

SUPPLEMENTARY NOTE 1
EXACT SOLUTION OF HARD SPHERES IN THE LIMIT OF INFINITE DIMENSIONS

This supplementary note reviews the exact solution of a hard-sphere system in high dimensions, which is obtained through the replica method in the full replica symmetry breaking (fullRSB) scheme [1]. We sketch here the main logical steps that allow one to obtain the results presented in this work. A detailed derivation will be presented elsewhere.

General formulation

Within the general RFOT framework, the disordered glass states of a particle system are assumed to be metastable and long-lived. Their lifetime is indeed assumed to diverge in the mean-field $d \rightarrow \infty$ limit, where d is the spatial dimension. These glass states therefore need to be described through appropriate extensions of standard statistical mechanics, which in practice consists of using the replica method, density functional (or Thouless-Anderson-Palmer) methods, or dynamical methods (see Ref. [2] for a complete review). Although all of these approaches are conceptually equivalent, in this paper we use the replica method, which is technically the simplest by far. The reader might be confused by the fact that the replica method is usually introduced to average over quenched disorder [3], which is absent from the interaction potential of standard glass formers. As it has long been recognized [4, 5], the main technical problem in these systems is that the emergence of metastable glassy states is not associated with a clear pattern of symmetry breaking, hence an individual glass state cannot be selected through a properly defined symmetry breaking field. This problem can, however, be surmounted by introducing a random external field, which is sent to zero at the end of the computation. The presence of this external field breaks translational symmetry and selects one among the many possible glass states. Replicas are therefore needed to properly take into account the presence of this external random field [4, 5]. This idea has been turned into a concrete computational scheme that exploits the tools from standard liquid theory [6]. Although a full description of this construction is beyond the scope of the current work, some of us have recently written detailed reviews that the reader may find useful [7, 8].

The infinite dimensional limit

We now focus on a system of identical d -dimensional particles, interacting through the hard-sphere potential $v(x)$. Temperature is irrelevant for this system and can be set to one, without loss of generality. The starting point is the virial expansion for the entropy \mathcal{S} as a function of the density field of hard-sphere particles. Taking the high-dimensional limit allows us to retain only the first two terms of the virial series, as Frisch and Percus have shown [9]. Hence the entropy of the system is a functional of the density profile $\rho(x)$ (that expresses the density of particles at point x) given by

$$\mathcal{S}[\rho(x)] = \int d^d x \rho(x) [1 - \log \rho(x)] + \frac{1}{2} \int d^d x d^d y \rho(x) \rho(y) f(x - y), \quad (1)$$

where $f(x) = e^{-v(x)} - 1 = -\theta(D - |x|)$ is the Mayer function and D is the diameter of the hard spheres. The first term in this expression is the ideal gas contribution, while the second term is the second virial correction and represents the mean-field density-density interaction. The equilibrium entropy of the system is obtained by maximizing the entropy, i.e., by solving the stationarity equation $\delta\mathcal{S}/\delta\rho(x) = 0$. At low density, the system is in a homogeneous liquid phase and the solution is $\rho(x) = \rho$. As density increases the system undergoes a first-order phase transition to a crystalline phase, whose symmetry is only known in low dimensions. If crystallization is avoided, the system instead enters a metastable supersaturated liquid phase [10]. In three dimensions, particular care must be taken both in numerical simulations and in experiments to avoid the crystal phase [8], but in $d > 3$, crystal nucleation is dynamically suppressed [11, 12], enabling the study and characterization of amorphous states.

As discussed above, a well-established theoretical approach to study these amorphous states consists of coupling the system to a spatial external random field that destabilizes the crystal and favors glassy configurations [4, 5]. One is then left with the problem of studying m copies (or replicas) of the original system infinitesimally weakly coupled together. In other words, each particle in the original problem now becomes a ‘‘molecule’’ made by m identical ‘‘atoms’’, each atom being a copy of the original particle. This molecular liquid can be studied with the standard tools of liquid theory [6, 7]. In high dimensions, the Frisch-Percus argument [9] that we discussed above for the non-replicated system also applies to the replicated one [8]. The entropy of the replicated system (or molecular liquid)

then reads

$$\mathcal{S}[\rho(\bar{x})] = \int d\bar{x} \rho(\bar{x}) [1 - \log \rho(\bar{x})] + \frac{1}{2} \int d\bar{x} d\bar{y} \rho(\bar{x}) \rho(\bar{y}) f(\bar{x} - \bar{y}), \quad (2)$$

where $\rho(\bar{x})$ is the single molecule density field [7, 8] and is a function of m d -dimensional coordinates $\bar{x} = \{x_1 \dots x_m\}$ that describe the configuration of a single molecule. Again the two terms represent the ideal gas term and the mean-field density-density interaction, and the density field is determined by maximizing the entropy, i.e., by solving the stationarity equations $\delta\mathcal{S}/\delta\rho(\bar{x}) = 0$. The phase diagram can be obtained by changing the parameter m after analytically continuing the expression to non integer values, following the approach described in Refs. [5–8].

A crucial remark is that the molecular liquid remains translationally and rotationally invariant, because the random external field is eliminated through the introduction of replicas. Requiring that the density profile be translationally and rotationally invariant leaves us with a function $\rho(\bar{x})$ that can only depend on the scalar products $q_{ab} = u_a \cdot u_b$, where $x_a = X + u_a$ with $X = m^{-1} \sum_a x_a$ being the center of mass of all x_a . A detailed study of this problem provides two important results [13]: (i) the analytical expression for the replicated entropy in Eq. (2) in terms of the matrix \hat{q} of the scalar products of the displacement vectors u_a in the infinite dimension limit, (ii) the proof that the exact solution of the stationarity equation gives the same replicated entropy as that computed within a Gaussian approximation for $\rho(\bar{x})$.

