Glass transition in granular media

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Abstract. – In the framework of schematic hard-spheres lattice models for granular media we investigate the phenomenon of the “jamming transition”. In particular, using Edwards’ approach, by analytical calculations at a mean-field level, we derive the system phase diagram and show that “jamming” corresponds to a phase transition from a “fluid” to a “glassy” phase, observed when crystallization is avoided. Interestingly, the nature of such a “glassy” phase turns out to be the same found in mean-field models for glass formers.

Gently shaken granular media exhibit a strong form of “jamming” [1–3], i.e., an exceedingly slow dynamics, which shows deep connections [4–6] to “freezing” phenomena observed in many thermal systems such as glass formers [7]. Although the idea of a unified description of these phenomena is emerging [5], the precise nature of jamming in non-thermal systems and the origin of its close connections to glassy phenomena in thermal ones are still open and very important issues [8].

Here, we discuss these topics in the framework of the statistical mechanics of powders introduced by Edwards [9–11] where, to allow theoretical calculations, it is assumed that time averages of a system subject to some drive (e.g., “tapping”) coincide with suitable ensemble averages over its “mechanically stable” states. In particular, we consider a schematic model for granular media recently shown [11] to be well described by Edwards’ assumption: a system of hard spheres under gravity confined on a cubic lattice. In this letter we first show that this model subject to a Monte Carlo (MC) “tap dynamics”, when crystallization is avoided, has a pronounced jamming similar to the one found in experiments [1–3]. We then discuss the nature of such a form of jamming by analytically solving Edwards’ partition function of the system at a mean-field level, by use of a Bethe approximation. This approach shows that the present model for granular media undergoes a phase transition from a (supercooled) “fluid” phase to a “glassy” phase, when its crystallization transition is avoided. The nature of such a “glassy” phase results to be the same found in mean-field models for glass formers [12,13]: a discontinuous replica symmetry breaking phase preceded by a dynamical freezing point. This finding quantitatively confirms early speculations about the structure of jamming in granular media [4,14] and clarifies the deep connections with glass formers [5].

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Our schematic model for granular media is a system of monodisperse hard spheres (with radius $a_0 = 1$) under gravity, constrained to move on the sites of a cubic lattice of spacing $a_0$. Its Hamiltonian is

$$H = H_{HC} + mg \sum n_iz_i,$$

where $z_i$ is the height of site $i$, $g = 1$ is gravity acceleration, $m = 1$ the grains mass, $n_i \in \{0, 1\}$ is an occupancy variable (absence or presence of a grain on site $i$) and $H_{HC} \{n_i\}$ is the hard-core term preventing the overlapping of nearest-neighbors grains [15].

$N$ grains are confined in a 3D box of linear horizontal size $L$ and height $H$ (in our MC simulations $L = 12$, $H = 20$, $N = 288$) between hard walls and periodic boundary conditions in the horizontal directions. They are initially prepared in a random loose stable pack and are subject to a dynamics made of a sequence of MC “taps” [4]: a single “tap” is a period of time, of length $\tau_0$ (the tap duration), where particles can diffuse laterally or upwards with a probability $p_{up} \in [0, 1/2]$ and downwards with $1 - p_{up}$; when the “tap” is off, grains can only move downwards (i.e., $p_{up} = 0$) and reach a blocked state (i.e., one of their “inherent states” [11]) where no one can move downwards without violating the hard-core repulsion. The parameter $p_{up}$ has an effect equivalent to keep the system in contact (for a time $\tau_0$) with a bath temperature $T_\Gamma = mga_0/\ln[(1 - p_{up})/p_{up}]$ (called the “tap amplitude”). Our measurements are performed when the shake is off and the system at rest. Time, $t$, is measured as the number of taps applied to the system.

The MC tap “dynamics” exhibits large relaxation times which grow as the tap amplitude decreases. In particular, we consider the density correlation function $C(t, t_w) = B(t, t_w)/B(t_w, t_w)$, where $B(t, t_w) = \sum_i [n_i(t+t_w)n_i(t_w) - \langle n_i(t+t_w) \rangle \langle n_i(t_w) \rangle]$. At high $T_\Gamma$, for $t_w$ long enough, $C(t, t_w)$ has a time translation invariant behavior, i.e., $C(t, t_w) = C(t)$. We do not consider here low values of $T_\Gamma$ as the model tends to crystallization [16]. The relaxation time, $\tau(T_\Gamma)$, plotted in fig. 1, has been obtained by fitting $C(t)$ as an exponential function at long time $t$. Even though we are at comparatively high $T_\Gamma$ values, an Arrhenius law (shown in the picture) or a Vogel-Tamman-Fulcher law fits the data. These properties
are very similar to those found in more refined models [4,11,17] and correspond to recent experimental results on granular media [2,3], which are found to exhibit a glassy behavior [7].

