Jamming transition in granular media: A mean field approximation and numerical simulations

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In order to study analytically the nature of the jamming transition in granular material, we have considered a cavity mean field theory, in the framework of a statistical mechanics approach, based on Edwards' original idea. For simplicity we have applied the theory to a lattice model and a transition with exactly the same nature of the glass transition in mean field models for usual glass formers is found. The model is also simulated in three dimensions under tap dynamics and a jamming transition with glassy features is observed. In particular two step decays appear in the relaxation functions and dynamic heterogeneities resembling ones usually observed in glassy systems. These results confirm early speculations about the connection between the jamming transition in granular media and the glass transition in usual glass formers, giving moreover a precise interpretation of its nature.

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I. INTRODUCTION

A deep connection between glass transition in molecular glass formers, structural arrest in colloidal systems, and jamming transition in granular media has often been stressed in the past few years. In spite of the fact that these systems are very different one from each other, varying suitably the control parameters, a slowdown and a subsequent structural arrest in a solid-like disordered state are found in each of them. In a possible phase diagram for jamming is suggested, which takes into account the fact that jamming is obtained either raising the volume fraction or lowering the temperature or lowering the applied stress. Colloidal suspensions and molecular glass formers are both thermal systems, and it is commonly accepted that both colloidal glass transition and molecular glass transition are of the same type despite of the fact that different control parameters may drive the transition. The case of granular materials is instead very different: They are athermal systems, since the thermal fluctuations are significantly less than the gravitational energy and the system cannot explore the phase space without any external driving. Nevertheless an exceedingly slowly down is observed when a granular material is shaken at low shaking amplitude, or flows under a low shear stress, with strong analogies with the slowing down observed in glass formers. Experimental and numerical studies have confirmed this connection, however its precise nature is still unclear.

In the present paper in order to study this connection we apply a statistical mechanics approach to granular media. This approach, which has been extensively developed in previous works, is based on an elaboration of the original ideas suggested by Edwards. The basic assumption is that for a granular system subject to an external drive (e. g. tapping), after having reached stationarity, time averages coincide with suitable ensemble averages over the “mechanically stable” states. We have shown that this assumption works for different lattice models namely that a generalized Gibbs distribution of the stable states describes with good approximation the stationary state attained by the system under tapping dynamics. Here each tap consists in raising the bath temperature to a finite value (called tap amplitude) and, after a lapse of time (called tap duration) quenching the bath temperature back to zero. By cyclically repeating the process the system explores the space of the mechanically stable states.

We thus consider one of the above lattice model for which the statistical mechanics approach works. The model is made up of hard spheres under gravity. Then we apply standard statistical mechanics methods in order to investigate analytically the existence and the nature of a possible jamming transition. More precisely we consider the Bethe-Peierls approximation using the cavity method: By changing the control parameter a phase transition from a fluid to a crystal is found, and, when crystallization is avoided, a glassy phase appears. The nature of this glassy phase is analogous to that found in mean field models for glass formers: In particular we observe a dynamical transition, where an exponentially high number of metastable states appears, and at a lower temperature a thermodynamic discontinuous phase transition to a glassy state. A brief account of these calculations was given in a previous Letter. We also studied the model in 3d by means of numerical simulations, and we found that the model under taps has a transition from a fluid to a crystal, in a very good agreement with he mean field approximation. However the numerical simulation was not suitable to study the glass transition since the model showed a strong tendency towards crystallization.

For this reason we study here a variant of the model
which has the virtue of avoiding crystallization. We find that the system under gravity evolved by Monte Carlo taps presents features characteristic of real granular media \cite{16,17}, and at low tap amplitudes a dynamical transition with properties recalling those of usual glass formers. In particular we observe a dynamical non linear susceptibility with a maximum at increasing time: This behavior, typical of glass formers, is usually interpreted as the sign of dynamic heterogeneities in the system.

In conclusions the results confirm early speculations about the deep connection between the jamming transition in granular media and the glass transition in usual glass formers, giving moreover a precise interpretation to its nature.

In Sect. II the mean field phase diagram is discussed. The details of calculations are presented in Appendices A and B In particular in App. B the self-consistency equations obtained using the cavity method are shown. In Sect. III the 3d model is presented and the numerical results are shown.

II. MEAN FIELD SOLUTION IN THE BETHE-PEIERLS APPROXIMATION

The model is a monodisperse hard sphere system (with diameter $\sqrt{2}a_0$) under gravity, constrained to move on the sites of a cubic lattice of spacing $a_0 = 1$. The Hamiltonian is given by:

$$\mathcal{H} = \mathcal{H}_{HC} + mg \sum_i n_i z_i$$

where $z_i$ is the height of site $i$, $g = 1$ is the gravity acceleration, $m = 1$ the grain mass, $n_i \in \{0, 1\}$ is the occupancy variable (absence or presence of a grain on site $i$) and $\mathcal{H}_{HC}(\{n_i\})$ is the hard core term preventing two nearest neighbor sites being simultaneously occupied.

We have shown in previous papers \cite{10} that the model, Eq. (1), evolving by means of a tap dynamics can be represented using the cavity method. In particular in App. B the self-consistency equations are shown. In Sect. III the mean field theory was first introduced.

in the Bethe-Peierls approximation (see \cite{11,12} and ref.s therein), based on a random graph (plotted in Fig. II) which keeps into account that the gravity breaks the symmetry along the $z$ axis. This lattice is made up by $H$ horizontal layers (i.e., $z \in \{1, \ldots, H\}$). Each layer is a random graph of connectivity, $k - 1 = 3$. Each site in layer $z$ is also connected to its homologous site in $z - 1$ and $z + 1$ (the total connectivity is thus $k + 1$). Locally the graph has a tree-like structure but there are loops whose length is of order in $N$, insuring geometric frustration. In the thermodynamic limit only very long loops are present. The details of calculations are given in appendices A and B (see also Ref.s \cite{15,18} where this mean field theory is first introduced).

![FIG. 1: In the mean field approximation, the grains are located on a Bethe lattice, sketched in the figure, where each horizontal layer is a random graph of given connectivity. Homologous sites on neighboring layers are also linked and the overall connectivity, $c$, of the vertices is $c \equiv k + 1 = 5.$](image)

We solve the recurrence equations found in the Bethe-Peierls approximation in three cases: 1) A fluid-like homogeneous phase; 2) a crystalline-like phase characterized by the breakdown of the horizontal translational invariance; 3) a glassy phase described by a 1-step Replica Symmetry Breaking (1RSB). The details of the calculations are shown in Appendices.