Let us write down the replicated entropy that was obtained this way in Refs. [13, 14]. We also define the Gaussian ansatz for the density field

$$\rho(\bar{u}) = \frac{\rho m^{-d}}{(2\pi)^{(m-1)d/2} \det(\hat{A}^{(m,m)})^{d/2}} \exp \left[-\frac{1}{2} \sum_{a,b}^{1,m-1} \left(\hat{A}^{m,m} \right)_{ab}^{-1} u_a \cdot u_b \right], \quad (3)$$

where $\langle \hat{q} \rangle = d\hat{A}$. Note that because of translational invariance, $\sum_a u_a = 0$, hence $\sum_a q_{ab} = 0$ and $\sum_a A_{ab} = 0$. Hence, the matrix \hat{A} is not invertible and thus $\rho(\bar{u})$ only depends on $\hat{A}^{m,m}$, which is the matrix obtained from \hat{A} by eliminating the last column and the last row. The replicated entropy in terms of a rescaled matrix $\hat{\alpha} = \frac{d^2}{D^2} \hat{A}$ is given in Eq. (45) of Ref. [13] as

$$s[\hat{\alpha}] = \frac{\mathcal{S}[\hat{\alpha}]}{N} = 1 - \log \rho + d \log m + \frac{(m-1)d}{2} \log(2\pi e D^2/d^2) + \frac{d}{2} \log \det(\hat{\alpha}^{m,m}) - \frac{d}{2} \hat{\varphi} \mathcal{F}(2\hat{\alpha}), \quad (4)$$

where s is the replicated entropy per particle. We have also introduced a reduced packing fraction $\hat{\varphi} = 2^d \varphi/d$ that remains finite at the glass transition, even when $d \rightarrow \infty$. The function $\mathcal{F}(\hat{\nu})$ is defined as follows

$$\mathcal{F}(\hat{\nu}) = \lim_{n \rightarrow 0} \sum_{n_1, \dots, n_m: \sum_a n_a = n} \frac{n!}{n_1! \dots n_m!} \exp \left[-\frac{1}{2} \sum_{a=1}^m v_{aa} \frac{n_a}{n} + \frac{1}{2} \sum_{a,b}^m v_{ab} \frac{n_a n_b}{n^2} \right]. \quad (5)$$

The above expression for the entropy must be maximized with respect to the matrix $\hat{\alpha}$ and one can therefore study the stationarity equations $\delta s[\hat{\alpha}]/\delta \hat{\alpha} = 0$. By constraining the form of $\hat{\alpha}$ one can restrict the parameter space over which to search for a solution. The simplest ansatz assumes that $\hat{\alpha}$ is completely symmetric under replica exchange, i.e., $\alpha_{ab} = \frac{1}{2} \Delta (\delta_{ab} - 1/m)$, and thus only depends on a single parameter Δ . It can be shown [5, 7, 8] that this structure corresponds to the standard 1-step replica symmetry breaking (1RSB) computation for models with quenched disorder, which is precisely the structure assumed in the original RFOT scenario [15, 16]. The hard-sphere phase diagram obtained this way was reported in Ref. [8]. Starting from Eq. (4), however, Ref. [14] showed that this 1RSB solution is unstable in some regions of the pressure-density phase diagram.

FullRSB equations

In the present paper we discuss the results obtained by assuming a fullRSB structure for the matrix $\hat{\alpha}$ that solves the stationarity equations. A review of the fullRSB construction is given in Ref. [3]. FullRSB matrices form a closed algebra and can be parametrized by a function over the interval $[0, 1]$, as we discuss below. By analogy with spin glass models, the fullRSB structure is expected to provide the exact solution of the model when the 1RSB solution is unstable. The correctness of the fullRSB solution can be proven by studying its (marginal) stability. We have obtained indications of marginal stability (by studying the relevant eigenvalue and found that it is identically zero in the fullRSB phase), but we leave a full discussion, i.e., a computation of all eigenvalues, for future work.

In order to illustrate the fullRSB construction we introduce the fundamental object of our theoretical approach, that is, the matrix of mean-square displacements between atoms in a molecule defined by

$$\Delta_{ab} = \frac{d}{D^2} \langle (u_a - u_b)^2 \rangle = \alpha_{aa} + \alpha_{bb} - 2\alpha_{ab}. \quad (6)$$

This matrix is analogous to the overlap matrix of the replica solution of mean-field spin glasses [3]. Not only does it encode the order parameter of the system, but its structure also reflects how the free energy minima are organized [1, 3, 17]. The 1RSB ansatz consists of taking a replica symmetric matrix $\Delta_{ab} = \Delta$ for $a \neq b$, which corresponds to the replica symmetric form of $\hat{\alpha}$ discussed above. The connection with dynamics is as follows. Consider a particle trajectory $x_i(t)$ and define the mean-square displacement

$$\Delta(t) = \frac{1}{N} \sum_{i=1}^N |x_i(t) - x_i(0)|^2. \quad (7)$$

At the 1RSB level we then have

$$\lim_{t \rightarrow \infty} \Delta(t) = \Delta, \quad (8)$$

where $t \rightarrow \infty$ means that we take the limit of the mean-square displacement for times that are large compared to the microscopic timescale but no larger than the lifetime of the metastable state in which the dynamics is trapped.

