Abstracts – Posters

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"Nucleation pathways in systems of non-Brownian spheres"

A confined system of non-Brownian particles, affected by the gravity field but not by thermic fluctuations, resembles the phenomenology of thermodynamic systems when they are subjected to external shaking. Here we report evidence of nucleation pathways in monodisperse spheres systems when the container (square box) is subjected to an annealing process driven by horizontal periodic vibrations. Limiting the system to a small accessible phase space (by forcing the container to vibrate in only one dimension during the annealing), a first nucleation pathway leads the system to an ordered structure, identified as a body centred tetragonal (bct) crystal, but if the system have access to a larger phase space (cuasi-two dimensional vibrations are applied to the container during the annealing), a second nucleation pathway is induced and, at the end of the annealing the system arrives to the densest packing, where a face centred cubic (fcc) crystal is obtained. A high temporal resolution camera, mounted perpendicularly to one of the walls of the container, was used to obtain the dynamics of the fluctuations in the horizontal and vertical coordinates of the particles closest to the wall, this give us a way to indirectly quantify the accessible phase space of the system along the two nucleation pathways. The changes in the coordination number and the velocity field are also reported. Finally, our results suggest that the controlled reversible structural phase transition (bct-fcc or fcc-bct) corresponds to a first order phase transition.

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"Polydisperse hard rectangles: A simple model for vibrated monolayers of granular rods"

We study the effect of length-polydispersity on the phase behavior of freely-rotating hard rectangular particles. Recent experiments on monolayers of quasi-two-dimensional granular rods vibrated in the vertical direction showed the presence of different liquid-crystal textures like isotropic (I), nematic (N), tetratic (T), and smectic (S) phases. Granular particles often exhibit large degree of polydispersity in length, so it is important to quantify its effect on the phase behavior. As a first approximation we used a hard-particle mean-field model based on the free-energy density functional. We have taken particles with rectangular shape because many experiments usually employ monolayers of metallic cylinders which have rectangular projected areas.

The rectangles can freely rotate in 2D and are polydisperse in length while their thickness is kept constant. We have taken a Schultz length-distribution function and also a distribution with a Gaussian tail to model the polydispersity and calculated the phase diagrams (density vs. particle aspect ratio) for different degrees of polydispersity (quantified through the mean square deviation of the density distributions). We found that the T phase stability decreases with polydispersity, while the I-N phase transition becomes strongly of first order. The I-N tricritical point, already present in the one-component system, moves to higher aspect ratios. Our calculations suggest the existence of a terminal polydispersity above which the I-N transition becomes always of first order. We found strong, driven by polydispersity, particle fractionation between the coexisting I and N phases. We also studied in detail the orientational ordering of particles in both, N and T phases, as a function of polydispersity. Our results might help to understand the phase behavior of granular monolayers of rods in recent experiments conducted by our group.

Nonequilibrium dynamics of a dry friction model subjected to coloured noise

Paul M. Geffert and Wolfram Just

We investigate a model with pure dry friction and coloured (exponentially correlated) noise

$$\dot{v} = -\Delta\sigma(v) + n.$$

Δ is the friction coefficient, $\sigma(v)$ is the sign function, representing the dry friction and n denotes the coloured noise $\langle n(t)n(s)\rangle = (D/\tau)\exp(-|t-s|/\tau)$.
By using the unified coloured noise approximation, developed by P. Jung and P. Hänggi, an approximate expression for the stationary probability density $P(v)$ can be obtained, which becomes delta-peaked for an increasing correlation time of the noise, signalling a nonequilibrium localisation phenomenon, related to stick-slip transitions in systems with dry friction. These results show good agreement with the numerical simulations.
To gain deeper insight to the model, we studied the equivalent two-dimensional system (v, n), computing the stationary distribution as well as the direct computation of the probability current. The latter is a clear signature of the nonequilibrium properties of the underlying dynamics.
By computing the power spectral density and increasing the correlation time of the noise τ, we observe a decrease of the full width at half maximum, starting around a "critical" value of τ, which indicates the above mentioned stick-slip transition.

