems using a new non-local interfacial Hamiltonian. This model, which may be derived systematically from a more microscopic theory and also applied to wetting at structured (non-planar) substrates such as wedges, allows for the presence of two-body interfacial interactions in the wetting layer. These are characterised by an additional diverging coherence length, missing in previous descriptions of wetting. This serves to cut-off the spectrum of interfacial fluctuations that describe the repulsion of the interface from the wall. This slows down the onset of critical effects (non-universality) and explains why the transition is not driven first-order thus preserving the structure of the global surface phase diagram.

The existence of hidden symmetries which precisely connect fluid adsorption in different geometries is also discussed. These point to profound connections between contact angles and geometrical angles which has not been previously appreciated or exploited. These are not only of fundamental interest to statistical physics but may also allow us to probe fluid adsorption properties in novel ways.

Elastic contribution to the free energy of a nematic in presence of a structured substrate: beyond Berreman's approach

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The behaviour of liquid crystals close to structured surfaces has attracted much attention on the last years due to their potential applications, such as bistable LCDs [1]. The presence of microstructured surfaces can frustrate the long-ranged orientational ordering of a nematic phase. Associated to the deformation of the director field of a nematic phase we can identify an elastic contribution of the free energy, which may play an important role in the interfacial behaviour of nematic phases. If the director field deformation is smooth, Berreman's approach [2] or its generalizations [3] account for the elastic contribution. In some cases topological defects also appear in the nematic phase. The presence of defects –with complex structure and dynamics– is a new ingredient and an additional source of surface inhomogeneity, not present in the adsorption of simple liquids. Indeed, colloidal particles dispersed in bulk nematics are known to give rise to complex nematic-mediated colloidal interactions, in which topological defects play an important role [4]. The inteplay between defects and surface structure is not still well understood.

We have considered a nematic phase in contact with a saw-shaped substrate of period L with favours (local) homeotropic alignment. We assume that the nematic phase can be described by the Landau-de Gennes free-energy, and the equilibrium order parameter profile is obtained by using the Finite Element Method (FEM) with adaptive meshing [5]. The analysis of the nematic free energy and its dependence on the periodicity of the substrate shows that under strong anchoring conditions (i.e. large L) the elastic contribution is not described by Berreman approach, but it has a geometry-dependent, log(L) contribution. Using a modified Frank-Oseen elastic Hamiltonian approach, we ascribe this elastic contribution to the appearance of non-half-integer topological defects on the cusps (edges and wedges) of the substrate [6]. This non-Berreman elastic contribution explains the large deviations of the wetting transition parameters with respect to the Wenzel law prediction [7], and it may lead to novel nematic-mediated interactions between prism-like colloidal particles [8].

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Rheological study on diluted micellar solutions of CTAB/NaSal/KBr

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Cetyltrimethylammonium Bromide (CTAB) in water forms spherical micelles, which upon addition of salts (NaSal or KBr) elongate to form entangled wormlike structures. The "worms" are stabilized by charge screening (NaSal and KBr), and by changes in the micellar surface energy as salicylate ions of (NaSal) intercalate in the CTAB micelles. Solutions of wormlike micelles exhibit dramatically increased viscosity, and visco-elasticity in the gel-like, highly entangled state. In this work we present a systematic rheological study for this surfactant, using Sodium Salicylate (NaSal) and Potassium Bromide (KBr) as added salts, with the aim of producing a fluid system exhibiting tuneable rheology. The influences of temperature and salt concentration were also observed and characterized in this work.

Electrorheological study of low molecular weight nematic liquid crystals: experimental and theoretical results

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The experimental and theoretical study of the electrorheological effect (ER) observed in the nematic phase of low molecular weight cyanobiphenyls is the aim of this work.

We will present the flow curves of our samples for different temperatures and under the influence of an external electric field, ranging from 0 to 3kV/mm, applied perpendicular to the flow direction. We will also present the viscosity as a function of the temperature, for the same values of electric field, obtained for different shear rates.