The fullRSB solution can be constructed as a sequence of k RSB solutions in the limit where k diverges. The first step is a 2RSB solution. In this case we divide the values that can be assumed by the replica indexes a and b into m/m_1 groups each of them containing m_1 possible values. We pose that $\Delta_{ab} = \Delta_2$ if both a and b are in the same group and $\Delta_{ab} = \Delta_1$ otherwise. The 2RSB entropy can be obtained by plugging this ansatz in Eq. (4) and optimizing the result over Δ_1 and Δ_2 . In order to go beyond the 2RSB ansatz we can construct a 3RSB matrix by dividing each of the m/m_1 blocks into m_1/m_2 blocks each containing m_2 values and by saying that $\Delta_{ab} = \Delta_3$ if we are in the same sub block. Iterating this procedure constructs a k RSB solution. In the fullRSB limit, where $k \rightarrow \infty$, the matrix Δ_{ab} can be parametrized by a continuous function $\Delta(x)$ over the interval $x \in [m, 1]$. Roughly speaking, the ‘‘index’’ x (corresponding to the continuum limit of the m_1 indices) selects a given hierarchical level, associated to the hierarchical structure of the subbasins sketched in Fig. 1. The replicated entropy, which can then be written as a function of $\Delta(x)$, is given by

$$\mathcal{S}_{\text{fullRSB}} = -m \int_m^1 \frac{dx}{x^2} \log \left[\frac{x\Delta(x)}{m} + \int_x^1 dz \frac{\Delta(z)}{m} \right] - \hat{\varphi} e^{-\Delta(m)/2} \int_{-\infty}^{\infty} dh e^h [1 - e^{mf(m,h)}], \quad (9)$$

where the function f satisfies the equation

$$\frac{\partial f(x, h)}{\partial x} = \frac{1}{2} \dot{\Delta}(x) \left[\frac{\partial^2 f(x, h)}{\partial h^2} + x \left(\frac{\partial f(x, h)}{\partial h} \right)^2 \right], \quad (10)$$

with initial condition $f(1, h) = \log \left(\frac{1}{2} + \frac{1}{2} \text{erf} \left[\frac{h}{\sqrt{2\Delta(1)}} \right] \right)$. Note that Eq. (10) was first obtained by one of us in the solution of the Sherrington-Kirkpatrick model [1, 3] and is the key connection between hard spheres and spin glasses.

The expressions above give the replicated entropy within a fullRSB ansatz as a function of $\Delta(x)$. To obtain thermodynamic results, we must, however, optimize the function over $\Delta(x)$. To write (and solve numerically) the stationarity equations, it is convenient to introduce in Eqs. (9) and (10) a rescaled variable $y = x/m$ and a rescaled function $\hat{f}(y, h) = mf(x, h) = -\frac{h^2 \theta(-h)}{2\gamma(y)} + \hat{j}(y, h)$, and to introduce Lagrange multipliers $\hat{P}(y, h)$ and $\hat{P}(1/m, h)$ that enforce both the Parisi equation (Eq. (10)) and its initial condition. The final variational equations for the fullRSB

solution are

$$\begin{aligned}
\Delta(y) &= \frac{\gamma(y)}{y} - \int_y^{1/m} \frac{dz}{z^2} \gamma(z), \quad \Leftrightarrow \quad \gamma(y) = y\Delta(y) + \int_y^{1/m} dz \Delta(z), \\
\widehat{j}(1/m, h) &= m \log \left[\frac{1}{2} \left(1 + \operatorname{erf} \left(\frac{h}{\sqrt{2m\gamma(1/m)}} \right) \right) \right] + \frac{h^2 \theta(-h)}{2\gamma(1/m)}, \\
\frac{\partial \widehat{j}(y, h)}{\partial y} &= \frac{1}{2} \frac{\dot{\gamma}(y)}{y} \left[-\frac{\theta(-h)}{\gamma(y)} + \frac{\partial^2 \widehat{j}(y, h)}{\partial h^2} - 2y \frac{h\theta(-h)}{\gamma(y)} \frac{\partial \widehat{j}(y, h)}{\partial h} + y \left(\frac{\partial \widehat{j}(y, h)}{\partial h} \right)^2 \right], \\
\widehat{P}(1, h) &= e^{-\Delta(1)/2 - \frac{h^2 \theta(-h)}{2\gamma(1)} + \widehat{j}(1, h)}, \\
\frac{\partial \widehat{P}(y, h)}{\partial y} &= -\frac{1}{2} \frac{\dot{\gamma}(y)}{y} e^{-h} \left\{ \frac{\partial^2 [e^h \widehat{P}(y, h)]}{\partial h^2} - 2y \frac{\partial}{\partial h} \left[e^h \widehat{P}(y, h) \left(-\frac{h\theta(-h)}{\gamma(y)} + \frac{\partial \widehat{j}(y, h)}{\partial h} \right) \right] \right\}, \\
\kappa(y) &= \frac{\widehat{\varphi}}{2} \int_{-\infty}^{\infty} dh e^h \widehat{P}(y, h) \left(-\frac{h\theta(-h)}{\gamma(y)} + \widehat{j}'(y, h) \right)^2, \\
\frac{1}{\gamma(y)} &= y\kappa(y) - \int_1^y dz \kappa(z).
\end{aligned} \tag{11}$$