The results of the calculations are summarized in Fig. II, where the bulk density at equilibrium, $\Phi = N_s/(2(z) - 1)$ \cite{19} (where $\langle z \rangle$ is the average height) is plotted as a function of the configurational temperature, $T_{conf}$, for a given value of the number of grains per unit surface, $N_s$. We found that at high $T_{conf}$ a homogeneous solution corresponding to the fluid-like phase is found. By lowering $T_{conf}$ at $T_m$ a phase transition to a crystal phase (an anti-ferromagnetic solution with a breakdown of the translation invariance) occurs. The fluid phase still exist below $T_m$ as a metastable phase corresponding to a supercooled fluid when crystallization is avoided. Finally a 1RSB solution (found with the cavity method \cite{11}), characterized by the presence of a large number of local minima in the free energy \cite{11}, appears at $T_D$, and becomes stable at a lower point $T_K$, where a thermodynamic transition from the supercooled fluid to a 1RSB glassy phase takes place. The temperature $T_D$, which is interpreted in mean field as the location of a dynamical transition where the relaxation time diverges, in real sys-
tems might instead correspond to a crossover in the dynamics (see [12, 14, 20] and Ref.s therein). $\Phi(T_{\text{conf}})$ has a shape very similar to that observed in the “reversible regime” of tap experiments [16, 21]. The location of the glass transition, $T_K$, corresponds to a cusp in the function $\Phi(T_{\text{conf}})$. The dynamical crossover point $T_D$ might correspond to the position of a characteristic shaking amplitude $\Gamma^*$ found in experiments and simulations where the “irreversible” and “reversible” regimes approximately meet.

FIG. 2: The density, $\Phi \equiv N_s/(2\langle z \rangle - 1)$, for $N_s = 0.6$ as a function of $T_{\text{conf}}$. $\Phi_{\text{max}}$ is the maximum density reached by the system in the crystal phase.

In Fig. 2 the phase diagram obtained by varying $N_s$ is shown. The dashed vertical line in figure corresponds to the value of $N_s$ chosen in Fig. 2.

FIG. 3: The system mean field phase diagram is plotted in the plane of its two control parameters ($T_{\text{conf}}, N_s$).

The model, Eq. (4), simulated in 3d by means of Monte Carlo tap dynamics [15] presents a transition from a fluid to a crystal as predicted by the mean field approximation, density profiles in good agreement with the mean field ones, and in the fluid phase a large increase of the relaxation time as a function of the inverse tap amplitude. In the following section we study a more complex model for hard spheres, where an internal degree of freedom allows to avoid crystallization [13].

III. HARD SPHERES WITH AN INTERNAL DEGREE OF FREEDOM

The Hamiltonian of the model is

$$H = \sum_{\langle ij \rangle} n_i n_j \phi_{ij}(\sigma_i, \sigma_j) + mg \sum_i n_i z_i, \quad (4)$$

where $z_i$ is the height of site $i$, $g = 1$ is the gravity acceleration, $m = 1$ the grain mass, $n_i \in \{0, 1\}$ is the occupancy variable (absence or presence of a grain on site $i$), $\sigma_i \in \{1, \ldots, q\}$ represents the internal degree of freedom (which we call spin), and $\phi_{ij}(\sigma_i, \sigma_j)$ is the interaction energy between spins. Different values of the spin correspond to different positions of the particle inside the cell. It is reasonable that a few number of internal states might be enough to catch the main features of real systems.

As in Ref. [13] we study a simple realization of the model described by Eq. (4). Interpreting the spin as position of the particle in the cell, our choice can be easily visualized in 2d, as shown in Fig. 4. We partition the space in square cells, and subdivide each cell into four internal positions (namely $q = 4$). When a cell is occupied by a particle in any given position, a hard-core repulsion excludes the presence of particles in some of the internal states of the neighboring cells (namely the interaction $\phi_{ij}(\sigma_i, \sigma_j)$ is chosen zero if the positions $\sigma_i$ and $\sigma_j$ are “compatible”, and infinite otherwise). This choice can be interpreted as a coarse grained version of a hard sphere system in the continuum. In 3d we subdivide the space into cubic cells, and considers six internal positions instead of four.

FIG. 4: The model in two dimensions: the space is partitioned in square cells, and each cell can be occupied by at most one particle in anyone of the four shown positions (little circles). A particle in any given position (large shaded circle) excludes the presence of particles in any of the black colored positions.
We perform a standard Metropolis algorithm on the system. The particles, initially prepared in a random configuration, are subject to taps, each one followed by a relaxation process. During a tap, for a time $\tau_0$ (called tap duration), the temperature is set to the value $T_T$ (called tap amplitude), so that particles have a finite probability, $p_{up} \sim e^{-mg/T_T}$, to move upwards. During the relaxation the temperature is set to zero, so that particles can only reduce the energy, and therefore can move only downwards. The relaxation stops when the system has reached a blocked state, where no grain can move downwards. Our measurements are performed at this stage when the shake is off and the system is at rest. The time, $t$, is the number of taps applied to the system.

In the following the tap duration is fixed, $\tau_0 = 10\text{MCsteps/particle}$, and different tap amplitudes, $T_T$, are considered. In Fig. 6 the bulk density, $\Phi \equiv N/L^2 (2(z) - 1)$, is plotted as a function of $T_T$ for $\tau_0 = 10 \text{MCsteps/particle}$. The empty circles correspond to stationary states, and the black stars to out of stationarity ones. $\Phi_{max}$ is the maximum density reached by the system in the crystal phase, $\Phi_{max} = 6/7$.

In conclusions the system here studied presents a jamming transition at low tap amplitudes as found in real granular media. In order to test the predictions of the mean field calculations, in the following we measure quantities usually important in the study of glass transition: The relaxation functions, the relaxation time and the dynamical susceptibility, connected to the presence a dynamical correlation length.