Nematic liquid crystals with positive dielectric anisotropy, which is the case of our samples, show a significant increase of the apparent viscosity upon application of the external electric field, for small shear rate values, which is due to the molecular alignment in the direction perpendicular to the flow field, in consequence of the application of the electric field. For higher shear rates a progressive decrease of the viscosity is observed, reflecting the director alignment balance between the electric field and the flow direction. For sufficiently high shear rates, the flow field completely dominates and the viscosities of the different flow curves converge into the curve obtained without electric field applied.

Theoretical interpretation of the observed behaviours is proposed in the framework of the continuum theory of Leslie-Ericksen for low molecular weight nematic liquid crystals. In this description the director alignment angle is a function of the electric field and the flow field - boundary conditions are neglected. Some Leslie viscosity coefficients and Miesowicz viscosities and the dielectric anisotropy ε_a are estimated for each temperature, by fitting the theoretical model to the experimental data.

Wedge Filling: Local and Non-Local Hamiltonians

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We study fluid adsorption in a linear wedge by means of different effective interfacial Hamiltonians, including a non-local model recently proposed.

Wetting of hairy surfaces

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The leaves of a Lady's Mantle are densely covered with hairs that display a rather surprising wetting behaviour: droplets of water can rest on the hairs, without contact with the leaf's surface, even though the hairs are hydrophilic [Otten & Herminghaus, Langmuir 20, 2405 (2004)]. It was suggested that this behaviour is due to an interplay of capillary interactions and the elasticity of the hairs. We put these arguments into a more quantitative framework to try to understand better the origin of this behaviour, and estimate the criteria for a furry hydrophilic surface to behave as effectively hydrophobic.

Structure, dynamics and manipulation of colloidal systems

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Colloidal systems are widely used as a model system to study many fundamental issues in condensed matter physics and statistical mechanics. The great advantage is that the colloidal time- and length scales are experimentally very well accessible. In addition, colloidal systems can be readily manipulated using for example optical tweezers, magnetic and electric fields. In this presentation, I will highlight various experiments that illustrate the unique properties of colloids. The main part of the talk will be about experiments in which we used optical tweezers to drag a large probe particle through a two-dimensional colloidal crystal of smaller particles. Here we varied the orientation with respect to the crystal axis and the drag-speed. I will also show recent work on crystallisation and column-formation in confined magnetic systems.

Liquid crystals in contact with structured substrates

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The contact of soft matter with solid surfaces offers the possibility to imprint external lateral structures deep into the bulk of the adjacent complex fluid and thus to manipulate it in a controlled way. For fluids consisting of non-spherical particles in the presence of confining substrates, the competition between fluid-substrate and fluid-fluid interactions leads to application-relevant surface-driven changes of both the mean local densities and the orientations of the particles [1]. Examples are the patterned alignment of bistable liquid-crystal display devices and liquid-crystal based detection of biomolecular and chemical events occurring at surfaces. Various technical developments allow the controlled fabrication of tailored solid surfaces at the nano- to micrometer range.

Here we use the Frank-Oseen theory and density functional theory to study the properties of liquid crystals in contact with patterned substrates. We discuss the phase behavior of a nematic liquid crystal confined between a flat substrate with strong anchoring and a patterned substrate whose structure and local anchoring strength is varied. By first evaluating an effective surface free energy function characterizing the patterned substrate we derive an expression for the effective free energy of the confined nematic liquid crystal. Then we determine phase diagrams involving a homogeneous state in which the nematic director is almost uniform and a hybrid aligned nematic state in which the orientation of the director varies through the cell. Direct minimization of the free energy functional are performed in order to test the predictions of the effective free energy method. We find remarkably good agreement between the phase boundaries calculated from the two approaches [2]. In addition the effective free energy method allows one to determine the energy barriers between two states in a bistable nematic device. The calculations reveal that phase transitions between two states can be triggered by applying a voltage between the substrates. Both dielectric interaction and flexoelectric polarization are taken into account, and in the numerical calculations particular attention is paid to the fact that the electric field is not constant throughout the cell [3].

Moreover, we use a microscopic density functional theory to study rod fluids near a right-angled wedge or edge as well as near a geometrically patterned substrate. Density and orientational order profiles, excess adsorptions, as well as surface and line tensions are determined. Near a hard wall which is periodically patterned with rectangular barriers, complete wetting of the wall by a nematic film occurs as a two stage process in which first the nematic phase fills the space between the barriers. In addition, the calculations exhibit an enrichment [depletion] of rods lying parallel and close to the corner of an individual right-angled wedge [edge].