The nature of the glassy region is, anyway, very difficult to be numerically established and further insight can be obtained by analytical treatments. This can be accomplished in Edwards’ approach [9–11] which we now assume to hold in our model, at least as a good approximation. This assumption is grounded on some recent results [11] showing that “time averages” of the system observables over the “tap” dynamics coincide with those over an ensemble average where only “mechanically stable” states (i.e., those where the system is found at rest) are counted. More specifically, the weight of a given state $r$ is [11] $e^{-βH(r)} \cdot Π_r$, where $T_{\text{conf}} = β^{-1}$ is a thermodynamic parameter, called “configurational temperature”, characterizing the distribution ($T_{\text{conf}}$ can be related to the shaking amplitude $T_Γ$, for instance, from the equality between the time average of the energy, $⟨e⟩(T_Γ)$, and the ensemble average, $⟨e⟩(T_{\text{conf}})$). The operator $Π_r$ selects mechanically stable states: $Π_r = 1$ if $r$ is “stable”, else $Π_r = 0$. The system partition function à la Edwards is thus the following [11]:

$$\sum_r e^{-βH(r)} \cdot Π_r,$$

where the sum runs over all microstates $r$.

Since the exact calculation of $Z$ for the above lattice model is hardly feasible, we now discuss a mean-field theory (see [13, 18] and references therein) based on a random graph version of such a lattice which is sketched in fig. 2. More specifically, we consider a 3D lattice box with $H$ horizontal layers (i.e., $z \in \{1, \ldots, H\}$) occupied by hard spheres. Each layer is a random graph of given connectivity, $k−1$ (we take $k = 4$). Each site in layer $z$ is also connected to its homologous site in $z−1$ and $z+1$ (the total connectivity is thus $k+1$). The Hamiltonian is the one of eq. (1) plus a chemical potential term to control the overall density. Hard core repulsion prevents two connected sites from being occupied at the same time. In the present lattice model we adopt a simple definition of “mechanical stability”: a grain is “stable” if it has a grain underneath. For a given grains configuration $r = \{n_i\}$, the operator $Π_r$ has thus a simple expression: $Π_r = \lim_{K→∞} \exp[-K-series]$, where $H_{\text{Edw}} = \sum_i δ_{n_i(z),1}δ_{n_i(z−1),0}δ_{n_i(z−2),0}$ (for clarity, we have shown the $z$-dependence in $n_i(z)$).
Fig. 3 – The system mean-field phase diagram is plotted in the plane of its two control parameters ($T_{\text{conf}}, N_s$): $T_{\text{conf}}$ is Edwards’ “configurational temperature” and $N_s$ the average number of grains per unit surface in the box. At low $N_s$ or high $T_{\text{conf}}$, the system is found in a fluid phase. The fluid forms a crystal below a melting transition line $T_m(N_s)$. When crystallization is avoided, the “supercooled” (i.e., metastable) fluid has a thermodynamic phase transition, at a point $T_K(N_s)$, to a replica symmetry breaking “glassy” phase with the same structure found in mean-field theory of glass formers. In between $T_m(N_s)$ and $T_K(N_s)$ a dynamical freezing point, $T_D(N_s)$, is located, where the system characteristic time scales diverge.

The local tree-like structure of our lattice allows to write down iterative equations à la Bethe for the probability of fields acting on the lattice sites [19]. In the “cavity method” [18], the recurrence equations are found by iteration of the lattice structure where $k$ “branches” (i.e., graphs where a root site, denoted by $j \in \{1, \ldots, k\}$, has only $k$ neighbors) are merged to a new site $i$, leading to a lattice with the same structure as before but with one more site. Three kinds of “branches” exist here: “up” (respectively, “down”) branches where the root site has $k - 1$ neighbors on its same layer and one in the upper (respectively, lower) layer; and “side” branches where the root has $k - 2$ neighbors on its layer, one in the upper and one in the lower layer. Correspondingly, three kinds of merging are possible where: an “up” (respectively, “down”) branch with root at height $z + 1$ (respectively, $z - 1$) and $k - 1$ “side” branches with root at height $z$ merge into a new “up” (respectively, “down”) branch with root in site $i$ at height $z$; an “up”, a “down” and $k - 2$ “side” branches merge into a new “side” branch.