In particular we calculate the two-time autocorrelation functions:

$$C(t, t_w) = \frac{1}{N} \sum_i \langle n_i(t) n_i(t_w) \vec{\sigma}_i(t) \cdot \vec{\sigma}_i(t_w) \rangle,$$

where $\vec{\sigma}_i$ are unit length vectors, pointing in one of the six coordinate directions, representing the position of the particles inside the cell; the average $\langle \ldots \rangle$ is done over $16 - 32$ different realizations of the model obtained varying the random number generator in the simulations, and the errors are calculated as the fluctuations over this statistical ensemble. For values of $t_w$ long enough, the system reaches a stationary state, where the time translation invariance is recovered, i.e., $C(t, t_w) = C(t - t_w)$. In this time region, by averaging $C(t', t_w)$ over $t'$ and $t_w$ such that $t = t' - t_w$ is fixed, we calculate the “equilibrium” autocorrelation functions

$$\langle q(t) \rangle = \langle C(t' - t_w) \rangle,$$

and the dynamical non linear susceptibility

$$\chi(t) = \langle q(t)^2 \rangle - \langle q(t) \rangle^2.$$

As shown in Fig. 7 at low values of the tap amplitudes, $T_T$, two-step decays appear, well fitted in the intermediate time region, by the $\beta-$correlator predicted by the mode coupling theory for supercooled liquids [24, 25] (the...
FIG. 7: The “equilibrium” autocorrelation function, \( \langle q(t) \rangle \), plotted as function of \( t \), for tap amplitudes \( T_\Gamma = 0.60, 0.50, 0.425, 0.40, 0.385, 0.365, 0.36 \) (from bottom to top). The continuous line in figure is the \( \beta \)-correlator of the mode coupling theory with exponent parameters \( a = 0.30 \) and \( b = 0.52 \). The dashed line is a stretched exponential \( \propto \exp[-(t/\tau)^\beta] \) with \( \beta = 0.70 \).

FIG. 8: The relaxation time, \( \tau \), as function of the bulk density, \( \Phi \). The continuous line is a Vogel-Fulcher, \( e^{A/(\Phi_c - \Phi)} \), with \( \Phi_c = 0.81 \pm 0.01 \) and \( A = 0.49 \pm 0.10 \). The dashed line is a power law, \( (\Phi_D - \Phi)^{-\gamma_1} \), with \( \Phi_D = 0.76 \pm 0.01 \) and \( \gamma_1 = 2.04 \pm 0.10 \).

FIG. 9: The relaxation time, \( \tau \), as function of the tap amplitude inverse, \( T_\Gamma^{-1} \). The dashed line is a power law, \( (T_\Gamma - T_D)^{-\gamma_2} \), with \( T_D = 0.40 \pm 0.01 \) and \( \gamma_2 = 1.52 \pm 0.10 \). The continuous line is an Arrhenius fit, \( e^{A/T_\Gamma} \), with \( A = 17.4 \pm 0.5 \) (the data in this region are also well fitted by both a super-Arrhenius and Vogel-Fulcher laws).

The dynamical non linear susceptibility, \( \chi(t) \), plotted in Fig. 10 at different \( T_\Gamma \), exhibits a maximum at a time, \( t^*(T_\Gamma) \). The presence of a maximum in the dynamical non linear susceptibility is typical of glassy systems [25, 26]. Their findings are in fact consistent with an Arrhenius behavior as function of the experimental tap amplitude intensity. However a direct comparison with our data is not possible since we do not know the relation between the experimental tap amplitude and the tap amplitude in our simulations. A more direct comparison would be possible if the experimental data were plotted as function of the bulk density, as we did in Fig. 8.

The dynamical non linear susceptibility, \( \chi(t) \), plotted in Fig. 10 at different \( T_\Gamma \), exhibits a maximum at a time, \( t^*(T_\Gamma) \). The presence of a maximum in the dynamical non linear susceptibility is typical of glassy systems [25, 26]. In particular the value of the maximum, \( \chi(t^*) \), diverges in the p-spin model [27] as the dynamical transition is approached from above, signaling the presence of a diverging dynamical correlation length. In the present case the...
value of the maximum increases as $T_T$ decreases (except at very low $T_T$ where the maximum seems to decrease\textsuperscript{27}). The growth of $\chi(t^*)$ in our model suggests the presence of a growing dynamical length also in granular media.

![Image of Figure 10](https://via.placeholder.com/150)

**FIG. 10:** The dynamical non linear susceptibility, $\chi(t)$, (normalized by $\chi(t_0)$, the value at $t_0 = 1$) as a function of $t$, for tap amplitudes $T_T = 0.60$, $0.50$, $0.425$, $0.41$, $0.40$, $0.385$, $0.3825$ (from left to right).

![Image of Figure 11](https://via.placeholder.com/150)

**FIG. 11:** Three kinds of branches exist here: 1) “Side” branch: the root site is connected to $k-2$ neighbors on its layer, one in the upper and one in the lower layer; 2) “Up” branch: the root site is connected to $k-1$ neighbors on its layer and one in the upper layer; 3) “Down” branch: the root site is connected to $k-1$ neighbors on its layer, one in the lower layer.

### IV. CONCLUSIONS

In conclusions using standard methods of statistical mechanics we have investigated the jamming transition in a model for granular media. We have shown a deep connection between the jamming transition in granular media and the glass transition in usual glass formers. As in usual glass formers the mean field calculations obtained using a statistical mechanics approach to granular media predict a dynamical transition at a finite temperature, $T_D$, and, at a lower temperature, $T_K$, a thermodynamics discontinuous phase transition to a glass phase. In finite dimensions 1) the dynamical transition becomes only a dynamical crossover as also found in usual glass formers\textsuperscript{12, 14, 20} (here the relaxation time, $\tau$, as a function of both the density and the tap amplitude, presents a crossover from a power law to a different regime); and 2) the thermodynamics transition temperature, $T_K$, seems to go to zero (the relaxation time, $\tau$, seems to diverge only at $T_T \approx 0$, even if a very low value of the transition temperature is consistent with the data).

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### APPENDIX A: MEAN FIELD SOLUTION

We consider the Hamiltonian, Eq. \textsuperscript{11}, plus a chemical potential term which controls the overall density. Hard Core repulsion prevents two connected sites to be occupied at the same time. We adopt a simple definition of “mechanical stability”: a grain is “stable” if it has a grain underneath. For a given grain configuration $r = \{n_i\}$, the operator $\Pi_r$ has a simple expression: $\Pi_r = \lim_{K \to \infty} \exp \{-K \mathcal{H}_{Edw}\}$, where $\mathcal{H}_{Edw} = \sum_i \delta_{n_i(z),1} \delta_{n_i(z-1),0} \delta_{n_i(z-2),0}$ (for clarity, we have shown the $z$ dependence in $n_i(z)$).

