

Numerical test of the Edwards conjecture shows that all packings are equally probable at jamming

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In the late 1980s, Sam Edwards proposed a possible statistical-mechanical framework to describe the properties of disordered granular materials¹. A key assumption underlying the theory was that all jammed packings are equally likely. In the intervening years it has never been possible to test this bold hypothesis directly. Here we present simulations that provide direct evidence that at the unjamming point, all packings of soft repulsive particles are equally likely, even though generically, jammed packings are not. Typically, jammed granular systems are observed precisely at the unjamming point since grains are not very compressible. Our results therefore support Edwards' original conjecture. We also present evidence that at unjamming the configurational entropy of the system is maximal.

In science, most breakthroughs cannot be derived from known physical laws: they are based on inspired conjectures². Comparison with experiment of the predictions based on such a hypothesis allows us to eliminate conjectures that are clearly wrong. However, there is a distinction between testing the consequences of a conjecture and testing the conjecture itself. A case in point is Edwards' theory of granular media. In the late 1980s, Edwards and Oakeshott¹ proposed that many of the physical properties of granular materials ('powders') could be predicted using a theoretical framework that was based on the assumption that all distinct packings of such a material are equally likely to be observed. The logarithm of the number of such packings was postulated to play the same role as entropy does in Gibbs' statistical-mechanical description of the thermodynamic properties of equilibrium systems. However, statistical-mechanical entropy and granular entropy are very different objects. Until now, the validity of Edwards' hypothesis could not be tested directly—mainly because the number of packings involved is so large that direct enumeration is utterly infeasible—and, as a consequence, the debate about the Edwards hypothesis has focused on its consequences, rather than on its assumptions. Here we present results that show that now, at last, it is possible to test Edwards' hypothesis directly by numerical simulation. To our own surprise, we find that the hypothesis appears to be correct precisely at the point where a powder is just at the (un)jamming threshold. However, at higher densities, the hypothesis fails. At the unjamming transition, the configurational entropy of jammed states appears to be at a maximum.

The concept of 'ensembles' plays a key role in equilibrium statistical mechanics, as developed by J. Willard Gibbs, well over a century ago³. The crucial assumption that Gibbs made to arrive at a tractable theoretical framework to describe the equilibrium properties of gases, liquid and solids was that, at a fixed total energy, every state of the system is equally likely to be observed. The distinction between, say, a liquid at thermal equilibrium and a granular material is that in a liquid, atoms undergo thermal motion whereas in a granular medium (in the absence of outside perturbations)

the system is trapped in one of (very) many local potential energy minima. Gibbsian statistical mechanics cannot be used to describe such a system. The great insight of Edwards was to propose that the collection of all stable packings of a fixed number of particles in a fixed volume might also play the role of an 'ensemble' and that a statistical mechanics-like formalism would result if one assumed that all such packings were equally likely to be observed, once the system had settled into a mechanically stable 'jammed' state. The nature of this ensemble has been the focus of many studies^{1,4–6}.

Jamming is ubiquitous and occurs in materials of practical importance, such as foams, colloids and grains when they solidify in the absence of thermal fluctuations. Decompressing such a solid to the point where it can no longer achieve mechanical equilibrium leads to unjamming. Studies of the unjamming transition in systems of particles interacting via soft, repulsive potentials have shown that this transition is characterized by power-law scaling of many physical properties^{7–12}. However, the exact nature of both the ensemble of jammed states and the unjamming transition remains unclear.

Here, we report a direct test of the Edwards conjecture, using a numerical scheme for computing basin volumes of distinct jammed states (energy minima) of N polydisperse, frictionless discs held at a constant packing fraction ϕ . Uniquely, our numerical scheme allows us to compute Ω , the number of distinct jammed states, and the individual probabilities $p_{i \in \{1, \dots, \Omega\}}$ of each observed packing to occur. Figure 1a shows a snapshot of a section of the system, consisting of particles with a hard core and a soft shell. We obtain jammed packings by equilibrating a hard-disc fluid and inflating the particles instantaneously to obtain the desired soft-disc volume fractions (ϕ), followed by energy minimization (see Methods). The minimization procedure finds individual stable packings with a probability p_i proportional to the volume v_i of their basin of attraction. Averages computed using this procedure, represented by $\langle \dots \rangle_B$, would then lead to a bias originating from the different v_i values. Recent advances in numerical methods^{13–16} have now enabled direct computation of v_i , and therefore, an unbiased characterization of the phase space. A summary of the technique is provided in the Methods.