Clustering effects in vibrated monolayers of rods

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Thermal systems of rectangular particles interacting solely through exclusion (entropy) show interesting behaviours [1]. At high density the isotropic (orientationally disordered) phase transforms to a nematic phase, where the long axes of the particles tend to orient parallel to each other and a globally oriented direction (the director) arises. When the particle aspect ratio is low an exotic, tetratic phase, possessing two perpendicular, equivalent directors, becomes more stable [2]. Mean-field studies predict the tetratic phase to destabilise with respect to the uniaxial phase for aspect ratios above 2.6 [3] or 3.1 [4], indicating that tetratic correlations are prevalent for particles close to a square shape. Surprisingly, some experiments on granular rods indicate that these correlations may survive for relatively long rods [5].

Vibrated monolayers of dissipative particles have been shown to exhibit patterns that resemble those of thermal systems. In particular, granular rods show liquid-crystal particle arrangements. Here we exploit these similarities to explore the existence of tetratic and smectic correlations in dense monolayers of granular rods. By focusing on clustering properties, we analyse differences and similarities between descriptions based on particles and clusters, and explain the existence of long-lived tetratic correlations for rather elongated rods in terms of the preference of particles to form squared-like cluster arrangements. Additionaly to the monocomponent system we have also explored mixtures of rods with different aspect ratios. In this case we see demixing and coexistence of phases with different ordering properties.

Experiments were performed on quasimonolayers of metallic rods vertically vibrated in a circular container with radius $R = 7$ cm and dimensionless acceleration $\Gamma \equiv a/g \sim 4$. Rods of length L and width $D = 1$ mm were used, with aspect ratios $\kappa \equiv L/D = 4, 6, 8, 10, 12$ and 14. Rod positions and orientations were identified as a function of time. When the packing fraction ϕ (projected area covered by rods with respect to total area) is sufficiently high, rods tend to locally orient parallel to each other, and domains of nematic, smectic and tetratic order are apparent. The tendency of particles to locally align is described in two ways: (i) by means of the standard *uniaxial* and *tetratic* order parameters $Q_2 = \langle \cos 2\varphi \rangle$ and $Q_4 = \langle \cos 4\varphi \rangle$, respectively, where φ is the angle between the long particle axis and the local director; (ii) by means of the cluster distribution $h(n)$, measuring the number of clusters of a given size n. Here we compare both but focus on the latter, as we believe it contains a more relevant structural information on the ordering properties.

Figure 1 (top left) shows a configuration of particles with $\kappa = 10$ and $\phi \simeq 0.82$. To clearly identify clusters, different colours are used. In figure 1 (top right) the corresponding steady-state average cluster distribution $h(n)$ is shown. In all experiments the distribution functions at short and intermediate/large cluster sizes have different functional forms:

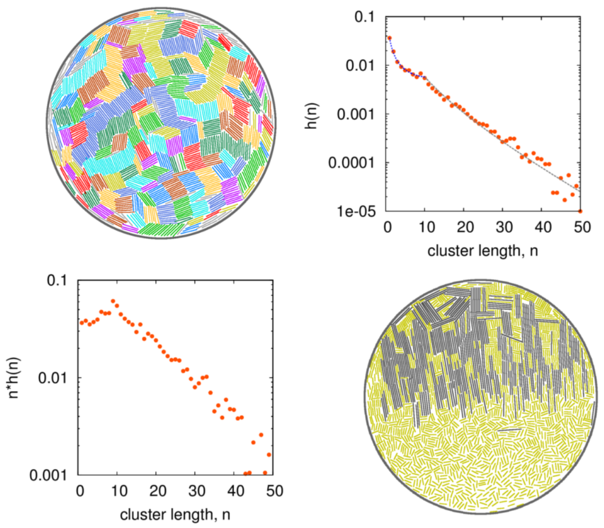

Figure 1: **Top-left**: Particle configuration for vibrated rods of $\kappa = 10$. Rods belonging to the same cluster are depicted as lines with the same colour. Different colours are used for different neighbouring clusters. **Top-right**: Distribution of cluster length in the steady state. Two fittings corresponding to two different mechanisms of cluster formation for $n < \kappa$ and $n > \kappa$. **Bottom-left**: Cluster length distribution multiplied by cluster length. **Bottom-right**: Segregation in mixtures of particles. Dark rods have $\kappa = 14$ and light ones $\kappa = 4$.

for short sizes the better fitting is obtained by an exponential power distribution, while at intermediate/large sizes a simple exponential or a log-normal distribution perform better. Interestingly, the number of rods belonging to a cluster of size n, namely $nh(n)$, exhibits a maximum at a cluster size n close to the aspect ratio κ, i.e. $n_{max} \simeq \kappa$, figure 1 (bottom left), suggesting that clusters with a square shape are particulary favoured (this feature is observed for all aspect ratios studied). Finally figure 1 (bottom right) shows a segregated pattern for a mixture of rods with different aspect ratios. Nematic and isotropic phases coexist for long and short rods respectively.

