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Phys. Rev. Lett. **109**, 205501 — Published 13 November 2012

DOI: [10.1103/PhysRevLett.109.205501](https://doi.org/10.1103/PhysRevLett.109.205501)

Universal microstructure and mechanical stability of jammed packings

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Jammed packings’ mechanical properties depend sensitively on their detailed local structure. Here we provide a complete characterization of the pair correlation close to contact and of the force distribution of jammed frictionless spheres. In particular we discover a set of new scaling relations that connect the behavior of particles bearing small forces and those bearing no force but that are almost in contact. By performing systematic investigations for spatial dimensions $d=3-10$, in a wide density range and using different preparation protocols, we show that these scalings are indeed universal. We therefore establish clear milestones for the emergence of a complete microscopic theory of jamming. This description is also crucial for high-precision force experiments in granular systems.

PACS numbers: 64.70.Q-, 05.20.-y, 61.20.-p, 81.05.Kf

Introduction – The jamming phenomenon is ubiquitous – candies [1], coal [2], and colloids [3] all can jam, but its microscopic universality remains debated, even for the most ideal of systems. Like any other phase transition, the jamming transition can be approached from the unjammed phase, e.g. by compressing hard spheres (HS) [4], or from the jammed phase, e.g. by minimizing the energy of soft spheres (SS) [5]. Yet these two complementary approaches have mostly been developed independently from each other (see [6] for HS and [7, 8] for SS). Unlike standard phase transitions, however, the jamming transition is a non-equilibrium phenomenon that happens deep inside the glass phase [9, 10], and therefore different protocols generate different packings, which may result to conflicting observations. Indeed, all agree that marginally stable packings of frictionless spheres average $2d$ force-bearing contacts per particle [8], but jammed packings’ density [6, 11–14], parts of their microstructure [6, 15, 16], as well as their given name [6, 17] are contentious. Although the jamming “j” point was proposed to be unique in the thermodynamic limit [5, 18], there is a growing consensus that jamming occurs over a range of “j” points [6, 7, 9, 13, 14, 17]. Yet various physical origins have been attributed to the jamming density variation, including structural correlations in the initial configuration [7], and the presence of small crystalline regions only detectable by subtle order metrics whose minimization should result in a single “maximally random jammed” state [6, 17]. Others have proposed the intrinsic existence of a range of densities over which packings with an identically disordered structure could be found [9, 13, 14]. A power-law growth of the number of almost-touching particles near jamming has also been identified numerically, but different exponents have been found for HS [4] and SS [15]. If there is microscopic

universality, it has yet to fully emerge.

In this letter we bring a different point of view to the problem by systematically investigating how the jamming limit is approached from both sides of the transition and by varying the dimensionality of space from $d=3$ to 10. This approach allows us to obtain a series of important results. (1) Increasing $d \geq 4$ suppresses crystallization [19, 20] and the “spurious” contribution of “rattlers”. We can thus show that random jammed packings of *monodisperse* spheres with identical near-contact structural properties can be obtained over a *range* of densities (thus confirming results in $d=3, 4$ [4, 14, 17, 19, 21]), and that this range *broadens* with increasing d . (2) We confirm an earlier suggestion that two exponents α and θ , corresponding to different physical regimes, control the mechanical stability of jammed packings [22]. The first describes the “quasi-contact” regime in which particles are separated by very small gaps h , whose number scales as $h^{-\alpha}$ for small h ; the second describes the tail of the “contact” regime, where the number of particles bearing a small force f scales as f^θ . (3) We also provide a complete characterization of the microstructure of jammed packings. We show that matching the two above regimes provides scaling relations between the exponents and non-trivial scaling functions. We thus conclude that the mechanical stability of jammed packings is related to their very complex contact microstructure. (4) We find these results to be universal in the sense that they are robust to changes in preparation protocol, packing density, and, in particular, spatial dimension.