We report a detailed analysis of the distribution of v_i for a fixed number of discs $N = 64$ (all maximum system sizes in our study were set by the current limits on computing power). We compute v_i using a thermodynamic integration scheme^{13–16}, and compute the average basin volume $\langle v \rangle(\phi)$. The number of jammed states is, explicitly, $\Omega(\phi) = V_J(\phi)/\langle v \rangle(\phi)$, where $V_J(\phi)$ is the total available phase-space volume at a given ϕ . A convenient way to check equiprobability is to compare the Boltzmann entropy $S_B = \ln \Omega - \ln N!$, which counts all packings with the same weight, and the Gibbs entropy $S_G = -\sum_i p_i \ln p_i - \ln N!$ (refs 17–19). The Gibbs entropy satisfies $S_G \leq S_B$, saturating the bound when all p_i are equal: $p_{i \in \{1, \dots, \Omega\}} = 1/\Omega$. As shown in Fig. 2a, S_G approaches

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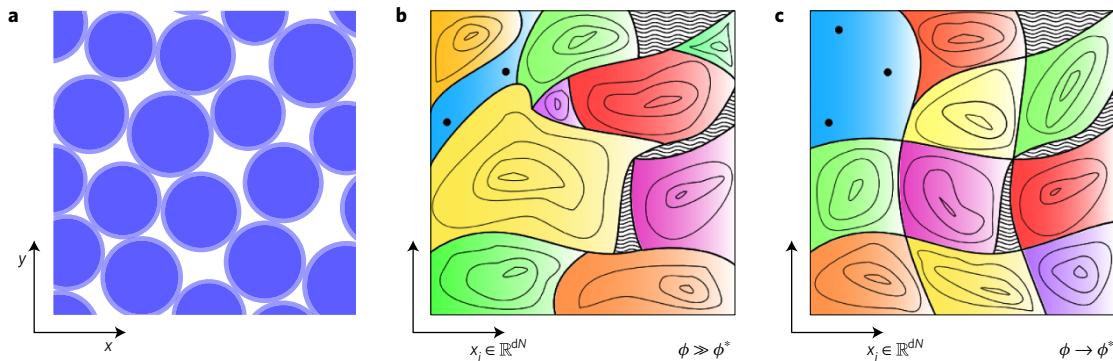


Figure 1 | Snapshot of the system studied and illustration of the associated energy landscape at different volume fractions. **a**, Snapshot of a jammed packing of discs with a hard core (dark shaded regions) plus soft repulsive corona (light shaded regions). **b,c**, Illustration of configurational space for jammed packings. The hatched regions are inaccessible due to hard-core overlaps. Single-coloured regions with contour lines represent the basins of attraction of distinct minima. The dark blue region with solid dots indicates the coexisting unjammed fluid region and hypothetical marginally stable packings, respectively. The volume occupied by the fluid V_{unj} is significant only for finite-size systems at or near unjamming. When $\phi \gg \phi^*$ (**b**) the distribution of basin volumes is broad but as $\phi \rightarrow \phi^*$ (**c**) the distribution of basin volumes approaches a delta function satisfying Edwards' hypothesis.