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"Decoupling phenomenon and replica symmetry breaking in the glass transition of binary fluids"

We theoretically investigate the glass transition of binary mixtures of large and small particles. Several experimental and numerical studies show that there exists the partially frozen phase, where only the large particles are vitrified whereas the small particles remain liquid, when the size ratio between the large and small particles is very large. In this talk, I present a thermodynamic theory which can describe this partially frozen phase. Our theory is an extension of the conventional replica liquid theory (RLT). The RLT describes the glass transition using the one-step replica symmetric breaking (1RSB) ansatz. The 1RSB RLT qualitatively and quantitatively describes well the experimental and numerical results when the size ratio is not very large. However, the 1RSB RLT can not describe the partially frozen phase if the size ratio is very large. To overcome this problem, we assume the two-step replica symmetric breaking (2RSB). Using the 2RSB replica liquid theory, we investigate the phase diagram of the binary harmonic spheres in the high dimensional limit, and show that the resultant phase diagram is a qualitatively similar to those obtained by experimental and numerical studies.

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"Dynamic facilitation in binary hard disk systems"

We investigate numerically the applicability of dynamic facilitation (DF) theory for glass-forming binary hard disk systems where supercompression is controlled by pressure. By using novel efficient algorithms for hard disks, we are able to generate equilibrium supercompressed states in an additive non-equimolar binary mixture, where micro-crystallization and size segregation do not emerge at high average packing fractions. Above an onset pressure where collective heterogeneous relaxation sets in, we find that relaxation times are well described by a "parabolic law" with pressure. We identify excitations, or soft-spots, that give rise to structural relaxation, and find that they are spatially localized, their average concentration decays exponentially with pressure, and their associated energy scale is logarithmic in the excitation size. These observations are consistent with the predictions of DF generalized to systems controlled by pressure rather than temperature.

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An itinerant oscillator model with cage inertia for weakly vibrated granular media

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April 27, 2016

Recent experiments with a rotating probe immersed in weakly fuidized granular materials show acomplex behavior on a wide range of timescales [1] (see fig 1). Viscous-like relaxation at high frequency is accompanied by an almost harmonic dynamical trapping at intermediate times, with possibly anomalous long time behavior in the form of super-diffusion. Inspired by the Itinerant Oscillator model for diffusion in molecular liquids, and other models with coupled thermostats acting at different timescales, here we discuss a new model able to account for fast viscous relaxation, dynamical trapping and super-diffusion at long times. The main difference with respect to liquids, is a non-negligible cage inertia for the surrounding (granular) fluid, which allows it to sustain a slow but persistent motion for long times. The computed velocity power density spectra and mean-squared displacement qualitatively reproduce the experimental findings. We also discuss the linear response to external perturbations and the tail of the distribution of persistency time, which is associated with superdiffusion, and whose cut-off time is determined by cage inertia [2] .

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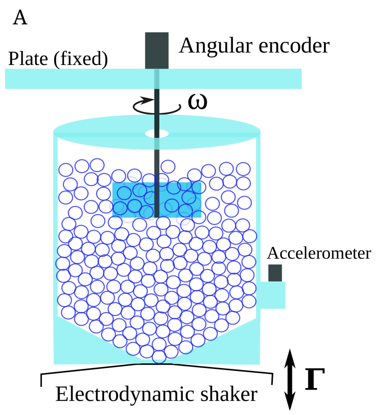

Figure 1: Sketch of the experimental setup.

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"A jamming transition of a finite-size nonequilibrium system"

Microcanonical analysis is a powerful method that can be used to generalize the concept of phase transitions to finite-size systems. However, microcanonical analysis has only been applied to equilibrium systems. I show that it is possible to conduct the microcanonical analysis of a finite-size nonequilibrium system by generalizing the concept of microcanonical entropy. An asymmetric diffusion process in a one-dimensional periodic lattice is known to exhibit a jamming transition, and this system is studied as an example for which a generalized entropy can be explicitly found. The microcanonical method is then used to define a generalized nonequilibrium phase transition of this finite-size system.