The observation that jammed packings’ properties are independent of d suggests that a mean-field theory should be able to capture the jamming phenomenology [23, 24]. One such treatment, the Gaussian replica theory (GRT) [10, 13], unifies the description of the glass transition

and of jamming by exploiting an analogy with discrete random optimization problems [9, 25]. In this treatment, the HS and SS approaches to jamming are unified under the assumption that jammed states are the infinite pressure (for HS) or zero temperature (for SS) limit of long-lived metastable glassy states [10, 13]. The theory predicts a growing jamming density range with d [13], the existence of scaling relations for energy and pressure relating the two sides of the jamming transition [10], and makes structural scaling predictions that are remarkably satisfied at short distances [10, 13]. Yet we show here that (5) G-RT completely fails to describe the structural regime that controls jammed packings' mechanical stability. Our results (1)-(5) will thus guide both theory and experiments (through high-precision force measurements [26]) towards a better understanding of the jamming transition.

Packing Generation – We consider a system of $N \geq 8000$ identical spherical particles of diameter σ in a fixed volume V , under periodic boundary conditions. The packing fraction $\varphi = NV_d(\sigma/2)/V$, where $V_d(r)$ is the volume of a d -dimensional sphere of radius r , measures the fraction of space occupied by particles. Jammed packings are prepared using two different numerical protocols (see Appendix for details and reduced units definitions). (i) Approaching jamming from densities below it by Lubachevsky-Stillinger (LS) compressions of HS undergoing Newtonian dynamics while σ grows at a fixed rate $\gamma = \dot{\sigma}$ [4]. The compression, which is tuned to prevent crystallization [20, 27], stops when particles are very near contact, defining the packing fraction φ_p^γ at which the HS reduced pressure becomes infinite. (ii) Approaching jamming from densities above or below it by minimizing the energy E of a random configuration of harmonic SS. Initial bounds σ_- and σ_+ that bracket jamming are evolved iteratively by choosing an intermediate value σ_m and minimizing the energy of the current configuration at σ_+ (procedure from above) or at σ_- (procedure from below). The final jammed configurations at the onset of $E \neq 0$ have φ_e^\downarrow from above and φ_e^\uparrow from below. From above, the energy vanishes with $e = E/N \sim \Delta\varphi^2$ and the static pressure $P \sim \Delta\varphi$, where $\Delta\varphi$ is the distance from jamming [5].

We find the initial σ_\pm to have no measurable effect on φ_e^\uparrow . We formally define $\varphi_e^{\min} = \min_{\sigma_\pm} \varphi_e^\uparrow(\sigma_\pm)$, but any reasonable σ_\pm results in the same final density. By contrast, φ_e^\downarrow strongly depends on σ_+ (Fig. 1), but is also independent of σ_- . We therefore define $\varphi_e^{\max} = \max_{\sigma_\pm} \varphi_e^\downarrow(\sigma_\pm)$. A practical way of constructing both φ_e^{\min} and φ_e^{\max} is to run the energy minimization (respectively from below and from above) starting from $\sigma_- = 0$ and σ_+ large enough to saturate φ_e^\downarrow to its maximum. Intermediate packing fractions can then be obtained by reducing σ_+ (Fig. 1). By varying σ_\pm in protocol (ii) we can thus construct packings over a density interval $[\varphi_e^{\min}, \varphi_e^{\max}]$ that roughly corresponds in protocol (i) to

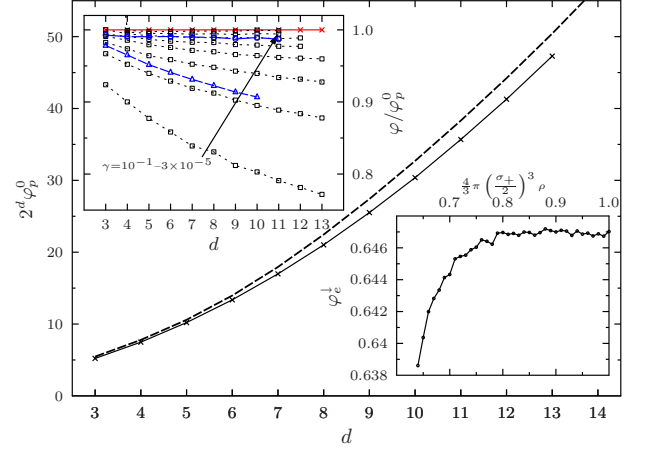


FIG. 1. The extrapolated jamming density $\varphi_p^{\gamma \rightarrow 0}$ following the protocol described in Ref. [27] is extended to higher d (solid line and crosses), and compared with the G-RT prediction for φ_{GCP} (dashed line). (top inset) The range of jamming densities φ_p^γ (squares) is compared to φ_e^{\max} (circles) and φ_e^{\min} (triangles). Note that $\varphi_e^{\max} \sim \varphi_p^{\gamma=3 \times 10^{-4}}$ and $\varphi_e^{\min} \sim \varphi_p^{\gamma=3 \times 10^{-2}}$. (bottom inset) The $d=3$ increase of φ_e^\downarrow with σ_+ , in terms of the initial effective packing fraction.