The partition function of the new branch ending in site $i$ can be recursively written in terms of the partition functions of the merged branches. Define $Z_{0,s}^{(i,z)}$ and $Z_{1,s}^{(i,z)}$ the partition functions of the “side” branch restricted, respectively, to configurations in which the site $i$ is empty or filled by a particle; analogously, $Z_{1,u}^{(i,z)}$ and $Z_{0,u}^{(i,z)}$ (respectively, $Z_{0,u}^{(i,z)}$) are the partition functions of the “up” branch restricted to configurations in which the site $i$ is filled or empty with the upper site filled (respectively, empty); finally, $Z_{1,d}^{(i,z)}$ and $Z_{0,d}^{(i,z)}$ (respectively, $Z_{0,d}^{(i,z)}$) are those of the “down” branch when site $i$ is filled or empty with the upper site filled (respectively, empty). For more details see [17]. It is convenient to introduce five local “cavity fields” $h_{1,s}^{(i,z)}, h_{1,u}^{(i,z)}, h_{1,d}^{(i,z)}, g_{0,u}^{(i,z)}$ and $g_{d}^{(i,z)}$ defined by: 

$$e^{\beta h_{1,s}^{(i,z)}} = Z_{1,s}^{(i,z)}/Z_{0,s}^{(i,z)}; \quad e^{\beta h_{1,u}^{(i,z)}} = Z_{1,u}^{(i,z)}/Z_{0,u}^{(i,z)}; \quad e^{\beta h_{1,d}^{(i,z)}} = Z_{1,d}^{(i,z)}/Z_{0,d}^{(i,z)}; \quad e^{\beta g_{0,u}^{(i,z)}} = Z_{0,u}^{(i,z)}; \quad e^{\beta g_{d}^{(i,z)}} = Z_{0,d}^{(i,z)}/Z_{0,u}^{(i,z)}.$$
Fig. 4 – For a system with a given number of grains (i.e., a given $N_s$), the overall number density, $\Phi \equiv N_s/2\langle z \rangle$ ($\langle z \rangle$ is the average height), calculated in mean-field approximation is plotted as a function of $T_{\text{conf}}$; $\Phi(T_{\text{conf}})$ has a shape very similar to the one observed in the “reversible regime” of tap experiments and MC simulations of the cubic lattice model for $\Phi(T_T)$. The location of the glass transition, $T_K$ (filled circle), corresponds to a cusp in the function $\Phi(T_{\text{conf}})$. The passage from the fluid to supercooled fluid is $T_m$ (filled square). The dynamical crossover point $T_D$ is found around the flex of $\Phi(T_{\text{conf}})$ and well corresponds to the position of a characteristic shaking amplitude $\Gamma^*$ found in experiments and simulations where the “irreversible” and “reversible” regimes approximately meet.

In these new variables the recursion relations are more easily written [20]:

$$e^{\beta h_{i,z}^{(i,z)}} = e^{\beta(\mu-mgz)} \prod_{j=1}^{k-2} \left(1 + e^{\beta h_{j,z}^{(j,z)}}\right)^{-1} \left(1 + e^{\beta g_{u,j,z}^{(j,z)\pm 1}}\right) \times$$

$$\times \left[1 + e^{\beta h_{d,j,z}^{(j,z)\pm 1}} + e^{\beta g_{d,j,z}^{(j,z)\pm 1}} + e^{\beta h_{d,j,z}^{(j,z)\pm 1} + \beta h_{u,j,z}^{(j,z)\pm 1}}\right]^{-1},$$

$$e^{\beta h_{u,i,z}^{(i,z)}} = e^{\beta(\mu-mgz)} \left(1 + e^{\beta g_{u,i,z}^{(i,z)\pm 1}}\right) \prod_{j=1}^{k-1} \left(1 + e^{\beta h_{u,j,z}^{(j,z)}}\right)^{-1},$$

$$e^{\beta g_{u,i,z}^{(i,z)}} = e^{\beta h_{u,i,z}^{(i,z)\pm 1}},$$

$$e^{\beta h_{d,i,z}^{(i,z)}} = e^{\beta(\mu-mgz)} e^{-\beta h_{d,i,z}^{(i,z)\pm 1}} \prod_{j=1}^{k-1} \left(1 + e^{\beta h_{u,j,z}^{(j,z)}}\right)^{-1},$$

$$e^{\beta g_{d,i,z}^{(i,z)}} = \left(1 + e^{\beta g_{d,i,z}^{(i,z)\pm 1}}\right) e^{-\beta h_{d,i,z}^{(i,z)\pm 1}}.$$  

(3)

From the iterative solution of these equations it is possible to compute the system free energy [17, 18]. Figure 3 shows the system phase diagram in the plane of the two control parameters ($T_{\text{conf}}, N_s$), where $N_s$ is the number of grains per unit surface in the box.

At low $N_s$ or high $T_{\text{conf}}$, a fluid-like phase is found, characterized by a homogeneous replica symmetric (RS) solution (in replica theory terminology) of the recursion equations (3), in which only one pure state exists and the local fields are the same for all the sites of the lattice (translational invariance). For a given $N_s$, by lowering $T_{\text{conf}}$ (see figs. 3, 4), a phase transition to a crystal phase (an RS solution with no space translation invariance) is found at
$T_m$ [21]. Notice that the fluid phase still exists below $T_m$ as a metastable phase corresponding to a supercooled fluid found when crystallization is avoided.