[1] Julian Lee, "Microcanonical analysis of a finite-size nonequilibrium system", Physical Review E (2016), in press.

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"Turning intractable counting into sampling: Computing the configurational entropy of three-dimensional jammed packings"

We present a numerical calculation of the total number of disordered jammed configurations for systems of three dimensional spheres at fixed volume fraction. To make these calculations tractable, we increase the computational efficiency of the approach of Xu *et al.* [Phys. Rev. Lett. **106**, 245502 (2011)] and Asenjo *et al.* [Phys. Rev. Lett. **112**, 098002 (2014)] and we extend the method to allow computation of the configurational entropy as a function of pressure. The approach that we use computes the configurational entropy by sampling the absolute volume of basins of attraction of the stable packings in the potential energy landscape. We find a surprisingly strong correlation between the pressure of a configuration and the volume of its basin of attraction in the potential energy landscape. This relation is well described by a power law. Furthermore, thanks to a novel numerical technique we analyse the effect of structural disorder on the basins of attraction of mechanically stable packings of soft repulsive spheres.

Equation of State and Equipartition Relations for the Limit State of Isotropic Compression in Granular Media

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(Dated: May 30, 2016)

Two basic strategies has been proposed to build up statistical mechanical descriptions of granular media: Edward's volumetric entropy and the force network ensemble, and both of them show evidences of elementary volume and force elements. By working out a recent proposal by Aste, Di Matteo et. al. [Phys.Rev. E 77, 021309 (2008)] to measure Edwards' compactivity from the gamma distribution of volumes of Voronoï or Delaunay cells, and assuming that the total volume divides into elementary cells of fixed minimal volume, we derive an equation of state relating the compactivity to the packing fraction, and show by extensive molecular dynamics simulations that this equation describes well the volumetric aspects of the limit state of isotropic compression for three-dimensional ensembles of mono-disperse spheres, for a broad range of the sliding and rolling friction coefficients [Europhys. Lett, 114, 14004 (2016)]. Similarly, Monte Carlo simulations at constant angoricity for the forces on a single grain in mechanical equilibrium (including steric exclusions and with and without friction), both in two and three dimensions, show us that the pressure per grain is also well described by a gamma distribution. In addition, an equipartition relation holds, relating the angoricity with the number of degrees of freedom for the forces on the grain and, by extrapolation, this equipartition relation agrees with previous proposals [J. Stat. Mech. P04002 (2011)]. These results are forward steps in the way to build a statistical description of granular media.

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"Three-Phase Flow and Fracturing of Deformable Granular Media"

The invasion of gas via fractures into a water-saturated porous medium is a process that occurs in numerous geo-engineering and natural circumstances: fracturing for enhanced contaminant remediation, stimulation of hydrocarbon reservoirs, fracturing of soft tissue in arterial walls, soil drying and outgassing of crystal rich magmas for example. However, it is challenging to typify and predict complex flows through deformable fractured media.

We create a simple model system to illuminate these processes. A wet unconsolidated granular packing confined in a Hele-Shaw cell is subject to a slow invasion of gas, causing fractures. We study the influence of granular properties (size/shape), and gas injection rate on the system, as well as the layering of different granular material. We image the complete fracture pattern as it forms, allowing us to investigate the dynamics of its growth and the properties of the resulting pattern (fracture density, branching frequency etc).

Fractures are triggered by initial pore invasion followed by fluidization of the compaction front and they grow in an intermittent, stick slip manner, interspersed with inactive periods. Growth is impeded by friction from local compaction fronts that form around the growing fracture branches. We describe a simple analytical model that predicts the fracture density from basic granular medium properties, and also demonstrate a transition from fracturing to capillary fingering in the presence of less permeable layers.