$[\varphi_p^{\gamma_-}, \varphi_p^{\gamma_+}]$ with $\gamma_- \approx 3 \times 10^{-2}$ and $\gamma_+ \approx 3 \times 10^{-4}$ (larger γ generate mechanically unstable packings). The resulting density range is remarkably found to grow steadily from about 2% in $d = 3$ to nearly 10% in $d = 11$ (Fig. 1). We therefore confirm the similar observation made for $d = 3$ binary mixtures [14], where the limited available density range and the subtle crystal order had left some room for debate [6]. Note that this range is achieved by only implementing procedures that compact liquid configurations. Ref. [21] has shown that enlarging the space of procedures enlarges the range of jammed packings, but the resulting packings likely have a different microstructure.

The similarity between the jamming density results of the two protocols suggests an underlying physical connection between them. G-RT indeed predicts that packings exist over a finite packing fraction range, whose upper limit is the “glass close packing” φ_{GCP} [13]. By analogy with random combinatorial optimization problems [25], the densest packing at φ_{GCP} is conjectured to require a time $\sim \exp(N^a)$ to generate, the exponent being possibly $a \approx (d-1)/d$, based on a nucleation analysis. The maximal density that can be reached by the protocols above, which both run in polynomial time in N , should therefore be strictly smaller than φ_{GCP} . Figure 1 shows it to be the case for all d , in agreement with G-RT.

Scaling functions – To determine the universal structure of disordered jammed structures, we consider the pair correlation function $g(r) = (\rho N)^{-1} \langle \sum_{i \neq j} \delta(\mathbf{r} + \mathbf{r}_i - \mathbf{r}_j) \rangle$, which is the only relevant structural correlation in

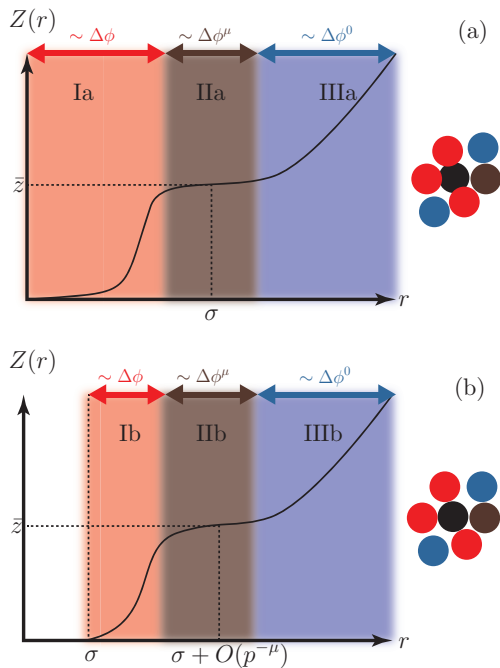


FIG. 2. Schematic of $Z(r)$ when approaching jamming from above (a) with protocol (ii), and from below (b) with protocol (i). Three distinct scaling regimes can be identified. The first regime is related to the growth of $Z(r)$ from 0 to \bar{z} . It corresponds to interparticle gaps $h = |r - \sigma| \sim \Delta\varphi$, and hence to particles that are in contact when $\Delta\varphi \rightarrow 0$. The last regime corresponds to gaps h that remain finite for $\Delta\varphi \rightarrow 0$. These particles remain separated at jamming, but these small gaps, $Z(r) - \bar{z} \propto h^{1-\alpha}$, form a “quasi-contact” regime. The intermediate regime corresponds to gaps $h \sim \Delta\varphi^\mu$. It matches the two other regimes and disappears when $\Delta\varphi \rightarrow 0$.

high d fluids [28]. For numerical convenience, we compute the cumulative structure function

$$Z(r) = \rho S_{d-1} \int_0^r ds s^{d-1} g(s), \quad (1)$$

where S_{d-1} is the surface of a d dimensional sphere of unit radius. The function $Z(r)$ thus provides the average number of neighbors within r of a given particle. Rattlers are first excluded from the analysis (Appendix), but we come back to this point below.