Here dots denote derivatives with respect to y and primes denote derivatives with respect to h . These equations can be solved numerically either by discretizing them on a grid, or by going to their corresponding finite k RSB iterative representation, that is

$$\begin{aligned}
\widehat{\Delta}_i &= \frac{\widehat{\gamma}_i}{y_i} + \sum_{j=i+1}^k \left(\frac{1}{y_j} - \frac{1}{y_{j-1}} \right) \widehat{\gamma}_j, \\
\widehat{j}(1/m, h) &= m \log \Theta \left(\frac{h}{\sqrt{2m\widehat{\gamma}_k}} \right) + \frac{h^2 \theta(-h)}{2\widehat{\gamma}_k}, \\
\widehat{j}(y_i, h) &= \frac{1}{y_i} \log \left[\int_{-\infty}^{\infty} dz K_{\widehat{\gamma}_i, \widehat{\gamma}_{i+1}, y_i}(h, z) e^{y_i \widehat{j}(y_{i+1}, z)} \right], \quad i = 1 \dots k-1, \\
\widehat{P}(y_1, h) &= e^{-\widehat{\Delta}_1/2 - \frac{h^2 \theta(-h)}{2\widehat{\gamma}_1} + \widehat{j}(y_1, h)}, \\
\widehat{P}(y_i, h) &= \int dz K_{\widehat{\gamma}_{i-1}, \widehat{\gamma}_i, y_{i-1}}(z, h) \widehat{P}(y_{i-1}, z) e^{z-h} e^{-y_{i-1} \widehat{j}(y_{i-1}, z) + y_{i-1} \widehat{j}(y_i, h)} \quad i = 2, \dots, k, \\
\widehat{\kappa}_i &= \frac{\widehat{\varphi}}{2} \int_{-\infty}^{\infty} dh e^h \widehat{P}(y_i, h) \left(-\frac{h\theta(-h)}{\widehat{\gamma}_i} + \widehat{j}'(y_i, h) \right)^2, \\
\frac{1}{\widehat{\gamma}_i} &= y_{i-1} \widehat{\kappa}_i - \sum_{j=1}^{i-1} (y_j - y_{j-1}) \widehat{\kappa}_j,
\end{aligned} \tag{12}$$

where

$$K_{\widehat{\gamma}, \widehat{\gamma}', y}(h, z) = \frac{\exp \left[-\frac{y}{2} \left(\frac{(z-h)^2}{\widehat{\gamma} - \widehat{\gamma}'} - \frac{h^2 \theta(-h)}{\widehat{\gamma}} + \frac{z^2 \theta(-z)}{\widehat{\gamma}'} \right) \right]}{\sqrt{2\pi(\widehat{\gamma} - \widehat{\gamma}')/y}}. \tag{13}$$

When k is sufficiently large, the results of the discrete k RSB equations should converge to the continuum fullRSB ones, which is the numerical strategy we employ here.

Numerical solution of the fullRSB equations, and the emergence of a scaling regime at large pressure

The fullRSB equations are formulated in terms of a function $\Delta(y)$ for $y = x/m \in [1, 1/m]$. It can be shown that the pressure associated with a given glass basin is $p \propto 1/m$ [8, 14], and therefore taking the limit $m \rightarrow 0$ corresponds to bringing the system to the jamming limit $p \rightarrow \infty$. In this limit the variable y extends over the range $[1, \infty)$.

To gain insights into the behavior of the fullRSB solution in the jamming limit, we numerically solve Eqs. (12). To simplify the numerical analysis, we fix $m = 0$ in the equation, while keeping a finite cutoff $y < y_{\max} \equiv 1/m$, as is obviously needed for numerical purposes. We indeed expect that the most important role of m , when $m \rightarrow 0$, is to fix the cutoff scale, the other contributions being but small perturbations in that limit. The results of this numerical computation are given in Fig. 3 of the main text. We observe two important effects. First, repeating the procedure for several values of k (recall that k is the number of RSB steps) reveals that the result does not depend on k when k is large. We find $k = 100$ to be a good choice and can be taken as representative of the fullRSB limit $k = \infty$. Second, when $y_{\max} = 1/m \rightarrow 0$, the solution converges to a limit curve and we observe that $\Delta(y) \sim y^{-1-c}$ when $y \rightarrow \infty$, with c close (but not equal) to 0.5. Note that from Eq. (11) one has $\dot{\gamma}(y) = y\dot{\Delta}(y)$ and therefore $\gamma(y \rightarrow \infty) \sim y^{-c}$.

The second observation is crucial for the subsequent analysis. Based on the results of the numerical solution of Eq. (12), we can look for an asymptotic scaling solution of the fullRSB equations (11) when $m = 0$ and $y \rightarrow \infty$ that has the form

$$\Delta(y) \sim \Delta_{\infty} y^{-1-c}, \quad (14)$$

$$\gamma(y) \sim \gamma_{\infty} y^{-c}, \quad (15)$$

$$\hat{j}(y, h) \sim -\frac{c}{2y} J(hy^b/\sqrt{\gamma_{\infty}}), \quad (16)$$

$$\hat{P}(y, h) \sim \begin{cases} y^c p_0(hy^c) & \text{for } h \sim -y^{-c}, \\ y^a p_1(hy^b) & \text{for } |h| \sim y^{-b}, \\ p_2(h) & \text{for } h \gg y^{-b}. \end{cases} \quad (17)$$

In the following, we define rescaled variables $z = hy^c$ and $t = hy^b/\sqrt{\gamma_{\infty}}$.