The random graph, Fig. \textsuperscript{11} keeps into account that the gravity breaks up the symmetry along the $z$ axis. This lattice is made up by $H$ horizontal layers\textsuperscript{28} occupied by hard spheres (two numbers identify a site of the lattice: The height of the layer, $z \in \{1, \ldots, H\}$, and the position in the layer, $i$). Each layer is a random graph of connectivity, $k - 1 = 3$. Each site in layer at height $z$ is also connected to its homologous site in $z-1$ and $z+1$ (the total connectivity is thus $k+1$). The local tree-like structure of the lattice allows to write down iterative equations à la Bethe, where the partition function of each site is written in terms of the partition functions of the neighbor sites. We have to introduce the concept of “branch”: a branch is a graph where a root site, $i$, has only $k$ neighbors. In the present case three kinds of branches exist (see Fig. \textsuperscript{111}: “up” (resp. “down”) branch where the root site has $k-1$ neighbors on its same layer and one in the upper (resp. lower) layer; and “side” branch where the root has $k-2$ neighbors on its layer, one in the upper and one in lower layer.

Define $Z_{0,s}^{i,z}$ and $Z_{1,s}^{i,z}$ the partition functions of a
“side” branch with root site \( i \) at height \( z \) restricted respectively to configurations in which the site \( i \) is empty or filled by a particle. \( Z^{(i,z)}_{1,u} \) and \( Z^{(i,z)}_{0,u} \) (resp. \( \overline{Z}^{(i,z)}_{0,v} \)) are the partition functions of the “up” branch restricted respectively to configurations in which the site \( i \) is filled by a particle, or empty with the upper site filled (resp. empty). Finally \( Z^{(i,z)}_{1,d} \) and \( Z^{(i,z)}_{0,d} \) (resp. \( \overline{Z}^{(i,z)}_{0,d} \)) are the partition functions of the “down” branch restricted respectively to configurations in which the site \( i \) is filled by a particle, or empty with the lower site empty (resp. filled).

The partition function of the branch ending in site \( i \) can be recursively written in terms of the partition functions of the neighbor sites. Summing over all the possible configurations of the neighbor sites, we obtained that the partition function of a “side” branch with root site \( i \) at height \( z \) is:

\[
Z^{(i,z)}_{0,s} = \prod_{j=1}^{k-2} \left( Z^{(j,z)}_{0,s} + Z^{(j,z)}_{1,s} \right) \times \left[ Z^{(i+z+1)}_{1,u} \left( Z^{(1,z-1)}_{0,d} + e^{-K} \overline{Z}^{(i,z-1)}_{0,d} \right) \right] \times \left( Z^{(i+z+1)}_{0,u} + e^{-K} Z^{(i,z+1)}_{0,u} \right)
\]

(A1)

In the same way we can write the recursion relations for the “up” branch:

\[
Z^{(i,z)}_{0,u} = \prod_{j=1}^{k-1} \left( Z^{(j,z)}_{0,s} + Z^{(j,z)}_{1,s} \right) Z^{(i,z+1)}_{1,u}
\]

\[
Z^{(i,z)}_{0,u} = \prod_{j=1}^{k-1} \left( Z^{(j,z)}_{0,s} + Z^{(j,z)}_{1,s} \right) \overline{Z}^{(i,z+1)}_{0,u}
\]

(A2)

Finally for the “down” branch we have:

\[
Z^{(i,z)}_{0,d} = \prod_{j=1}^{k-1} \left( Z^{(j,z)}_{0,s} + Z^{(j,z)}_{1,s} \right) \left( Z^{(i,z-1)}_{0,d} + \overline{Z}^{(i,z-1)}_{0,d} \right)
\]

\[
Z^{(i,z)}_{0,d} = \prod_{j=1}^{k-1} \left( Z^{(j,z)}_{0,s} + Z^{(j,z)}_{1,s} \right) Z^{(i,z-1)}_{1,d}
\]

(A3)

\[
Z^{(i,z)}_{1,d} = e^{\beta (\mu - mg)} \prod_{j=1}^{k-1} Z^{(j,z)}_{0,s} \left( Z^{(i,z+1)}_{0,u} + Z^{(i,z+1)}_{0,u} \right)
\]

Note that in the case \( k = 1 \) the problem reduces to a simple one-dimensional chain: In this case the recursive method is equivalent to the transfer matrix method and gives the exact solution.

From the iterative solution of Eqs. (A1) it is possible to compute the system free energy. Generalizing the procedure followed in [11] we calculate the free energy density, \( F \), in the thermodynamic limit from the variation of the free energy going from a random graph with \( H \) layers and \( N \) sites on each layer to one with \( H \) layers and \( N + 2 \) sites on each layer. In order to do that we define the following intermediate object: a random graph with \( H \) layers and \( N \) sites in each plane such that \( 2(k+1) \) sites on each plane are connected only to \( k \) neighbors instead of \( k + 1 \). In particular on each layer 2 sites are not connected to sites on the higher layer (“down” branches), 2 sites are not connected to sites on the lower layer (“up” branches) and the other \( 2(k-1) \) are connected only with \( k-2 \) sites in the plane instead of \( k-1 \) (“side” branches). From this intermediate object a random graph with \( H \) layers and \( N + 2 \) sites on each layer (all connected to \( k+1 \) sites) can be obtained adding 2 new sites to each plane and connecting each of the new sites with \( k-1 \) side branches on their respective planes, one up branch in the upper layer and one down branch in the lower layer (see Fig. 12). This operation is called “site addition”. A random graph with \( H \) layers and \( N \) sites on each layer (all connected to \( k+1 \) sites) is instead obtained from the intermediate object adding for each layer 2 links between the up branches at height \( z \) and the down branches at height \( z-1 \), and \((k-1)\) links between the sides branches
on each layer (see Fig. 12). This operation, which allows to saturate all the missing links, is called “link addition”.