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Cellulosic Spirals and Helices

Godinho, M.H.[1], Canejo, J.P.[1], Borges, J.P.[1] and Teixeira, P.I.[2]
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Cellulose, along with polypeptides and DNA, belongs to a family of organic molecules that can form cholesteric liquid crystalline (LC) phases, where the direction of preferential molecular alignment rotates in a helical pattern [1]. Recently it was found that helical micro and nano helices can be obtained from cellulose liquid crystalline phases by the electrospinning technique [2]. The twisting is on a supramolecular scale, and similar to what has been seen in other systems such as amyloid (polypeptide) nanofibrils [3] and cellulose from Micrasterias denticulate [4]. In fact, cellulose acetate was the first fiber reported to have been electrospun and is the most popular cellulosic material for electrospinning today. The fibre diameter can be significantly reduced from micrometres to a few nanometres using this technique, and suspended fibres with helical structures can also be prepared by careful choice of target. In this work we show that nano and microfibers electrospun from liquid crystalline cellulosic solutions will curl into spirals if they are supported at just one end, or, if they are supported at both ends, a helix hand reversal can be found - the spontaneous switching of a helical structure of one handedness to its mirror image. This same behaviour is known to be exhibited by the tendrils of climbing plants such as Passiflora edulis, three to four orders of magnitude larger than our fibres [5]. The results obtained will be discussed in the framework of a model proposed by Goriely et al. [6].

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Can one obtain a yield-locus from a single DEM simulation?

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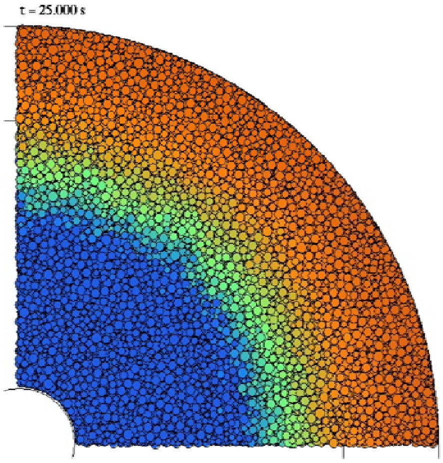
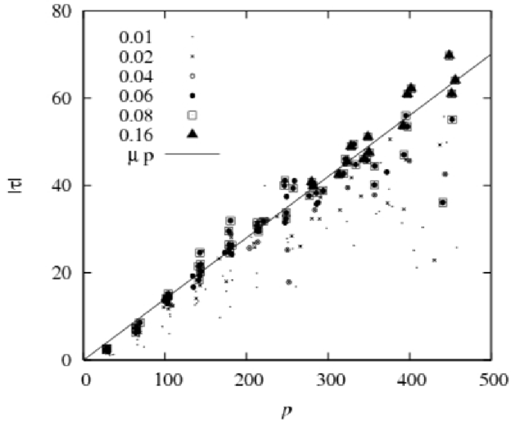
DEM simulations of ring shear cells (right) allow to study the non-equilibrium behavior of granular materials under shear close to jamming. More specific, the density, the stresses and the velocity gradient are extracted.
In the split-bottom ring geometry, this data are plotted (below) as shear stress vs. normal stress (pressure). If only the large shear rate data are given (large symbols) one already has a yield locus.

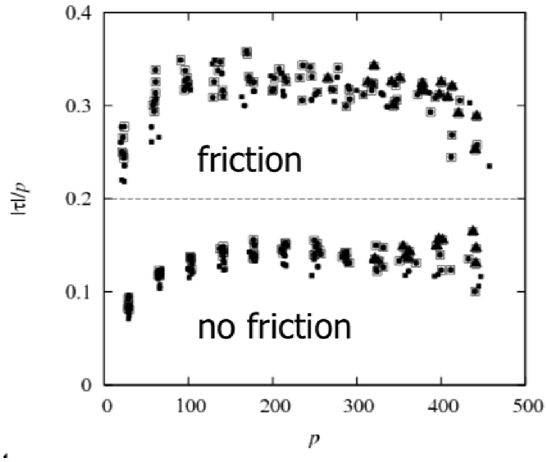




Scaling the shear stress by p displays clearly the non-linear nature of the yield locus.