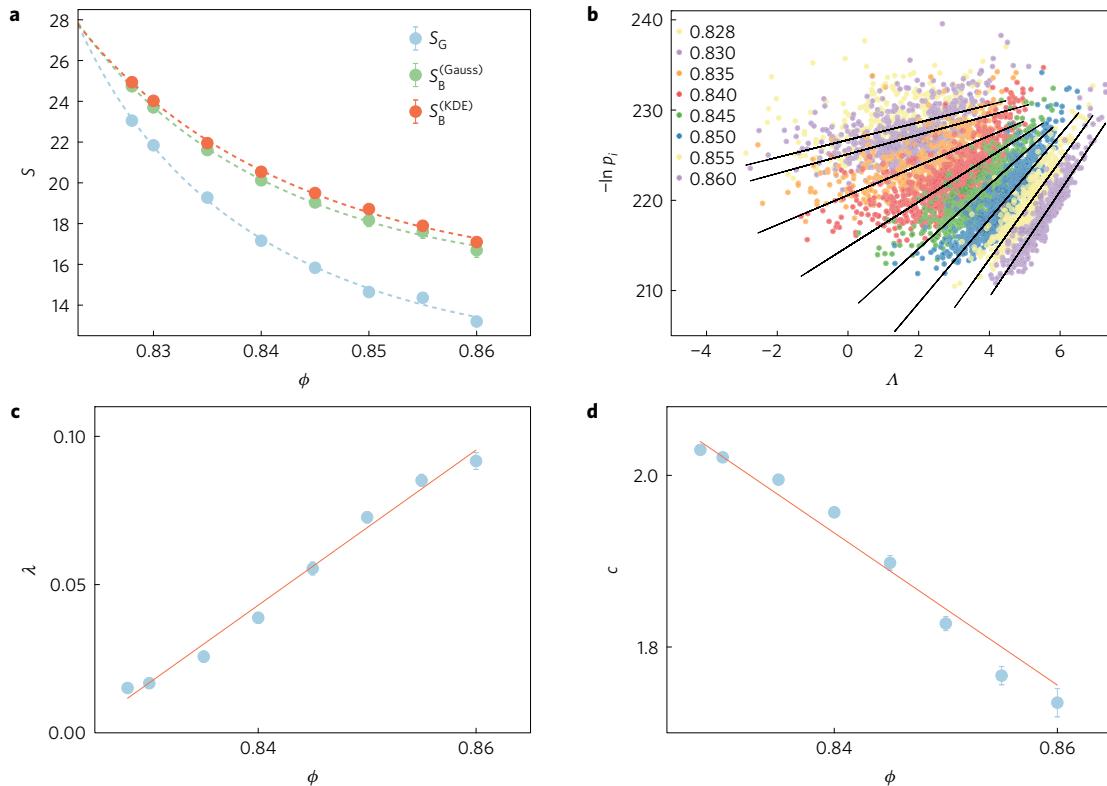


Figure 2 | Numerical results obtained by basin-volume calculations for jammed packings of $N=64$ discs with a hard core and a soft shell. **a**, Gibbs entropy S_G and Boltzmann entropy S_B as a function of volume fraction. S_B is computed both parametrically by fitting $B(f)$ with a generalized Gaussian function (Gauss) and non-parametrically by computing a kernel density estimate (KDE) as in ref. 13. The dashed curves are a second-order polynomial fit. **b**, Scatter plot of the negative log-probability of observing a packing, $-\ln p_i = F_i + \ln V_j(\phi)$, where V_j is the accessible fraction of phase space (see Methods) as a function of log-pressure, Λ . The black solid lines are lines of best fit computed by linear minimum mean square error using a robust covariance estimator and bootstrap (see Methods). **c,d**, Slopes $\lambda(\phi)$ (**c**) and intercepts $c(\phi)$ (**d**) of linear fits for equation (16). Solid lines are lines of best fit and error bars refer to the standard error computed by bootstrap²⁸.

S_B from below as $\phi \rightarrow \phi_{N=64}^{*(S)} \approx 0.82$. Fig. 1b,c schematically illustrates the evolution of the basin volumes as the packing fraction is reduced.

To characterize the distribution of basin volumes, we analyse the statistics of v_i along with the pressure P_i of each packing. It is convenient to study $F_i \equiv -\ln v_i$ as a function of $\Lambda_i \equiv \ln P_i$. As shown in Fig. 2b, we observe a strong correlation between F_i and Λ_i , which we quantify by fitting the data to a bivariate Gaussian distribution. The conditional expectation of F given Λ then yields a linear rela-

tionship (denoted by solid lines in Fig. 2b) such that $\langle F \rangle_B(\phi; \Lambda) \propto \lambda(\phi) \Lambda$, where $\langle F \rangle_B(\phi; \Lambda)$ represents the average over all basins at a given Λ . Previous studies at higher packing fractions¹³ indicate that this relationship is preserved in the thermodynamic limit. Defining $f = F/N$, we have (see Methods for details)

$$\begin{aligned} \langle f \rangle_B(\phi; \Lambda) &= \lambda(\phi) \Lambda + c(\phi) \\ &= \lambda(\phi) \Delta \Lambda + \langle f \rangle_B(\phi) \end{aligned} \quad (1)$$