Therefore the variation of the free energy when going from $NH$ to $(N + 2)H$ sites (i.e. a random graph with two sites more on each layer) is related to the free energy shifts (see Fig. 12) for a site addition ($\Delta F_{site}^{(z)}$) and for two different kinds of link addition ($\Delta F_{link,1}^{(z)}$ and $\Delta F_{link,2}^{(z)}$):

$$F_{N+2} - F_N = 2 \sum_{z=1}^{H} \Delta F_{site}^{(z)} - (k - 1) \sum_{z=1}^{H} \Delta F_{link,2}^{(z)}$$

$$- 2 \sum_{z=1}^{H-1} \Delta F_{link,1}^{(z)},$$

where $F_{N+2} - F_N$ is obtained as $(F_{N+2} - F_0) - (F_N - F_0)$, and $F_0$ is the free energy of the intermediate object described above. We assume that in the thermodynamic limit the free energy is linear in $N$. The free energy density is then:

$$F = \sum_{z=1}^{H} \Delta F_{site}^{(z)} - \frac{(k - 1)}{2} \sum_{z=1}^{H} \Delta F_{link,2}^{(z)} - \sum_{z=1}^{H-1} \Delta F_{link,1}^{(z)}.$$  

(A5)

In terms of the local fields the free energy shifts due to the addition of a site $i$ at height $z$ reads:

$$e^{-\beta \Delta F_{site}^{(z)}} = \left[ \prod_{j=1}^{k-1} \left( 1 + e^{\beta h_{j}^{(i,z)}} \right) \right] \times \left( 1 + e^{\beta h_{u}^{(i,z)}} + e^{\beta h_{d}^{(i,z)}} e^{\beta h_{u}^{(i,z)}} \right) + e^{\beta (N-mg_{s})} \left( 1 + e^{\beta h_{(i,z)}} \right).$$  

(A6)

The free energy shift due to a link addition between a down branch with the root site at height $z$ and an up branch with the root site at height $z + 1$ is given by:

$$e^{-\beta \Delta F_{link,1}^{(z)}} = 1 + e^{\beta h_{d}^{(i,z)}} + e^{\beta h_{u}^{(i,z) + 1}} + e^{\beta h_{d}^{(i,z) + 1}} (1 + e^{\beta h_{u}^{(i,z) + 1}}).$$  

(A7)

Finally the free energy shift due to a link addition between two side branches with root sites $i$ and $j$ at height $z$ is:

$$e^{-\beta \Delta F_{link,2}^{(z)}} = 1 + e^{\beta h_{d}^{(i,z)}} + e^{\beta h_{d}^{(j,z)}}.$$  

(A8)

In order to compute the free energy of the system we have to compute the mean values of the free energy shifts for all the sites at a given height and for all the possible realization of the lattice. In the following these mean values will be computed in three different cases: 1) A fluid-like homogeneous phase; 2) A crystalline-like solution characterized by the break down of the horizontal translational invariance; 3) A glassy phase by a 1-step Replica Symmetry Breaking.

The fluid-like solution is obtained by setting that the local fields on each layer are the same for all sites of the layer ($\{h^{(i,z)} \} = \{h^{(z)} \}$ ∀$i$). In this case Eq.s (A4) become $5H - 1$ algebraic coupled equations and they are easily solved finding the fixed points. This homogeneous (Replica Symmetric) solution is characterized by horizontal translational invariance and is found to be stable for high values of the configurational temperature, $T_{conf}$, or for low values of the number of grains per unit surface, $N_{s}$. In this case the free energy is easily computed from Eq.s (A6), (A8) and (A9), since in this case all the quantities are site independent. From the free energy, $F$, we derive the density profile, $\sigma(z) \equiv \langle n_i(z) \rangle$:

$$\sigma(z) = \frac{e^{\beta (\mu - mg_{s})} \left( 1 + e^{\beta h_{u}^{(i,z)}} \right)}{e^{-\beta \Delta F_{site}^{(z)}},}$$  

(A9)

the number of particles per unit of surface, $N_s \equiv \sum_{z=1}^{H} \sigma(z)$, and the gravitational energy density, $E \equiv \sum_{z=1}^{H} mg_{s} \sigma(z)$. From the relation $F = E - TS - \mu N_s$, we also calculate the entropy per lattice site, $S = -\beta F - \beta \mu N_s + \beta E$.

In the crystalline (Replica Symmetric) solution the local fields are different on different sites (breakdown of translational invariance), but do not fluctuate from site to site. This is achieved by the introducing two sub-lattices, $a$ and $b$, and different local fields on each lattice. The merging is done taking into account the structure of the crystalline phase. In our case, each site of the sub-lattices $a$ (resp. $b$) is connected with $k + 1$ sites of the sub-lattice $b$ (resp. $a$). The crystal periodicity is thus two lattice spacings. Schematically Eq.s (A4) for each layer become:

$$\left\{ \{h_b \} = f(\beta, \mu, \{h_a \} \right\}$$

$$\left\{ \{h_a \} = f(\beta, \mu, \{h_b \} \right\}$$

FIG. 12: Site addition: a new central site at height $z$ is connected to $k - 1$ side branches (s) with the root sites in the same layer, to one up (u) branch with the root site in the higher layer and to one down (d) branch with the root site in the lower layer; Link addition (1): a link between a down branch with the root site at height $z$ and an up branch with the root site in the higher layer is added; Link addition (2): a link between two side branches with the root site in the same layer is added.
where \{h_{u}\} and \{h_{d}\} are the sets of all local fields respectively on the two sub-lattices. This is a system of \(2(5H-1)\) algebraic coupled equations. The free energy is computed from the fixed points of these equations. For a given \(N_s\), by lowering \(T_{conf}\), a phase transition from the fluid to the crystal is found at \(T_m\) (see Fig. B).

The fluid phase still exist below \(T_m\) as a metastable phase corresponding to a supercooled fluid when crystallization is avoided. Nevertheless, the entropy per site predicted by the fluid solution becomes negative when the temperature is lowered, or the packing fraction is increased. Hence, this solution is not appropriate to describe the high \(N_s\) or low \(T_{conf}\) region. A solution characterized by the presence of a large number of local minima of the free energy is found in this region. In this case the local fields may fluctuate. To describe this situation we have to introduce three probability distributions on each layer \(P^u_{i,z}(h_{u},g_{u}), P^s_{i,z}(h_{s}), P^d_{i,z}(h_{d},g_{d})\) defined as the probability of finding the fields \(h_{u,i,z}\) and \(g_{u,i,z}\) (or respectively \(h_{s,i,z}\), or \(h_{d,i,z} \) and \(g_{d,i,z}\) on site \(i\) at height \(z\) equal to \(h_{u}\) and \(g_{u}\) (or respectively to \(h_{s}\), or to \(h_{d}\) and \(g_{d}\)). 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 \(\{P^u_{i,z,d} \equiv P^u_{i,z,d}\}\).