Material parameters that can be varied involve particle size, size-distributions, fricton (right) and adhesion – among many others.

The peculiar evolution of the anisotropy of stress and structure will be discussed.



• S. Luding,
The effect of friction on wide shear bands
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• S. Luding,
Constitutive relations for the Shear Band Evolution in Granular Matter under Large Strain [Particuology 6, 501-505, 2008], [PDF file] .

Dense colloids and flow through porous structures

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I will present simulations of particles dragged by a Non-Newtonian fluid through a porous structure. A generalization of Darcy's law is possible. The filtering efficiency will be discussed. Three dimensional numerical simulations of model clay consisting of aluminium oxide spheres interacting via DLVO potentials yield viscosity, pair correlation and cluster structure. We find shear thinning in quantitative agreement with experiment. Considering only the hydrodynamic interactions between the particles we produce time series of up to 10**10 time steps under shear and obtain distributions for the velocity components over six orders of magnitude. These compare very well with a simple mean-field theory and show a Gaussian behaviour for small velocities and an exponential tail for large velocities. We can scale them in concentration, viscosity and shear rate and also study the effect of gravity. We also studied the collapse of a fragile granular suspension due to the penetration of an object and the subsequent difficulty in pulling this object out again. This has direct application to quicksand.

In and out of equilibrium inverse freezing

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I will present two microscopic mechanisms for the viscosity increase of a complex fluid under forcing, and discuss their entropic and kinetic origin..

Kinetic theory of mixtures of inelastic rough hard spheres

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The simplest model of a granular fluid consists of identical, inelastic smooth hard spheres with a constant coefficient of normal restitution. Kinetic theory tools have successfully been applied to this model and interesting properties have been analyzed. Obviously, the model can be made closer to reality by introducing more ingredients, such as polydispersity and/or roughness. These two ingredients are especially interesting because they unveil an inherent breakdown of energy equipartition in granular fluids, even in homogeneous and isotropic states. The aim of this talk is to explore the combined effect of both ingredients in a kinetic theory description. We will consider a dilute mixture of inelastic rough hard spheres of arbitrary number densities, masses, diameters, moments of inertia, and mutual coefficients of normal and tangential restitution. After constructing the Boltzmann equation for the mixture, the collisional moments associated with the translational and rotational temperatures will be expressed in terms of average values. Next, those average values will be estimated by assuming a Maxwellian velocity distribution, allowing us to express the cooling rates in terms of the partial temperatures and the mechanical parameters of the mixture. Finally, the results will be applied to the homogeneous cooling state of a binary mixture and the influence of inelasticity on the temperature ratios will be analyzed.

Superdiffusion of massive partices induced by multi-scale flow

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In this work, we study the statistics of diffusion of massive particles in scale-free velocity fields. We show that the key feature underlying superdiffussive nature of the transport of the particles is the multi-scale vortical structure. However, other mechanisms such as dissipation are needed to account for preferential concentration in the distribution of the particles.

Rectification and Fluctuations of granular tracers

Marini Bettolo Marconi, U.[1]
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We consider a massive inelastic piston, whose opposite faces have different coefficients of restitution, moving under the action of an infinitely dilute gas of hard disks maintained at a fixed temperature. The dynamics of the piston is Markovian and obeys a continuous Master Equation: however, the asymmetry of restitution coefficients induces a violation of detailed balance and a net drift of the piston, as in a Brownian ratchet. Numerical investigations of such non-equilibrium stationary state show that the velocity fluctuations of the piston are symmetric around the mean value only in the limit of large piston mass, while they are strongly asymmetric in the opposite limit. Only taking into account such an asymmetry, i.e. including a third parameter in addition to the mean and the variance of the velocity distribution, it is possible to obtain a satisfactory analytical prediction for the ratchet drift velocity.