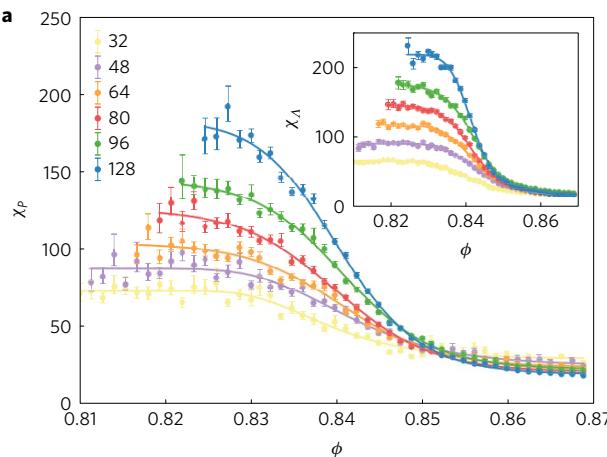


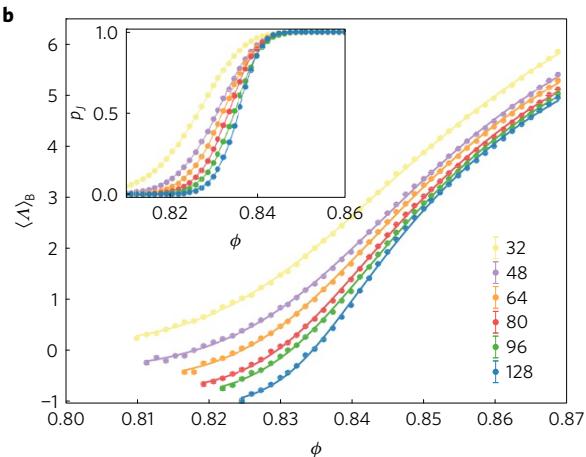
Figure 3 | Finite-size scaling analysis. **a**, $\chi_P \equiv N\sigma^2(P/\langle P \rangle_B)$ and (inset) $\chi_A \equiv N\sigma_A^2$, plotted as a function of volume fraction ϕ . By finite-size scaling (see Supplementary Information) we show that the curves diverge in the thermodynamic limit as $\phi \rightarrow \phi^{*(A)}$, implying $\phi_{N \rightarrow \infty}^* = \phi_{N \rightarrow \infty} = 0.841(3)$ (see main text for discussion). For $\phi \gg \phi_N^*$, χ_P approaches a constant value indicating the absence of extensive correlations far from the transition. **b**, Observed average log-pressure $\langle \Lambda \rangle_B$ and (inset) probability of obtaining jammed packings by our protocol, as a function of volume fraction ϕ . By finite-size scaling (see Supplementary Information) we show that $\langle \Lambda \rangle_B \rightarrow -\infty$ as $\phi \rightarrow \phi_{N \rightarrow \infty}^{*(\Lambda)} = 0.841(3)$ and p_j collapses for $\phi \rightarrow \phi_{N \rightarrow \infty}^{*(p_j)} = 0.844(2)$, thus locating the unjamming point. Error bars, computed by BCa bootstrap²⁹, refer to 1σ confidence intervals. The solid lines are generalized sigmoid fits of the form $f(\phi) = a - (a - b)/(1 + \exp(-w\Delta\phi))^{1/u}$. We show only values of ϕ where the probability of finding a jammed packing is at least 1%, so that the observables are computed over sufficiently large sample sizes.

where $\Delta \Lambda = \Lambda - \langle \Lambda \rangle_B(\phi)$. For Edwards' hypothesis to be valid, we require that in the thermodynamic limit: the distribution of volumes approaches a Dirac delta, which follows immediately from the fact that the variance $\sigma_f^2 \sim 1/N$ (ref. 15) (see Supplementary Information); and F_i needs to be independent of Λ_i , as well as of all other structural observables (see Supplementary Information), and therefore $\lambda(\phi)$ must necessarily vanish. As can be seen from Fig. 2c,d, within the range of volume fractions studied, $\lambda(\phi)$ decreases but saturates to a minimum as $\phi \rightarrow \phi_{N=64}^{*(\lambda)}$. We argue below that the saturation is a finite-size effect. An extrapolation using the linear regime in Fig. 2c indicates that $\lambda \rightarrow 0$ at packing fraction $\phi_{N=64}^{*(\lambda)} = 0.82 \pm 0.07$, remarkably close to where our extrapolation yields $S_G = S_B$. The analysis of basin volumes, therefore, strongly suggests that equiprobability is approached only at a characteristic packing fraction and that the vanishing of $\lambda(\phi)$ can be used to estimate the point of equiprobability.