Within the one-step Replica Symmetry Breaking ansatz of the cavity method (see appendix B) the recursion relations for the fields are replaced by self consistent integral equations for the probability distribution of the fields.

For the “up” merging the self consistent integral equation reads:

\[
P^u_{i,z}(h_{u},g_{u}) = C_1 \int \prod_{j=1}^{k-1} \left[ dh_{s,j,z} P^s_{j,z}(h_{s,j,z}) \right] \prod_{j=1}^{k-1} \left[ dh_{d,j,z+1} P^d_{j,z+1}(h_{u,j+1,z+1},g_{d,j+1,z+1}) \right] \delta(h_z-h_{u,i,z}) \delta(g_z-g_{u,i,z}) e^{-\beta m \Delta F_{up}(i,z)}, \tag{A10}
\]

where \(C_1\) is a constant insuring the normalization of \(P^u_{i,z}\), \(h_{u,i,z}\) and \(g_{u,i,z}\) are the local fields defined by Eqs. \[A1\], \(m \in [0,1]\) is the usual 1RSB parameter to be obtained by the maximization of the free energy with respect to it, and \(\Delta F_{up}\) is the free energy shift in the “up” merging process. This quantity is computed by using that the addition of a site \(i\) at a certain height \(z\) (“site addition”) is the result of an “up” merging process, which bring to a new “up” branch with root site \(i\), plus a link addition between this branch and a down branch at height \(z - 1\):

\[
\Delta F_{site}^{(i,z)} = \Delta F_{up}^{(i,z)} + \Delta F_{link,2}^{(i,z-1,z)} \tag{A11}
\]

From this equation we obtain that:

\[
e^{-\beta \Delta F_{up}^{(i,z)}} = \frac{Z_{0,u}^{(i,z)}}{Z_{0,u}^{(i,z+1)} \prod_{j=1}^{k-2} Z_{0,s}^{(j,z)}} \tag{A12}
\]

From Eqs. \[A11\] \[A3\] the free energy shift \(\Delta F_{up}^{(i,z)}\) has a simple expression in terms of the local fields.

In the same way we can determine the self consistency equations for the other two kinds of merging:

\[
P^s_{i,z}(h_{s},g_{s}) = C_2 \int \prod_{j=1}^{k-2} \left[ dh_{s,j,z} P^s_{j,z}(h_{s,j,z}) \right] \prod_{j=1}^{k-2} \left[ dh_{d,j,z+1} P^d_{j,z+1}(h_{u,j+1,z+1},g_{d,j+1,z+1}) \right] \delta(h_z-h_{s,i,z}) e^{-\beta m \Delta F_{side}(i,z)}, \tag{A13}
\]

and

\[
P^d_{i,z}(h_{d},g_{d}) = C_3 \int \prod_{j=1}^{k-1} \left[ dh_{s,j,z} P^s_{j,z}(h_{s,j,z}) \right] \prod_{j=1}^{k-1} \left[ dh_{d,j,z+1} P^d_{j,z+1}(h_{u,j+1,z+1},g_{d,j+1,z+1}) \right] \delta(h_z-h_{d,i,z}) \delta(g_z-g_{d,i,z}) e^{-\beta m \Delta F_{down}(i,z)}, \tag{A14}
\]

For the “side” and the “down” merging one has that:

\[
\Delta F_{site}^{(i,z)} = \Delta F_{side}^{(i,z)} + \Delta F_{link,1}^{(i,z,z+1)} \tag{A15}
\]

This yields to:

\[
e^{-\beta \Delta F_{side}^{(i,z)}} = \frac{Z_{0,u}^{(i,z+1)}}{Z_{0,u}^{(i,z)} \prod_{j=1}^{k-2} Z_{0,s}^{(j,z)}} \tag{A17}
\]

and

\[
e^{-\beta \Delta F_{down}^{(i,z)}} = \frac{Z_{0,d}^{(i,z+1)}}{Z_{0,d}^{(i,z)} \prod_{j=1}^{k-1} Z_{0,s}^{(j,z)}} \tag{A18}
\]

For any value of \(\beta, \mu\) and \(m\) we solve Eqs. \[A10\], \[A13\] and \[A14\] iteratively, discretizing the probability distributions until the whole procedure converged.

From the probability distributions we compute the free energy density of the system: according to Eq. \[A6\] we have to find the average values of the free energy shifts due to link and site additions. The free energy shift due to site addition is given by:

\[
\langle e^{-\beta m \Delta F_{site}(i,z)} \rangle = \int \prod_{j=1}^{k-1} \left[ dh_{s,j,z} P^s_{j,z}(h_{s,j,z}) \right] \prod_{j=1}^{k-1} \left[ dh_{d,j,z+1} P^d_{j,z+1}(h_{u,j+1,z+1},g_{d,j+1,z+1}) \right] \delta(h_z-h_{s,i,z}) \delta(g_z-g_{d,i,z}) e^{-\beta m \Delta F_{up}(i,z)}, \tag{A19}
\]
For the first kind of link addition we have:

\[
\langle e^{-\beta m \Delta F_{\text{link},1}^{(z)}} \rangle = \\
\int \left[ dh_d^{(i,z-1)} dg_d^{(i,z-1)} P_{z-1}^d(h_d^{(i,z-1)}, g_d^{(i,z-1)}) \right] \\
\times \left[ dh_u^{(i,z+1)} dg_u^{(i,z+1)} P_{z+1}^u(h_u^{(i,z+1)}, g_u^{(i,z+1)}) \right] \\
\times e^{-\beta m \Delta F_{\text{link},1}^{(i,z)}} .
\]  

(A20)

Finally for the second kind of link addition we find:

\[
\langle e^{-\beta m \Delta F_{\text{link},2}^{(z)}} \rangle = \prod_{j=1}^{2} \left[ dh_s^{(j,z)} P_s(h_s^{(j,z)}) \right] e^{-\beta m \Delta F_{\text{link},2}^{(j,z)}} .
\]  

(A21)

In the previous relations \(\Delta F_{\text{site}}(i, z)\), \(\Delta F_{\text{link},1}^{(i,z-1)}\) and \(\Delta F_{\text{link},2}^{(i,z)}\) are function of the local fields according to Eq. \(\text{A10}\), \(\text{A17}\) and \(\text{A15}\).