A comment on this scaling form is in order. The result for $\Delta(y)$ and $\gamma(y)$ has been motivated above. The form of $\hat{j}(y, h)$ can be guessed by first considering its asymptotic limits $h \rightarrow \pm\infty$, where, using Eq. (11) with Eq. (15), we can show that $\hat{j}(y, h \rightarrow -\infty) \sim -c/(2y)$ and that $\hat{j}(y, h \rightarrow \infty) = 0$. Then Eq. (16) is a natural guess, with a function $J(t)$ that goes from $J(t \rightarrow \infty) = 0$ to $J(t \rightarrow -\infty) = 1$ and varies on a scale y^b , that remains to be determined.

Motivating Eq. (17) is a bit harder and goes in three logical steps. First, the existence of three different scaling regimes is clearly visible in the numerical solution of Eq. (12). Second, the analysis of the continuum equation for $\hat{P}(y, h)$, under the assumption given in Eq. (15), allows one to prove the scalings associated to p_0 and p_2 in Eq. (17). This part of the analysis is technically involved and will be reported elsewhere. Third, the existence of a matching regime associated with p_1 is needed for consistency. The fact that exponent b is the same as the one for $\hat{j}(y, h)$ is a natural and simple choice that, as we will show, is consistent with the equations. The p_0 and p_1 regimes are matched by requiring that $p_0(z) \sim |z|^{\theta}$ for small z , and $p_1(z \rightarrow -\infty) \sim |z|^{\theta}$, with $\theta = \frac{c-a}{b-c}$ in such a way that the two power laws are matched. Similarly, matching the p_1 and p_2 regimes requires that $p_1(z \rightarrow \infty) \sim z^{-\alpha}$ with $\alpha = a/b$, and $p_2(h) \sim h^{-\alpha}$ for $h \rightarrow 0$. We therefore obtain information on the asymptotic behavior of the functions p_0, p_1, p_2 .

Analytical calculation of the exponents at jamming

The exponents a, b , and c can be now determined by inserting the scaling form given by Eqs. (14)-(17) in the fullRSB equations (11) in the limit $m \rightarrow 0$.

Plugging Eq. (15) and Eq. (16) into the equation for \hat{j} and taking the $y \rightarrow \infty$ limit, gives that a non trivial equation for the scaling function J exists if and only if $b = (1+c)/2$ and is given by

$$\frac{c}{2} J''(t) = -t J'(t) \left(\frac{1+c}{2} - c\theta(-t) \right) + J(t) - \theta(-t) + \frac{c^2}{4} J'(t)^2, \quad (18)$$

with the boundary conditions $J(-\infty) = 1$ and $J(\infty) = 0$. This equation admits a unique solution once the value of c has been fixed. This treatment thus provides a relation between b and c as well as an equation for $J(t)$.

We can now turn to the scaling of \hat{P} , focusing on the matching regime in Eq. (17), where $\hat{P}(y, h) \sim y^a p_1(hy^b)$. Plugging this asymptotic form in the equation for $\hat{P}(y, h)$ given in Eq. (11) and taking the $y \rightarrow \infty$ limit, we find once again that a non trivial result only exists for $b = (1+c)/2$. We can also write down an equation for the scaling function $p_1(t)$ that is given by

$$\frac{c}{2} p_1''(t) = (a - c\theta(-t)) p_1(t) + \left(\frac{1+c}{2} - c\theta(-t) \right) t p_1'(t) - \frac{c^2}{2} [p_1'(t) J'(t) + p_1(t) J''(t)]. \quad (19)$$

This equation is linear in p_1 and can be seen as an eigenvalue problem for a . We need to find the eigenfunction p_1 that behaves like $|t|^\theta$ when $t \rightarrow -\infty$ and like $t^{-\alpha}$ when $t \rightarrow \infty$, and is such that $p_1(t) > 0$. This eigenvalue problem admits a unique solution for a that depends on c through c itself and through $J(t)$. In this way at fixed c we can compute the other two exponents a and b , and the functions $J(t)$ and $p_1(t)$.

We last need to fix the value of c . A general consequence of the fullRSB equations is the following relation

$$1 = \frac{\widehat{\varphi}}{2} \int_{-\infty}^{\infty} dh e^h \widehat{P}(y, h) \widetilde{f}''(y, h)^2 \quad \widetilde{f}(y, h) = -\frac{h^2 \theta(-h)}{2} + \gamma(y) \widehat{j}(y, h), \quad (20)$$

which can be derived directly from Eq. (11) and is nothing but the mathematical statement of marginal stability of the fullRSB solution. By deriving this equation with respect to y , by using the fullRSB equations, and by plugging in the result for the scaling ansatz in the limit $y \rightarrow \infty$, we obtain the following relation

$$\frac{1}{2} = \frac{\int_{-\infty}^{\infty} dt p_1(t) [\theta(-t) + \frac{\epsilon}{2} J''(t)]^2 [\theta(t) - \frac{\epsilon}{2} J''(t)]}{\int_{-\infty}^{\infty} dt p_1(t) [\frac{d}{dt} (\theta(-t) + \frac{\epsilon}{2} J''(t))]^2}. \quad (21)$$

Because the right hand side is a function of c , this condition indeed fixes the value of c .