We next show that $\lambda(\phi)$ does indeed tend to zero in the thermodynamic limit. We use the fluctuations σ_f^2 , σ_Λ^2 , and the covariance $\sigma_{f,\Lambda}^2$, obtained from the elements of the covariance matrix $\hat{\sigma} = ((\sigma_f^2, \sigma_{f,\Lambda}^2), (\sigma_{f,\Lambda}^2, \sigma_\Lambda^2))$ of the joint distribution of f and Λ (see Methods for details), to define λ and c as:

$$\begin{aligned} \lambda(\phi) &\equiv \frac{\sigma_{f,\Lambda}^2(\phi)}{\sigma_\Lambda^2(\phi)} \\ c(\phi) &\equiv \langle f \rangle_B(\phi) - \frac{\sigma_{f,\Lambda}^2(\phi)}{\sigma_\Lambda^2(\phi)} \langle \Lambda \rangle_B(\phi) \end{aligned} \quad (2)$$

From Fig. 2b we observe that the decrease of λ is driven by σ_Λ^2 increasing to a maximum, while σ_f^2 and $\sigma_{f,\Lambda}^2$ decrease (see Supplementary Fig. 2). We expect the main features of these distributions to be preserved as the system size N is increased¹³, which suggests that for larger N , where basin volume calculations are still intractable for multiple densities, the maximum in σ_Λ^2 can be used to identify $\phi_N^{*(\lambda)}$. We have directly measured $\chi_A = N\sigma_A^2$ using our sampling scheme—which samples packings with probability proportional to the volume of their basin of attraction—for systems of up to $N = 128$ discs (see inset of Fig. 3a) and finite-size scaling indicates that χ_A diverges as $\phi \rightarrow \phi_{N \rightarrow \infty}^{*(\Lambda)} = 0.841(3)$ (see Supplementary Information). The saturation of λ to a minimum as $\phi \rightarrow \phi_N^{*(\lambda)}$, for small N , is determined by the fact that χ_A diverges only in the thermodynamic limit; a detailed discussion is given in the Methods.



Interestingly, we find evidence that in the thermodynamic limit, the point of equiprobability, $\phi_{N \rightarrow \infty}^*$, coincides with the point at which the system unjams, $\phi_{N \rightarrow \infty}^*$. We use two characteristics of the unjamming transition to locate $\phi_{N \rightarrow \infty}^*$: the average pressure of the packings goes to zero, and therefore $\langle \Lambda \rangle \rightarrow -\infty$ (see Fig. 3b); and the probability of finding jammed packings, p_j , goes to zero (see inset of Fig. 3b). A scaling analysis indicates that $\langle \Lambda \rangle \rightarrow -\infty$ as $\phi_{N \rightarrow \infty}^{*(\Lambda)} = 0.841(3)$, and $p_j \rightarrow 0$ as $\phi_{N \rightarrow \infty}^{*(p_j)} = 0.844(2)$ (see Supplementary Information). We thus find that $\phi_{N \rightarrow \infty}^* = \phi_{N \rightarrow \infty}^{*(\Lambda)}$ within numerical error and up to corrections to finite-size scaling²⁰. Our simulations therefore lead to the surprising conclusion that the Edwards conjecture appears to hold precisely at the (un)jamming transition. We note that our earlier simulations, which were performed at densities much above jamming^{13,15}, did not support the equiprobability hypothesis. The earlier simulations were in fact far enough away from unjamming that the emergence of equiprobability at this point could not be anticipated. Our earlier findings, therefore, do not contradict the more recent ones and are completely consistent with these.