The total free energy density of the system is, according to Eq. \(\text{A17}\):

\[
F[m] = -\frac{1}{\beta m} \left[ \sum_{z=1}^{H} \log e^{-\beta m \Delta F_{\text{site}}^{(z)}} \right] \\
- \sum_{z=1}^{H} \frac{(k-1)}{2} \log e^{-\beta m \Delta F_{\text{link},2}^{(z)}} \\
- \sum_{z=1}^{H-1} \log e^{-\beta m \Delta F_{\text{link},1}^{(z)}} .
\]  

(A22)

The parameter \(m\) is fixed by the maximization of the free energy with respect to it. The justification for that is in the replica method, since \(m\) turns out to be the break point in Parisi’s order parameter function at the 1-step RSB level. For a spin glass it has been rigorously proved that in the limit \(k \to \infty\), \(F[m]\) is a lower bound to the correct free energy, so it is natural to find the preferred value of \(m\) by the maximization of \(F[m]\).

**APPENDIX B: SELF-CONSISTENCY EQUATIONS IN THE CAVITY METHOD**

In this appendix we show how to obtain the self-consistency integral equations \(\text{A10}\), \(\text{A13}\) and \(\text{A11}\) using the cavity method in the 1-step RSB ansatz \(\text{I1}\), \(\text{I2}\). The region at high packing fraction (or at low configurational temperature) is characterized by the existence of many pure states. Let \(\mathcal{N}(F)\) the number of pure states for a given value of the free energy of the system. The function \(\Sigma(F) = \log \mathcal{N}(F)\) is called complexity. We assume that within one pure states \(\alpha\) the local fields \(h_{u,\alpha}^{(i,z)}\), \(g_{u,\alpha}^{(i,z)}\), \(h_{d,\alpha}^{(i,z)}\) and \(g_{d,\alpha}^{(i,z)}\) on different cavity sites are uncorrelated. Therefore Eq.s \(\text{A10}\) continue to hold in any given pure state. In this case we have to make a statistical description of the solutions of Eq.s \(\text{A10}\) in the different pure states, taking into account the number of pure states for a given value of the free energy.

Let us consider, for example, the “up” merging of \(k\) cavity sites in a site \(i\) at height \(z\). As said before, in each pure state \(\alpha\) the local fields in the \(k\) cavity sites are not correlated. Nevertheless in each pure state \(\alpha\) the local fields, \(h_{u,\alpha}^{(i,z)}, g_{u,\alpha}^{(i,z)}\), and the free energy shift, \(\Delta F_{u,\alpha}^{(i,z)}\), due to the merging are correlated, since they are both functions of the local fields in the neighbor sites in the state \(\alpha\), according to Eq.s \(\text{A17}\) and \(\text{A11}\). Let us define \(S_z(h_u^z, g_u^z, \Delta F_u^z)\) as the probability distribution of finding the fields \((h_{u,\alpha}^{(i,z)}, g_{u,\alpha}^{(i,z)})\) and the free energy shift \(\Delta F_u^z\) after an up merging at height \(z\). Because of the recursion relations of Eq.s \(\text{A10}\) and \(\text{A11}\), this distribution probability has to verify the following iteration relation:

\[
S_z(h_u^z, g_u^z, \Delta F_u^z) = \int_{k=1}^{k-1} \left[ dh_s^{(j,z)} P_s(h_s^{(j,z)}) \right] e^{-\beta m \Delta F_{\text{link},2}^{(j,z)}} \\
\times \left[ dh_u^{(i,z+1)} dg_u^{(i,z+1)} \right] \\
\times P_{z+1}^u(h_u^{(i,z+1)}, g_u^{(i,z+1)}) \\
\times \delta(h_u^z - h_{u,\alpha}^{(i,z)}) \delta(g_u^z - g_{u,\alpha}^{(i,z)}) \\
\times \delta(\Delta F_u^z - \Delta F_{u,\alpha}^{(i,z)}).
\]  

(B1)

In order to determine the probability distribution for the local fields self-consistently we have to make the integration over all possible free energy shifts:

\[
P_z^u(h_u^z, g_u^z) = \int d(\Delta F_u^z) S_z(h_u^z, g_u^z, \Delta F_u^z) \mathcal{N}(F - \Delta F) \\
= \int d(\Delta F_u^z) S_z(h_u^z, g_u^z, \Delta F_u^z) e^{\Sigma(F - \Delta F_u^z)}.
\]  

Since we are interested only in the local minima with the lowest free energies, we expand the exponent to the first order in \(\Delta F_u^z\):

\[
P_z^u(h_u^z, g_u^z) = C_1 \int d(\Delta F_u^z) S_z(h_u^z, g_u^z, \Delta F_u^z) \exp(-\beta m \Delta F_u^z),
\]  

(B2)

where the parameter \(m \in [0, 1]\) is:

\[
m = \frac{1}{\beta} \frac{\partial \Sigma}{\partial F},
\]  

(B3)

and \(C_1\) is a normalization constant. Actually the first order expansion means that the density of pure states for a given value of the free energy is \(\mathcal{N} \approx \exp(m(F - F_{\text{ref}}))\), where \(F_{\text{ref}}\) is a reference free energy whose value is completely irrelevant. This form of the density of states is the same found in the 1-step RSB formulation.

By integrating over \(\Delta F_u^{(i,z)}\), the delta function selects only the right value of the free energy shift given in Eq. \(\text{A12}\). We thus have:

\[
P_z^u(h_u^z, g_u^z) = C_1 \prod_{j=1}^{k-1} \left[ dh_s^{(j,z)} P_s(h_s^{(j,z)}) \right] \\
\times \left[ dh_u^{(i,z+1)} dg_u^{(i,z+1)} \right] \\
\times P_{z+1}^u(h_u^{(i,z+1)}, g_u^{(i,z+1)}) \\
\times \delta(h_u^z - h_{u,\alpha}^{(i,z)}) \delta(g_u^z - g_{u,\alpha}^{(i,z)}) \\
\times \delta(\Delta F_u^z - \Delta F_{u,\alpha}^{(i,z)}).
\]  

(B4)
We have thus obtained the self consistency Eq. (A10). In the same way it is possible to obtain the equations for the “side” and the “down” merging.