Investigating granular friction through vibration

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We perform experiments on a granular medium confined to a circular channel. The medium is excited both by the shearing action of a forced annular overhead plate and by vertical excitation. The vibration naturally causes the granular structure to lose rigidity and here we attempt to quantify what level of energy input is necessary to weaken the granular material. The results indicate that an extremely low level of vibration is sufficient to completely destroy the solidified state of the GM, though we find that one requires a much larger vibration to significantly reduce the viscosity of the resultant granular fluid.

Effects of hydrodynamic interaction on fibre suspension

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Fibres are used in industry as fillers in polymer matrices to control rheological properties, process conditions, quality of products and so on. There are some theories for rigid fibre dispersion; commonly used theories are based on the Jeffery model, with an evolution function of orientation and a constitutive equation. These models are normally modified to be applied to semi-dilute concentrations with fibre-fibre interactions. The first simulation research on this subject, treating dynamics of flexible fibre under flows, was done by PSM (particle simulation method)[1,2], where fibres are modelled as connected beads. Between adjacent beads, stretch force, bending and torsion torques are considered. It is possible to simulate fibre behaviour under flow by solving translational and rotational equations of motion with non-slip restriction between adjacent beads, which is important for producing tumbling phenomena. Still now, the effect of hydrodynamic interaction on fibre behaviours and rheological properties is not well known. This research focuses on fibre aspect ratio and flexibility. Fibres are modelled as a series of beads, following PSM and hydrodynamic interactions [3] are considered. The effects on hydrodynamic interaction on flexible fibres under flows will be demonstrated.

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Gel-forming patchy colloids

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I will discuss thermodynamic and dynamic properties of simple models of particles with patchy interactions. I will show that possibility of controlling the number of bonded nearest neighbors has interesting consequences on the thermodynamic of the system:
(i) It reduces the region of the phase diagram where liquid-gas coexistence is observed
(ii) it offers the possibility of generating liquid states (i.e. states with temperature l ower than the liquid-gas critical temperature) with a vanishing occupied packing fraction, a case can not be realized with spherically interacting particles;
(iii) it opens up the region of stability of the liquid phase, favoring the establishment of homogeneous disordered materials at small packing fraction, which can be named accordingly stable equilibrium gels or network glasses.

I will show also how the process of self-assembly of the network can be described theoretically in a rather precise and I will discuss the connections between physical and chemical gels.
Recent literature related to this presentation includes:

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Diffusion anomaly in a cell model for water

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Liquid water shows many unique and unusual properties and several scenarios have been proposed to interpret them: liquid-liquid critical point, singularity free, etc. Here, we present a simple Hamiltonian model that reproduces the basic properties of liquid water and covers various of these scenarios by a simple, physically motivated one-parameter tuning. In particular, it enables to distinguish between the singularity free scenario and the liquid-liquid critical point scenarios. Extensive Monte Carlo simulations of this model account for the density anomaly, the crossover from Arrhenius to non-Arrhenius behavior upon increasing pressure, the (recently observed in experiments) density minimum at low temperature, and the diffusivity anomaly. The two latter are independent from the existence of a 2nd critical point.

Trapped colloidal particle at constant speed

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In a dense colloidal system, a single particle can be used as a probe to provoke microscopic stresses and study their relaxation, i.e. for microrheology. Connection with bulk rheology can be made through the stationary relation z <v><F>, where the z is an effective friction coefficient and <v> and <F> are the average velocity and force, respectively. The tracer can be dragged at constant F, constant v or allowing fluctuations of both F and v. In this work, we study by means of Brownian dynamics simulations the microrheology and dynamics of a single tracer trapped in a harmonic potential which travels at constant speed through a system of hard spheres, and compare with experiments where a tracer is trapped with optical tweezers. The results are analyzed with a single particle model, where the bath properties are embedded in an "effective fluid". The stationary tracer position distribution yields the effective friction coefficient and temperature. The friction coefficient shows velocity thinning, with a low speed plateau which gives (in the simulations) the correct bulk shear viscosity of hard spheres, and a high velocity plateau which agrees (in the experiments) with the high shear bulk viscosity. The tracer position correlation function, on the other hand, shows two distinguishable relaxations, arising from the friction with the solvent and collisions with other particles. This relaxation cannot be rationalized within the effective fluid model.