The equations above can be solved numerically with arbitrary precision to obtain the exponents a , b , and c and

$$\kappa = 1 + c, \quad \alpha = a/b, \quad \theta = \frac{c - a}{b - c}. \quad (22)$$

The results are

$$\begin{aligned} a &= 0.29213 \dots, & b &= 0.70787 \dots, & c &= 0.41574 \dots, \\ \alpha &= 0.41269 \dots, & \theta &= 0.42311 \dots, & \kappa &= 1.41574 \dots, \end{aligned} \quad (23)$$

where the precision is given by the last digit and depends on the cutoff used to discretize the asymptotic equations given in Eqs. (18), (19), and (23).

Pair correlation function and the Coulomb gap

We now show that the three critical exponents α , θ , and κ are connected to measurable quantities.

First, recall that $\Delta(y) \sim y^{-1-c} \sim y^{-\kappa}$ when y is large. Within the fullRSB solution, the value of $\Delta(y)$ associated with the largest y is the so-called Edwards-Anderson order parameter $\Delta_{\text{EA}} = \Delta(y_{\text{max}})$, which can be connected to the long-time limit of the mean-square displacement (7) in the glass by $\lim_{t \rightarrow \infty} \Delta(t) = \Delta_{\text{EA}}$. In other words, Δ_{EA} is the Debye-Waller factor. Recalling that $y_{\text{max}} = 1/m \propto p$, we conclude that $\Delta_{\text{EA}} \propto p^{-\kappa}$, i.e., that the Debye-Waller factor of the glass vanishes with pressure with the anomalous exponent κ , contrary to what happens in a hard-sphere crystal where $\Delta_{\text{EA}} \propto p^{-2}$.

Second, it is possible to show that the function $\widehat{P}(y, h)$ is connected to the pair correlation function of the glass, but the derivation is fairly long, thus details will be given elsewhere. For now, we note that the pair correlation function $g(r)$ is given, for $r = D(1 + h/d)$ and $d \rightarrow \infty$, by

$$g(h) = \theta(h) \int_{-\infty}^{\infty} dz e^{z-h} \gamma_{\Delta(1/m)}(h-z) \widehat{P}(1/m, z) e^{-mf(1/m, z)}, \quad (24)$$

where $\gamma_{\Delta}(x)$ is a centered and normalized Gaussian of width Δ . From this relation, one can show that the exponent α controls the power-law divergence of the pair correlation function upon approaching contact through the relation $g(h) \sim h^{-\alpha}$, as was numerically observed in several studies [18].

One can also show that $g(h)$ develops a delta peak for $h \propto 1/p$ upon approaching jamming. The integral of this peak gives that the number of contacts is equal to $2d$. Jammed packings are thus *predicted* to be isostatic. Note that Eq. (20), i.e., marginal stability, plays a crucial role in the derivation of isostaticity. Upon approaching jamming, the contact peak is described by a scaling function [8], which is basically the Laplace transform of $p_0(z)$. Hence the exponent θ enters in the scaling of the delta peak, and is connected to the probability distribution of inter-particle forces $P(f)$ [8, 19]. In this way one can show that for small f , $P(f) \sim f^\theta$.

The three exponents, α , θ , and κ are therefore connected to the scaling of measurable quantities by $\Delta_{\text{EA}}(p \rightarrow \infty) \sim p^{-\kappa}$, $g(h \rightarrow 0) \sim h^{-\alpha}$, $P(f \rightarrow 0) \sim f^\theta$, and are related to the exponents a , b , and c that enter in Eq. (17) by the three relations (22). Note that within numerical error we find that $a + b = 1$ (see Eq. (23)) even if at the moment we are not capable of deriving this relation analytically. Coupling the relation $a + b = 1$ with all the other scaling relations implies that $\alpha = 1/(2 + \theta)$, a scaling relation that was first derived in Ref. [20].

Fractal structure of the basins

The function $\Delta(y)$ can also be used to look directly at the structure of hierarchically organized states [3]. In the 1RSB picture of the glass transition, at the dynamical or mode-coupling transition point the liquid minimum of the free energy landscape breaks down into an exponential number of minima organized according to their free energy (here, internal entropy). From this landscape one can study the number of metastable states having internal entropy s

$$\mathcal{N}(s) = e^{N\Sigma(s)}, \quad (25)$$

where N is the size of the system. In the fullRSB picture the state structure is organized in a hierarchical way. Suppose that we are able to sample configurations from a given state a . We then introduce the mean-square distance between two of these configurations, labeled a and b , as $\Delta_{ab} = \frac{1}{N} \sum_{i=1}^N |x_i^{(a)} - x_i^{(b)}|^2$. To be more concrete, let us “lump” all of the states that are at a mutual distance that is less than Δ within a metabasin in which the total internal entropy is s . We can then try to determine how many of them there are, $\mathcal{N}(s, \Delta)$. In this way we obtain a coarse-grained description of the configurational entropy on the scale Δ defined by

$$\mathcal{N}(s, \Delta) = e^{N\Sigma(s, \Delta)}. \quad (26)$$

From this definition it follows that $\Sigma(s, \Delta(1)) = \Sigma_L(s)$, where $\Sigma_L(s)$ is the configurational entropy of the largest metabasin. The connection between $\Sigma(s, \Delta)$ and the mean-square displacement profile $\Delta(y)$ can be obtained as follows. We first highlight the dependence on m of the profile $\Delta(y; m)$, and we introduce the inverse function $y(\Delta; m)$. The standard 1RSB expression that relates the configurational entropy of metabasins having internal entropy s to Δ is then given by

$$my(\Delta(1; m); m) = m = \frac{\partial \Sigma(s, \Delta(1; m))}{\partial s} = \frac{\partial \Sigma_L(s)}{\partial s}, \quad (27)$$

where we have used the fact that $y(\Delta(1; m); m) = 1$. This relation holds for the most coarse-grained version of the configurational entropy. If we reduce the coarse graining on states we have on a fixed scale Δ , then we obtain

$$my(\Delta, m) = \frac{\partial \Sigma(s, \Delta)}{\partial s}. \quad (28)$$

Equation (27) relates m to the total internal entropy s of the metabasins we are looking for, on a fixed scale of metabasin width Δ .