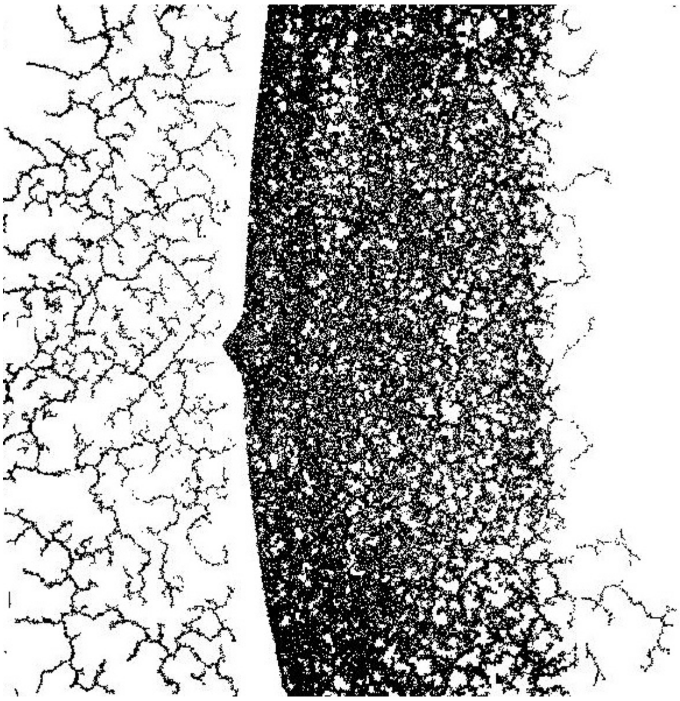

Fig. 1: Gas fractures and capillary fingering in wet granular packing of different grain sizes.

Fabien Paillusson
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"How can we test ergodicity in absence of a prior distribution?"

In thermodynamic systems, ergodicity refers to equating time averages of some observable with so-called ensemble averages of the same observable. These ensemble averages are often to be understood as being phase space averages corresponding to a time-independent Gibbs' ensemble probability distribution. For athermal systems and, in particular for granular systems undergoing a particular dynamical process, the lack of consensus about what ought to be the equivalent of the thermodynamic Gibbs' ensembles suggests that we might need alternative ways of testing ergodicity. One possible alternative relies on the so-called operational interpretation of ensembles and does not require per se any prior probability density. We will see how it can be used for tapped granular matter and discuss some open questions regarding the conclusions one can draw from it.

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"Diffusion of random walkers in periodic potentials, with applications to glasses."

We investigate the diffusion constant of a random walker in a periodic potential, as a function of the typical intercollision time t_c, and provide analytical predictions in the overdamped, $t_c \to 0$, and in the underdamped, $t_c \to \infty$, limits. We show that there are qualitative differences between the random walk dynamics, and the corresponding Langevin dynamics with viscous damping $\gamma = m/t_c$. As an application, we describe the temperature dependence of the diffusion coefficient of an amorphous system of harmonic spheres, assuming the dynamics to occurs through hops in phase space triggered by phonon scattering events. The resulting temperature dependence of the diffusion constant compares favorably with Molecular Dynamics Simulations.

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"An effective potential approach to thermal hard spheres"

Hard spheres (HS) under thermal agitation are a canonical model for many systems of interest in condensed matter, in particular colloidal glasses, and are routinely employed also in the study of the jamming problem, both from the theoretical and the numerical point of view. Despite this popularity, the hard-core character of the HS interaction produces difficulties which are not found in softer systems; for example the non-analyticity of the HS potential makes impossible the computation of the Dynamical Matrix which would encode the vibrational properties of jammed HS packings, which are in turn deeply linked to their critical properties and marginal stability as detailed by numerous recent studies.
Building up from a recent breakthrough which enables the inference of the force-laws of a generic packing of particles from a single visual image, we address this problem by using this approach to infer an effective force-law for thermal HS both at and away from the jamming point. We perform decompressions of jammed packings of hard disks and infer the effective force-law from the average positions of the disks, showing that it has a 1/h dependence (h being the gap between two disks) as found by previous approaches. Our method can in principle work everywhere the averaging procedure of disk positions is meaningful, i.e. in the whole glass phase, improving upon previous attempts at an effective potential description of HS. Besides curing the above exposed problems in the study of jammed HS packings, this novel approach will hopefully enable us to study soft excitations in thermal glassy systems (the foremost example being the celebrated Boson Peak) using tools which are normally confined to the study of athermal systems.