How patchy can one get and still condense?

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We investigate the influence of strong directional, or bonding, interactions on the phase diagram of complex fluids, and in particular on the liquid-vapour critical point. To this end we revisit a simple model and theory for associating fluids which consists of spherical particles having a hard-core repulsion, complemented by three short-ranged attractive sites on the surface (sticky spots), two of type A and one of type B. Results are interpreted in terms of the equilibrium cluster structures of the coexisting phases. In systems where there is no AB interaction, the critical point exists for all values of the BB interaction strength. By contrast, when there is no BB interaction, there is no critical point below a certain finite value of the AB interaction strength. These somewhat surprising results are rationalised in terms of the different network structures of the two systems: two long AA chains are linked by one BB bond (X-junction) in the former case, and by one AB bond (Y-junction) in the latter. The vapour-liquid transition may then be viewed as the condensation of these junctions and, we find that X-junctions condense for any fraction of BB bonds, whereas condensation of the Y-junctions requires a finite fraction of AB bonds.

When Glass and Gel Meet

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The structure and relaxation dynamics of dense glass-formers is nowadays relatively well-understood. Their behavior is characterized by a dramatic slowing down of the dynamics due to steric hindrance effects: particles are arrested within the cage formed by their neighbors. On the other hand, low-density frozen disordered structures, i.e. gels, are also observed in Nature. In this case particles become arrested when bonded to a macroscopic network structure which percolates through the system. The relaxation dynamics is less well-understood in gels than in dense glass-formers, and one finds a richer zoology. Certain systems can be studied both at low and high densities, and thus one can use them to investigate the glass and gel phases. What exactly happens at intermediate densities at which the two phases meet is not clear.

Here we numerically investigate a simple model system that allows to study the gel and the dense glass state, and hence to shed light on the interplay of two different arrest mechanisms. The model, first introduced in Phys. Rev. Lett. 98, 135503 (2007), is composed by particles and bridging polymers, and has a low-density equilibrium gel phase. The global structure of the gel is homogeneous, but the stress is only supported by a fractal network. As the density is increased, the systems enters into a glassy phase which interferes with the existing gel structure. In this regime the system exhibits a three-step relaxation process as a result of the competition between two different localization lengthscales: l_SH (associated to steric hindrance effects) and l_PN (related to the mesh size of polymer network). In some regions of parameter space this competition gives rise to an apparent logarithmic decay of correlation functions, which can be understood as a simple crossover effect. We propose a theoretical model that describes the observed behavior, sheding light on the origin of this lengthscales competition and opening the door to the investigation of a very large class of glass-forming systems with new and rich dynamics.

Complex depletion and gelation in surfactant+colloid mixtures

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Crystallization and glass formation in hard ellipsoids

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Suspensions of hard objects such as spheres, cylinders or ellipsoids are useful model systems for basic questions of statistical mechanics. We present computer simulation studies on the crystalline phases and glassy dynamics of hard ellipsoids of revolution. For aspect ratios > 3 the previously suggested stretched-fcc phase [D. Frenkel and B. M. Mulder, Mol. Phys. 55, 1171 (1985)] is replaced by a novel crystalline phase. The close-packed version of this crystal is a specimen of the family of superdense packings recently reported [Donev et al., Phys. Rev. Lett. 92, 255506 (2004)]. We also present evidence for glassy dynamics in suspensions of monodisperse hard ellipsoids. In equilibrium, almost spherical ellipsoids show a first order transition from an isotropic phase to a rotator phase. When overcompressing the isotropic phase into the rotator regime, we observe two-step relaxation in positional and orientational correlators, and super-Arrhenius slowing down of diffusion and relaxation. The effects are strong enough for asymptotic laws of mode-coupling theory to apply. Glassy dynamics are unusual in monodisperse systems. Typically, polydispersity in size or a mixture of particle species is prerequisite to prevent crystallization. Here, we show that a slight particle anisometry acts as a sufficient source of disorder.