It can be shown that at equilibrium the metabasins entropies on a scale Δ are *independent random variables* distributed according to $\mathcal{P}_\Delta(s) \propto e^{my(\Delta; m)s}$ [3, 17], and therefore the typical value of s on a scale Δ is $s_{\text{typ}}(\Delta) \propto 1/y(\Delta)$. From this result it follows that close to jamming, there is a large region of (small) Δ , where $y(\Delta) \sim \Delta^{1/\kappa}$. In this region, when increasing Δ from the smallest Δ_{EA} to the larger values, one finds that the total basin size grows as $s_{\text{typ}}(\Delta) \sim 1/y(\Delta) \sim \Delta^{1/\kappa} \sim \sqrt{\Delta}^{2/\kappa}$ (recalling that Δ is the squared distance between configurations). Hence the basins in phase space form a fractal with dimension $2/\kappa = 1.41267 \dots$.

Out-of-equilibrium dynamics

Following a quench from high temperature or, in the case of hard spheres, from low pressure, at initial time $t = 0$, a macroscopic system relaxes without reaching equilibrium. During this process, the two-time correlation function

$$\Delta(t, t_w) = \frac{1}{N} \sum_{i=1}^N |x_i(t) - x_i(t_w)|^2 \quad (29)$$

never becomes a function of $(t - t_w)$, where t_w is the waiting time after the quench. Instead, relaxation becomes progressively slower as t_w becomes larger, i.e., as the system *ages*. Rather surprisingly, one may infer from a static calculation some features of the out-of-equilibrium dynamics. This result follows from two different facts:

(i) The constant pressure dynamics relaxes up to a density at which the free energy landscape disconnects into separate basins. This *threshold* level [21] is also the one at which the basins lose their stability and become marginal.

(ii) At long times, the almost-stable states visited by the dynamics are sampled with equal probability. This property emerges in the mean-field out-of-equilibrium solution [21, 22], of which there is no clear general explanation yet.

If we compute the function $\Delta(y)$ with the value of m fixed not by maximizing the free energy (minimizing the entropy)

as in the equilibrium computation, but rather by demanding that for $m = m_{\text{th}}$ the stability of the solution be marginal (the replicon associated with the largest value of Δ in the Parisi ansatz vanishes), it may be shown that properties *i*) and *ii*) imply that the values of pressure, free energy, and other thermodynamic properties coincide with the asymptotic properties obtained from the dynamics. The fluctuation-dissipation ratio is then given by $m_{\text{th}}y(\Delta; m_{\text{th}})$, when the time-dependent mean-square displacement is $\Delta(t, t_w) = \Delta$ [22].

SUPPLEMENTARY NOTE 2 MOLECULAR DYNAMICS SIMULATIONS

Molecular dynamics simulations of $N=8000$ identical hard spheres in $d=3, 4, 6,$ and 8 evolving in a cubic box under periodic boundary conditions are performed using a modified version of the event-driven code described in Refs. [11, 18]. Hard spheres of unit diameter D and unit mass m naturally express time t in units of $\sqrt{\beta m D^2}$ at fixed unit inverse temperature β . Glasses are obtained from compressing very low-density fluids using a Lubachevski-Stillinger algorithm with, in $d > 3$, a slow particle growth rate of $\dot{\gamma} = 3 \times 10^{-4}$ [11]. Slow compaction of the fluid makes it fall out of equilibrium near the dynamical transition and evolves the resulting glass arbitrarily close to jamming, approximating an adiabatic state following [18]. In $d=3$, a rapid initial growth with $\dot{\gamma} = 3 \times 10^{-2}$, in order to prevent crystal formation [18], is followed by the slower growth rate once the system is well within the glass, i.e., $p \gtrsim 10^3$.

Using these glass configurations as starting point for fixed-density simulations, the mean-square displacement $\Delta(t) = \frac{1}{N} \sum_i \langle |x_i(t) - x_i(0)|^2 \rangle$ is obtained (Fig. 3(b) from the main text). Rattlers, which are identified by compressing each glass up to $p = 10^{10}$ [18] and identifying particles with fewer than $d+1$ force contacts, i.e., with pair distances that are smaller than $D + 100/p$, are removed from the averaging. The long-time plateau then gives $\lim_{t \rightarrow \infty} \Delta(t)/d = \Delta_{\text{EA}}$, where the Debye-Waller factor Δ_{EA} estimates the average cage size in the glass.