[1] A. Coniglio and H.J. Herrmann, Physica A 225, 1 (1996); M. Nicodemi, A. Coniglio and H.J. Herrmann, Phys. Rev. E 55, 3962 (1997).
[2] A.J. Liu and S.R. Nagel, Nature 396, 21 (1998).
[3] C.S. O’Hern, S.A. Langer, A.J. Liu, S.R. Nagel, Phys. Rev. Lett. 86, 111 (2001).
[4] G. D’Anna and G. Gremaud, Nature 413, 407 (2001); G. D’Anna, P. Mayor, A. Barrat, V. Loreto, and F. Nori, Nature 424, 909 (2003).
[5] A. Mehta and J. Berg, Europhys. Lett. 56, 784 (2001).
[6] C.S. O’Hern, L.E. Silbert, A.J. Liu, S.R. Nagel, Phys. Rev. E 68, 011306 (2003).
[7] M. Nicodemi and A. Coniglio, Phys. Rev. Lett. 82, 916 (1999).
[8] M. Nicodemi, Phys. Rev. Lett. 82, 3734 (1999). A. Barrat, J. Kurchan, V. Loreto, and M. Sellitto, Phys. Rev. Lett. 85, 5034 (2000). J.J. Brey, A. Prados, B. Sánchez-Rey, Physica A 275, 310 (2000). D. S. Dean and A. Legevri, Phys. Rev. Lett. 86, 5639 (2001). H. A. Makse and J. Kurchan, Nature 415, 614 (2002). J. Berg, S. Franz and M. Sellitto, Eur. Phys. J. B 26, 349 (2002). G. De Smedt, C. Godreche, J.M. Luck, Eur. Phys. J. B 32, 215-225 (2003). G. Tarjus and P. Viot, Phys. Rev. E 69, 011307 (2004).
[9] A. Coniglio and M. Nicodemi, Physica A 296, 451 (2001). A. Fierro, M. Nicodemi and A. Coniglio, Europhys. Lett. 59, 642 (2002); Europhys. Lett. 60, 684 (2002); Phys. Rev. E 66, 061301 (2002).
[10] S.F. Edwards and R.B.S. Oakeshott, Physica A 157, 1080 (1989). A. Mehta and S.F. Edwards, Physica A 157, 1089 (1989). S.F. Edwards, in Current Trends in the physics of Materials, (Italian Phys. Soc., North Holland, Amsterdam, 1990).
[11] M. Mézard and G. Parisi, Eur. Phys. J. B 20, 217 (2001).
[12] G. Biroli and M. Mézard, Phys. Rev. Lett. 88, 025501 (2002).
[13] M. Piccamarra, M. Tarzia, A. de Candia, and A. Coniglio, Phys. Rev. E 67, 057105 (2003); Phys. Rev. E 68, 066111 (2003).
[14] L.F. Cugliandolo and J. Kurchan, Phys. Rev. Lett. 71, 173 (1993). J. Kurchan, cond-mat/9812347 and in “Jamming and Rheology”, A.J. Liu and S.R. Nagel Eds., Taylor and Francis, London (2001).
[15] M. Tarzia, A. de Candia, A. Fierro, M. Nicodemi and A. Coniglio, Europhys. Lett. 66, 531 (2004).
[16] P. Philippe and D. Bideau, Europhys. Lett. 60, 677 (2002).
[17] E. Clement and J. Rajchenbach, Europhys. Lett. 16, 133 (1991).
[18] M. Tarzia, A. Fierro, M. Nicodemi and A. Coniglio, Phys. Rev. Lett. 93, 198002 (2004).
[19] In the case of uniform density profile, i.e. $\sigma(z) = const.$, we have $\sigma(z) = \Phi$ (where $\Phi \equiv N/L^2(2(z) - 1)$) below the maximum height and zero above.
[20] C. Toninelli, G. Biroli, D. S. Fisher, Phys. Rev. Lett. 92, 185504 (2004).
[21] J.B. Knight, C. G. Fandrich, C. N. Lau, H. M. Jaeger, and S. R. Nagel, Phys. Rev. E 51, 3957 (1995). E. R. Nowak, J. B. Knight, E. Ben-Naim, H. M. Jaeger, and S.R. Nagel, Phys. Rev.E 57, 1971 (1998).
[22] We add a fully empty layer in $z = -1$ and a fully occupied layer in $z = 0$ in order to simulate the box bottom, and a fully empty layer in $z = L + 1$ to allow the particles to occupy the top of the box without violating the hard core interaction.
[23] W. Gotze, in Liquids, Freezing and Glass Transition, eds. J.P. Hansen, D. Levesque, and Zinn-Justin, Elsevier (1991). T. Franosch, M. Fuchs, W. Gotze, M.R. Mayr and A.P. Singh, Phys. Rev. E 55, 7153 (1997). M. Fuchs, W. Gotze and M. R. Mayr, Phys. Rev. E 58, 3384 (1998).
[24] The $\beta$-correlator predicted by the MCT is given by $\Phi(t) = f_c + g(t/t_\sigma)$, where $g(t/t_\sigma) \propto (t/t_\sigma)^{-\alpha}$ for $t_\sigma < t < t_\sigma$, and $g(t/t_\sigma) \propto -(t/t_\sigma)^\alpha$ for $t_\sigma < t < t_\sigma$.
[25] S. Franz, C. Donati, G. Parisi and S. C. Glotzer, Philos. Mag. B 79, 1827 (1999). C. Donati, S. Franz, S. C. Glotzer and G. Parisi, J. Non-cryst. Solids, 307, 215 (2002).
[26] S. C. Glotzer, V. N. Novikov, and T. B. Schrøder, J. Phys. Chem. B 112, 509 (2000).
[27] Interestingly this anomalous behavior seems to occur around the crossover temperature $T_D$ previously calculated. The origin of this behavior, also observed in molecular dynamics simulations of a usual glass former [26], is still unclear.
[28] We add an auxiliary layer at height $H + 1$ where all sites are empty in order to allow the particles to occupy the top of the box without violating the hard core interaction. For the first two layers, $z = 1, 2$, we assume that the particles are always mechanically stable in order to simulate the presence of the bottom of the box.