The Cubatic Phase in Truncated Sphere and Square Platelet Systems

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The cubatic phase is a liquid crystalline phase with cubic orientational order, consisting of short stacks of four or five particles, with neighbouring stacks tending to be perpendicular to one another. This occurs in the truncated sphere system. However, it is by no means certain whether the cubatic phase is stable with respect to the columnar phase. We have attempted to answer this question by measuring the free energy of both phases using expanded ensemble Monte Carlo simulations.

We also show that a cubatic phase occurs in a system of rigid square platelets formed from fused spheres. We have investigated the dynamics of the cubatic phase in this system by means of molecular dynamics simulation.

Dynamical Properties of Cubatic Liquid Crystals

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The cubatic liquid crystalline phase is an exotic form of matter in which particles have no long range positional order but the orientations have a cubic symmetry, with particles preferentially forming stacks and pointing along the x-, y- and z- axes with equal probability. This phase was first observed in systems of truncated hard spheres. We have used molecular dynamics to study for the first time the dynamical properties of this phase, using a model system of rigid, square slabs formed from repulsive spheres.

We briefly present the form of the hydrodynamic equations for this phase, involving the coupling of the conserved variables to elastic fluctuations, and then show a selection of time correlation functions, clarifying the influence of the special symmetry of the phase on dynamical properties. We have also studied the effect of shearing the cubatic phase, finding that increasing the shear rate drives a phase transition to a nematic phase – a phase that is not stable at equilibrium. We present a preliminary phase diagram, showing the effects of shear.

Demixing in two-dimensional anisotropic fluids

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Hard anisotropic particles have played an important role as statistical mechanical models for liquid--crystal ordering. However, they are being used more recently to obtain liquid-crystal steady-state textures in vibrated monolayer experiments, where particles dissipate energy through inelastic collisions. In this communication we discuss some theoretical work, based on equilibrium statistical mechanics, which may help rationalise the steady-state textures observed in vibration experiments regarding their dependence with particle area fraction and mixture composition. One- and two-component particle mixtures are considered, and nematic ordering and demixing phenomena are analysed. Our focus is mainly on the isotropic and nematic phases, and specifically on an exotic variety of the latter, the so-called tetratic phase, possessing four-fold symmetry. We also present preliminary results of vibrated monolayer experiments, where two species of granular cylindrical particles of very different lengths exhibit strong demixing. Our theoretical work, based on equilibrium statistical mechanics, may help rationalise the steady-state textures observed in vibration experiments in terms of dependence on area fraction covered and mixture composition.

Effects of Confinement on Free Energy of Particles at Fluid Interfaces

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Two-dimensional colloids, formed by micron-sized particles trapped at fluid interfaces, have recently received a great deal of attention in view of the various possible applications such as controlled self-assembly, mesoscale structure formation and study of two-dimensional melting. In this work we investigate the effects of confinement and curvature on the free energy of a system composed of a particle floating at the surface of a sessile drop. Due to the presence of the substrate one has to solve the boundary value problem for the shape of the droplet, governed in the small deformation limit by the two-dimensional Helmholtz equation. To do this, we propose a capillary analogue of the image method, known from electrostatics. The full numerical minimization of the free energy agrees very well with the obtained analytical solution. We show, that the substrate provides a confining potential for the particle and that the equilibrium configuration depends on the type of the boundary conditions (pinned or free contact line). Moreover, on the contrary to the case of a flat interface, we find that the capillary interactions on a curved interface are non-monotonic, which may induce clustering in the many-particle case.

Rheological Experimental Data on Micellar CTAB Aqueous Solutions, using HSal and NaSal

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The surfactant CTAB (cetyltrimethylammonium bromide) in aqueous solution forms cationic micelles above a critical concentration, which grow in length if the charge of the head group is screened. In the present study, an acid (salicylic acid - HSal) and its conjugate base (sodium salicylate - NaSal) were used as additives. The presence of the acid changes the solution pH from neutral to acidic media.