In order to capture the state structure upon approaching jamming, we track the evolution of the overlap of the underlying force network $\langle f_{ij}^{(a)} f_{ij}^{(b)} \rangle$ for glasses at different pressures. The force network is obtained by performing pairwise comparisons between 100 configurations (*a* and *b*) that evolve from a glass initially obtained as described above. This configuration then undergoes a molecular dynamics simulation sufficiently long for the initial positions to decorrelate, but while staying within the same glass state, i.e., for their mean-square displacement to reach the plateau height of the Debye-Waller factor. Each of the configurations is then independently compressed to $p = 10^{10}$ at $\dot{\gamma} = 3 \times 10^{-4}$. At that pressure a very large fraction of the force network is already defined. Then if particles *i* and *j* are within a distance $D + 100/p$ from each other they are considered to be part of the force network and hence $f_{ij} = 1$; for all other pairs of particles $f_{ij} = 0$. Rattlers in configurations *a* and *b* are removed from the analysis. Note that the results from Fig. 3(a) are qualitatively insensitive to the choice of cutoff as long as it is near the crossover between weak contacts and quasi-contacts [18].

SUPPLEMENTARY REFERENCES

- [1] Giorgio Parisi, “Order parameter for spin-glasses,” *Physical Review Letters* **50**, 1946–1948 (1983).
- [2] Tommaso Castellani and Andrea Cavagna, “Spin glass theory for pedestrians,” *Journal of Statistical Mechanics: Theory and Experiment* **2005**, P05012 (2005).
- [3] M. Mézard, G. Parisi, and M. A. Virasoro, *Spin glass theory and beyond* (World Scientific, Singapore, 1987).
- [4] T. R. Kirkpatrick and D. Thirumalai, “Comparison between dynamical theories and metastable states in regular and glassy mean-field spin models with underlying first-order-like phase transitions,” *Phys. Rev. A* **37**, 4439–4448 (1988).
- [5] Rémi Monasson, “Structural glass transition and the entropy of the metastable states,” *Phys. Rev. Lett.* **75**, 2847–2850 (1995).
- [6] M. Mézard and G. Parisi, “A tentative replica study of the glass transition,” *Journal of Physics A: Mathematical and General* **29**, 6515–6524 (1996).
- [7] M. Mezard and G. Parisi, “Glasses and replicas,” in *Structural Glasses and Supercooled Liquids: Theory, Experiment and Applications*, edited by P.G.Wolynes and V.Lubchenko (Wiley & Sons, 2012).
- [8] Giorgio Parisi and Francesco Zamponi, “Mean-field theory of hard sphere glasses and jamming,” *Rev. Mod. Phys.* **82**, 789–845 (2010).
- [9] H. L. Frisch and J. K. Percus, “High dimensionality as an organizing device for classical fluids,” *Phys. Rev. E* **60**, 2942–2948 (1999).
- [10] A. Cavagna, “Supercooled liquids for pedestrians,” *Physics Reports* **476**, 51–124 (2009).
- [11] Monica Skoge, Aleksandar Donev, Frank H. Stillinger, and Salvatore Torquato, “Packing hyperspheres in high-dimensional Euclidean spaces,” *Phys. Rev. E* **74**, 041127 (2006).
- [12] Patrick Charbonneau, Atsushi Ikeda, Giorgio Parisi, and Francesco Zamponi, “Glass transition and random close packing above three dimensions,” *Phys. Rev. Lett.* **107**, 185702 (2011).

- [13] J. Kurchan, G. Parisi, and F. Zamponi, “Exact theory of dense amorphous hard spheres in high dimension. I. the free energy,” *Journal of Statistical Mechanics: Theory and Experiment* **2012**, P10012 (2012).
- [14] Jorge Kurchan, Giorgio Parisi, Pierfrancesco Urbani, and Francesco Zamponi, “Exact theory of dense amorphous hard spheres in high dimension. II. The high density regime and the gardner transition,” *J. Phys. Chem. B* **117**, 12979–12994 (2013).
- [15] T. R. Kirkpatrick and P. G. Wolynes, “Stable and metastable states in mean-field Potts and structural glasses,” *Phys. Rev. B* **36**, 8552–8564 (1987).
- [16] T. R. Kirkpatrick and D. Thirumalai, “Dynamics of the structural glass transition and the p -spin-interaction spin-glass model,” *Phys. Rev. Lett.* **58**, 2091–2094 (1987).
- [17] M Mézard, G Parisi, N Sourlas, G Toulouse, and M Virasoro, “Nature of the spin-glass phase,” *Physical Review Letters* **52**, 1156–1159 (1984).
- [18] Patrick Charbonneau, Eric I. Corwin, Giorgio Parisi, and Francesco Zamponi, “Universal microstructure and mechanical stability of jammed packings,” *Phys. Rev. Lett.* **109**, 205501 (2012).
- [19] Aleksandar Donev, Salvatore Torquato, and Frank H. Stillinger, “Pair correlation function characteristics of nearly jammed disordered and ordered hard-sphere packings,” *Physical Review E* **71**, 011105 (2005).
- [20] Matthieu Wyart, “Marginal stability constrains force and pair distributions at random close packing,” *Phys. Rev. Lett.* **109**, 125502 (2012).
- [21] L. F. Cugliandolo and J. Kurchan, “Analytical solution of the off-equilibrium dynamics of a long-range spin-glass model,” *Phys. Rev. Lett.* **71**, 173–176 (1993).
- [22] L. F. Cugliandolo and J. Kurchan, “On the out-of-equilibrium relaxation of the Sherrington–Kirkpatrick model,” *Journal of Physics A: Mathematical and General* **27**, 5749–5772 (1994).