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"Pore deformation mechanisms and configuration landscape of granular crystallisation"

Uncovering grain-scale mechanisms that underlie the disorder-order transition in assemblies of dissipative, athermal particles is an outstanding problem of fundamental physics with technological relevance. To date, the study of granular crystallisation has mainly focused on the symmetry of crystalline patterns while their emergence from initially irregular clusters of grains remains largely unexplored. Here crystallisation of three-dimensional packings of frictional spheres is studied at the grain-scale by using x-ray tomography and persistent homology. The latter provides a map of the different topological configurations of grains within the packings. This map encodes new information on the formation process of tetrahedral and octahedral pores: the two building blocks of perfect crystals. We describe four key formation mechanisms of these pores that reproduce the main changes of the map during crystallisation. We show how these mechanisms are connected to mechanical features of partially crystallised packings and give clues to interpret the observed dominance of face-centred cubic motifs.

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"Jamming of granular plugs in cylindrical confinement"

Multiphase granular-fluid flow in channels and tubes occur in a range of geophysical and engineering processes. Examples include transport of oil, gas and sand through sub-sea pipelines and conveying of powders and granular materials in civil and chemical engineering. Here we study a horizontal tube initially filled with water and grains, where a meniscus forms across the tube aperture. The granular material settles out of suspension, and the gas invasion dynamic is governed in part by the Coulomb friction associated with granular accumulation fronts ahead of the meniscus. We show that capillary and frictional forces combine to produce a characteristic flow pattern whereby plugs of grains are shed by the moving interface. The system undergoes a transition to full fluidisation of the granular mixture and complete evacuation of the granular suspension when the liquid withdrawal rate increases beyond a critical value.

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"Clustering and flow around a sphere moving into a grain cloud"

A bidimensional simulation of a sphere moving at constant velocity into a cloud of smaller spherical grains far from any boundaries and without gravity is presented with a non-smooth contact dynamics method. A dense granular ``cluster" zone builds progressively around the moving sphere until a stationary regime appears with a constant upstream cluster size. The key point is that the upstream cluster size increases with the initial solid solid fraction ϕ_0 but the cluster packing fraction takes an about constant value independent of ϕ_0. Although the upstream cluster size around the moving sphere diverges when ϕ_0 approaches a critical value, the drag force exerted by the grains on the sphere does not. The detailed analysis of the local strain rate and local stress fields made in the non parallel granular flow inside the cluster allows us to extract the local invariants of the two tensors: dilation rate, shear rate, pressure and shear stress. Despite different spatial variations of these invariants, the local friction coefficient μ appears to depend only on the local inertial number I as well as the local solid fraction, which means that a local rheology does exist in the present non parallel flow. The key point is that the spatial variations of I inside the cluster does not depend on the sphere velocity and explore only a small range around the value one.

2D foams jam differently than soft disks

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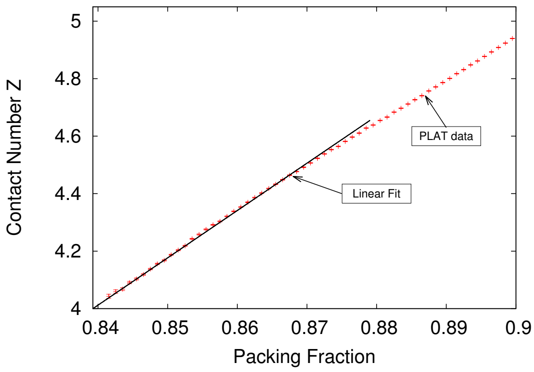
Abstract

For random packings of soft disks in two (and three) dimensions, it is well known that the average contact number Z increases with a square root in $\Delta\phi = \phi - \phi_c$ close to the critical packing fraction ϕ_c, when an affine compression is applied [1, 2, 3].

However, for an idealised two-dimensional foam we show here, using data from PLAT simulations [4, 5, 6], that Z increases linearly in ϕ. Our result is consistent with the different forms for the distributions of next nearest neighbour distances close to the jamming point that we find for 2D foams and polydisperse soft disk systems, respectively.



Our work contributes to the understanding that foams close to the wet limit are not well described as random packings of soft disks and raises theoretical questions which have still to be considered.

Acknowledgements J. Winkelmann acknowledges funding by the Irish Research Council (IRC). Further support by: COST actions MP1106 "Smart and green interfaces" and MP1305 "Flowing matter". ESA MAP Metalfoam (AO-99-075). Science Foundation Ireland (SFI) Grant Number 13/IA/1926.

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