Rheological measurements were carried out using two approaches: flow curves in a steady simple shear flow and temperature sweep tests. In order to study the additive concentration dependence, the flow curves were measured for shear rates from 0.1 to 2000 s-1 at 30ºC. The CTAB concentration was fixed at 100mM and additives concentration was varied between 22.5-40mM. The obtained flow curves showed different behaviours for each system, within the accessible shear rate range. The CTAB/NaSal system is predominantly in the shear thinning regime (some samples present a Newtonian plateau at low shear rates), and the viscosity increases with NaSal concentration. For CTAB/HSal, the addition of acid has a less dramatic effect on the viscosity values, but the system shows both shear thinning and thickening behaviour; the transition between the shear thinning to shear thickening regime is dislocated for higher shear rates as acid concentration increases.

Temperature sweep tests were carried out in the temperature range 20 – 50 ºC, for shear rate values 0.1; 0.5; 1; 5; 10; 50 and 100 s-1. A similar behaviour is observed for both systems but within different temperature ranges. The temperature dependence can be described as follows: after an initial plateau, viscosity increases with temperature until a viscosity peak is reached; for higher temperatures, the systems' viscosity is a decreasing function with T. Although after reaching the viscosity maximum all curves collapse in the same decreasing slope for the CTAB/NaSal system, while for the CTAB/HSal system this phenomena occurs gradually and is dependent of the shear rate value. The occurrence of the maximum viscosity value is dislocated to higher temperatures with the increase of the applied shear rate value.

Fourier states in a low density granular gas

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We describe in detail in this work the properties of the Fourier steady state in a low density granular gas. The system consists of a granular gas enclosed by two infinite parallel thermal walls. Our work is based on the theoretical classification of steady base states described in a recent work [F. Vega Reyes and J. S. Urbach, J. Fluid Mech., in press (2009)]. We show by means of computer simulations that, as we increase wall temperature difference, the temperature profiles transition from positive to negative curvature, passing through an intermediate state with linear temperature profile. We show these transitions occur in the same way for both low (Navier-Stokes regime) and moderate Knudsen number (non-linear regime). We show that the departure from Navier-Stokes hydrodynamics may be characterized with a critical parameter A_th, which we define ad hoc, that is a function of the degree of inelasticity, in strong analogy with the critical shear rate for uniform shear flow in Couette granular flows. The new critical parameter marks the point where the linear temperature occurs, which, as we show, is the point where the reduced time/length scales defined by wall temperature difference and inelasticity are balanced.

Analysis of the longitudinal uniform flow in a granular gas by means of computer grid DSMC simulations

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The uniform longitudinal flow [1] (ULF) is characterized by a linear longitudinal velocity field u_x (x, t) = a(t)x, where $a(t)=a_0/(1+a_0t)$, a uniform density $n(t) \propto a(t)$, and a uniform temperature T(t). In a granular gas characterized by a given value of the coefficient of normal restitution α, the relevant control parameter of the problem is the reduced deformation rate a* = a(t) / ν(t) (which plays the role of the Knudsen number), where $\nu(t) \propto n(t) \sqrt{T(t)}$ is an effective collision frequency. The relevant response parameter is a nonlinear viscosity function η*(a*) defined from the difference between the normal stress $P_{xx}(t)$ and the hydrostatic pressure p(t)=n(t)T(t).

In this work, we consider a single granular gas under conditions of uniform longitudinal flow and analyze the temporal evolution of the gas in the hydrodynamic stage. We compare the results for the nonlinear viscosity function η*(a*) obtained by means of a BGK-like kinetic model and by DSMC computer grid simulations. The results show a good agreement both for the steady-state point and for the whole non-Newtonian function η*(a*).

References

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Percolation threshold of acid-etched titanium from Minkowski's functionals

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Minkowski's functionals provide morphological and topological information of a rough surface such as connectivity. In the context of biomaterials, since the Euler characteristic relates to the possibility of fluid flow on a surface, it may be of interest in the prediction of biointegration. The Euler characteristic (third Minkowski's functional) can be used to define a percolation threshold from the height level where the Euler characteristic function has its zero crossing. A high percolation threshold suggests better fluid retention properties..

In this work, we studied the evolution of commercially pure titanium (grade IV) subjected to an acid etching process. Each set of samples was attacked for different times, from 0 to 750 s with hidrofluoridhric acid. Topographies of each sample were achieved by AFM (Nanoscope IV) in Tapping Mode.

We present the evolution of the maximum-density height for the peaks and valleys with etching time and the concerning percolation thresholds.