Why is χ_A related to the unjamming transition? As the particles interact via purely repulsive potentials, the pressure P is strictly positive, which implies that the fluctuations of P have a floor and go to zero at unjamming. The relative fluctuations $\chi_P \equiv N\sigma^2(P/\langle P \rangle_B)$ can be non-zero, and a diverging χ_P would then imply a diverging χ_A . Because of the bounded nature of P (refs 21–23), however, χ_P can diverge only at the unjamming transition where $\langle P \rangle_B \rightarrow 0$ (see Methods). We find that χ_P does diverge (Fig. 3a) and finite-size scaling yields $\phi_{N \rightarrow \infty}^{*(P)} = 0.841(3)$, in agreement with what has been found for χ_A . Returning to the $N = 64$ case that we have analysed using the basin volume statistics, we find that both χ_P and χ_A saturate to their maximum values over similar ranges of ϕ and our estimate $\phi_{N=64}^* \approx 0.82$, where $S_G = S_B$ and $\lambda \rightarrow 0$, falls in this region. In addition, the average number of contacts $\langle z \rangle_B(\phi_{N=64}^*) = 4.1 \pm 0.2$ is close to the isostatic value $z_{N=64}^{(iso)} \equiv 2d - 2/64 \approx 3.97$ (ref. 10) (see Supplementary Information).

Finally, we note that the states in the generalized Edwards ensemble^{5,21,24,25} characterized by ϕ and P have basin volumes that are similar, if not identical, over the full range of ϕ that we have explored (see scatter plot in Fig. 2b), indicating that equiprobability in the stress–volume ensemble^{5,24} is a more robust formulation

of the Edwards hypothesis. This observation is consistent with recent experiments²⁶.

Although, the equiprobability of jammed states at a given packing fraction was posited by Edwards for jammed packings of hard particles, our analysis shows that for soft particles, the Edwards hypothesis is valid only for the marginally jammed states at $\phi_{N \rightarrow \infty}^* = \phi_{N \rightarrow \infty}^j$, where the jamming probability vanishes, the entropy is maximized, and relative pressure fluctuations diverge. We have shown not only that there exists a practical ‘Edwardsian’ packing generation protocol, capable of sampling jammed states equiprobably, but we have uncovered an unexpected property of the energy landscape for this class of systems. At this stage, we cannot establish whether the same considerations are valid in three dimensions, although the already proven validity of equation (16) in three dimensions would suggest so¹³. The exact value of the entropy at unjamming, whether finite or not, also needs to be elucidated. The implications for ‘soft’ structural glasses is apparent: at ϕ^j the uniform size of the basins implies that the system, when thermalized, has the same probability of visiting all of its basins of attraction; hence, there are no preferred inherent structures. This could be a signature of the hard-sphere transition occurring at the same point²⁷. Our approach can, therefore, be extended to spin-glasses and related problems, and it would be clearly very exciting to explore the analogies and differences between ‘jamming’ in various systems for which the configuration space can break up into many distinct basins.

Methods

Methods, including statements of data availability and any associated accession codes and references, are available in the [online version of this paper](#).