The above RS fluid solution, however, is not appropriate to describe the high $N_s$ or low $T_{\text{conf}}$ region which is dominated by the presence of a large number of local minima of the free energy where the fields may fluctuate [18]. This situation is characterized by non-trivial probability distributions for the local fields on each layer $z$: $P_z^u(h_u, g_u)$, $P_z^s(h_s)$ and $P_z^d(h_d, g_d)$. Within the one-step replica symmetry breaking (1RSB) ansatz of the cavity method [18,22], the recursion relations for the fields are replaced by self-consistent integral equations for the distribution of the local fields:

$$P_z^u(h_u^z, g_u^z) = C_1 \int \prod_{j=1}^{k-1} \left[ dh_s^{(j,z)} P_z^s(h_s^{(j,z)}) \right] \times \left[ dh_u^{(i,z+1)} dg_u^{(i,z+1)} P_{z+1}^u(h_u^{(i,z+1)}, g_u^{(i,z+1)}) \right] \times$$

$$\times \delta(h_u^z-h_u^{(i,z)}) \delta(g_u^z-g_u^{(i,z)}) \exp \left[ -\beta m \Delta F_u^z \right], \quad (4)$$

where $C_1$ is a normalization constant, $h_u^{(i,z)}$, $g_u^{(i,z)}$ are the local fields defined by eqs. (3), $\Delta F_u^z$ is the free-energy shifts in the merging process [17,18] and $m$ is the usual 1RSB parameter to be obtained by maximization of the free energy with respect to it. Analogous equations are found for $P_s^u(h_s)$ and $P_d^u(h_d, g_d)$. We have solved all these equations iteratively, by discretizing the probability distributions, until the whole procedure converged.

A non-trivial solution of the 1RSB equations appears for the first time at a given temperature $T_D(N_s)$, signaling the existence of an exponentially high number of pure states. In mean-field theory $T_D$ is interpreted as the location of a purely dynamical transition as in mode coupling theory, but in real systems it might correspond just to a crossover in the dynamics (see [12,13,23] and references therein). The 1RSB solution becomes stable at a lower point $T_K$, where a thermodynamic transition from the supercooled fluid to a 1RSB glassy phase takes place (see fig. 3) in a scenario à la Kauzmann with a vanishing complexity of pure states (which stays finite for $T_K < T < T_D$).

The results of these calculations, summarized in the phase diagram of fig. 3, are further illustrated in fig. 4: in a system with a given number of grains (i.e., a given $N_s$), the overall number density, $\Phi$, is plotted as a function of $T_{\text{conf}}$ (here by definition $\Phi \equiv N_s / 2 \langle z \rangle$, where $\langle z \rangle$ is the average height). The shown curve, $\Phi(T_{\text{conf}})$, is the equilibrium function here calculated. It has a shape very similar to the one observed in tap experiments [1,3], or in MC simulations on the cubic lattice (see also [4]), where the density is plotted as a function of the shaking amplitude $\Gamma$ (along the so-called “reversible branch”).

Summarizing, in the present mean-field scenario of a granular medium with $N_s$ particles per surface, in general, at high $T_{\text{conf}}$ (i.e. high shaking amplitudes) a fluid phase is located (see fig. 3). By lowering $T_{\text{conf}}$, a phase transition to a crystal phase is found at $T_m$. However, when crystallization is avoided, the fluid phase still exists below $T_m$ as a metastable phase corresponding to a supercooled fluid. At a lower point, $T_D$, an exponentially high number of new metastable states appears, interpreted, at a mean-field level, as the location of a purely dynamical transition, which in real system is thought to correspond just to a dynamical crossover. Finally, at an even lower point, $T_K$, the supercooled fluid has a genuinely thermodynamics discontinuous phase transition to glassy state. MC simulations of a cubic lattice model show indeed the divergence of the relaxation time $\tau$ at low “shaking” amplitudes (see fig. 1). The structure of the glass transition of the present model for granular media, obtained in the framework of Edwards’ theory is the same found in the glass transition of the $p$-spin glass and in other mean-field models for glass formers [12,13].
The boundary conditions are insured by adding two auxiliary planes at height $z = -1$ and $z = H + 1$, where all sites are empty but stable (in Edwards’ sense).

In the present model the “melting” transition is continuous. This pathology can be cured as explained in [17] or in Weigt M. and Hartmann A. K., Europhys. Lett., 62 (2002) 533.

Since the glassy phase is expected to be translational invariant, we work in the factorized case in which the probability distributions at a given height are equal for all the sites of the layer.

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