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References

1. Edwards, S. F. & Oakeshott, R. B. S. Theory of powders. *Phys. A* **157**, 1080–1090 (1989).
2. Laughlin, R. *A Different Universe: Reinventing Physics from the Bottom Down* (Basic Books, 2006).
3. Gibbs, J. W. *Elementary Principles of Statistical Mechanics* (Charles Scribner’s Sons, 1902).
4. Edwards, S. F. & Grinev, D. V. Granular materials: towards the statistical mechanics of jammed configurations. *Adv. Phys.* **51**, 1669–1684 (2002).
5. Bi, D., Henkes, S., Daniels, K. E. & Chakraborty, B. The statistical physics of athermal materials. *Annu. Rev. Condens. Matter Phys.* **6**, 63–83 (2015).
6. Baule, A., Morone, F., Hermann, H. & Makse, H. A. *Edwards Statistical Mechanics for Jammed Granular Matter*. Preprint at <http://arXiv.org/abs/1602.04369> (2016).
7. Olsson, P. & Teitel, S. Critical scaling of shear viscosity at the jamming transition. *Phys. Rev. Lett.* **99**, 178001 (2007).
8. Wyart, M., Nagel, S. R. & Witten, T. A. Geometric origin of excess low-frequency vibrational modes in weakly connected amorphous solids. *Europhys. Lett.* **72**, 486–492 (2005).
9. Silbert, L. E., Liu, A. J. & Nagel, S. R. Structural signatures of the unjamming transition at zero temperature. *Phys. Rev. E* **73**, 041304 (2006).
10. Goodrich, C., Liu, A. J. & Sethna, J. P. Scaling ansatz for the jamming transition. *Proc. Natl Acad. Sci. USA* **113**, 9745–9750 (2016).
11. Ramola, K. & Chakraborty, B. Disordered contact networks in jammed packings of frictionless disks. *J. Stat. Mech.* **2016**, 114002 (2016).
12. Ramola, K. & Chakraborty, B. Scaling theory for the frictionless unjamming transition. *Phys. Rev. Lett.* **118**, 138001 (2017).
13. Martiniani, S., Schrenk, K. J., Stevenson, J. D., Wales, D. J. & Frenkel, D. Turning intractable counting into sampling: computing the configurational entropy of three-dimensional jammed packings. *Phys. Rev. E* **93**, 012906 (2016).
14. Xu, N., Frenkel, D. & Liu, A. J. Direct determination of the size of basins of attraction of jammed solids. *Phys. Rev. Lett.* **106**, 245502 (2011).
15. Asenjo, D., Paillusson, F. & Frenkel, D. Numerical calculation of granular entropy. *Phys. Rev. Lett.* **112**, 098002 (2014).
16. Martiniani, S., Schrenk, K. J., Stevenson, J. D., Wales, D. J. & Frenkel, D. Structural analysis of high-dimensional basins of attraction. *Phys. Rev. E* **94**, 031301 (2016).
17. Swendsen, R. H. Statistical mechanics of colloids and Boltzmann’s definition of the entropy. *Am. J. Phys.* **74**, 187–190 (2006).
18. Frenkel, D. Why colloidal systems can be described by statistical mechanics: some not very original comments on the Gibbs paradox. *Mol. Phys.* **112**, 2325–2329 (2014).
19. Cates, M. E. & Manoharan, V. N. Testing the foundations of classical entropy: colloid experiments. *Soft Matter* **11**, 6538–6546 (2015).
20. Vagberg, D., Valdez-Balderas, D., Moore, M. A., Olsson, P. & Teitel, S. Finite-size scaling at the jamming transition: corrections to scaling and the correlation-length critical exponent. *Phys. Rev. E* **83**, 030303 (2011).
21. Henkes, S. & Chakraborty, B. Statistical mechanics framework for static granular matter. *Phys. Rev. E* **79**, 061301 (2009).
22. Lois, G. *et al.* Stress correlations in granular materials: an entropic formulation. *Phys. Rev. E* **80**, 060303 (2009).
23. Tighe, B. P. *Force Distributions and Stress Response in Granular Materials*. PhD thesis, Duke Univ. (2006).
24. Blumenfeld, R. & Edwards, S. F. On granular stress statistics: compactivity, angoricity, and some open issues. *J. Phys. Chem. B* **113**, 3981–3987 (2009).
25. Henkes, S., O’Hern, C. S. & Chakraborty, B. Entropy and temperature of a static granular assembly: an ab initio approach. *Phys. Rev. Lett.* **99**, 038002 (2007).
26. Puckett, J. G. & Daniels, K. E. Equilibrating temperaturelike variables in jammed granular subsystems. *Phys. Rev. Lett.* **110**, 058001 (2013).
27. Charbonneau, P., Kurchan, J., Parisi, G., Urbani, P. & Zamponi, F. Glass and jamming transitions: from exact results to finite-dimensional descriptions. *Annu. Rev. Condens. Matter Phys.* **8**, 265–288 (2017).
28. Efron, B. Bootstrap methods: another look at the jackknife. *Ann. Statist.* **7**, 1–26 (1979).
29. Efron, B. Better bootstrap confidence intervals. *J. Am. Stat. Assoc.* **82**, 171–185 (1987).

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Author contributions

S.M., D.F. and B.C. designed the study. S.M. and K.J.S. developed the software and performed the numerical simulations. S.M., K.R., B.C. and D.F. analysed the data and wrote the manuscript.

Additional information

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Competing financial interests

The authors declare no competing financial interests.