For both protocols, $Z(r)$ jumps from 0 to a plateau at \bar{z} on a scale proportional to the distance to jamming $\Delta\varphi$, where \bar{z} is the isostatic average number of contacts $2d$ plus a correction $\bar{z} - 2d \propto \Delta\varphi^\zeta$ (Fig. 2). For HS, we find $\zeta=0.36(2)$, while $\zeta=0.53(3)$ for SS (Fig. 3) [5]. The approach to the isostatic plateau is characterized by a long power-law tail with exponents $\theta=0.28(3)$ for HS and $\theta=0.42(2)$ for SS, but the exponent is independent of d for a given model. The plateau is extended by a second power-law regime that corresponds to particles in “quasi-contact”, carrying no force at jamming. We find that in this regime the scaling is the same for both pro-

ocols, growing as $Z(r) - \bar{z} \propto (r - \sigma)^{1-\alpha}$ with a universal exponent $\alpha = 0.42(2)$ until it reaches the trivial large r regime. Interestingly, the two power-law regimes can be matched by a scaling function \mathcal{H}_\pm , which defines an additional intermediate regime. This intermediate regime shrinks to a point at jamming, but smoothly crosses over from one power-law regime to the other at finite $\Delta\varphi$. Consistency therefore sets clear scaling requirements for the different regimes (see Appendix for scaling analysis) as detailed in Fig. 2, and verified in Fig. 3.

Force distribution and mechanical stability – The consequences of these universal scaling relations on mechanical properties can be gleaned from the probability distribution of inter-particle forces f . Here again, we consider the cumulative distribution $G(f) = \int_0^f P(f') df'$ rather than the pair force distribution $P(f)$, for numerical convenience.

For HS approaching jamming, the average force $\bar{f} \propto p$. In the contact regime the force and distance distributions are also related through a Laplace transform (Appendix) [4]. The low-force distribution is thus consistent with $G(f) \propto f^{1+\theta}$ and $\theta = 0.28(3)$. For SS approaching jamming from above, the pair potential sets the relation between the force and the pair distributions [29] (Appendix). Here again, the low-force tail is consistent with $\theta = 0.42(2)$. For both protocols, however, the regime intermediate between contacts and quasi-contacts results in deviations from this power-law decay at very weak forces away from jamming.

The large force regime has been thoroughly studied [4, 5, 18, 29–32], but the weak force distribution is much less well characterized. Yet it has been proposed by Wyart [22] that $\alpha \geq 1/(2 + \theta)$ is required for mechanical stability. Both the SS values ($\alpha = 0.39(1)$, $\theta = 0.42(2)$) and the HS ones ($\alpha = 0.42(2)$, $\theta = 0.28(3)$), however, indicate a slight violation of this condition. A generalized stability condition of the form $\alpha \geq (1 - \delta/2)/(2 + \theta - \delta/2)$ [22] is consistent with our findings for $\delta \gtrsim 0.2$, but a direct test of this extended relation is beyond the scope of the current analysis.

Rattlers – Rattlers, i.e., particles with no mechanical contacts, must be considered before concluding that the dimensional and protocol robustness of these results strongly support a universal microscopic description of jamming. Because their fraction rapidly decreases with increasing d (Appendix) [19], and their structural contribution is clearly distinct from that of the other particles when $\Delta\varphi \rightarrow 0$, it is reasonable to remove them from the analysis. Rattlers indeed play essentially no role in the scaling regimes in high d , while in low d , their inclusion introduces noise in $Z(r)$ and $G(f)$ that obscures the scaling relations, which may explain why $\alpha \approx 0.5$ was obtained in Ref. [15]. Removing the rattlers reveals the robust relationship between microstructure and mechanical properties, in support of jamming having a critical dimension $d_c = 2$ [24].

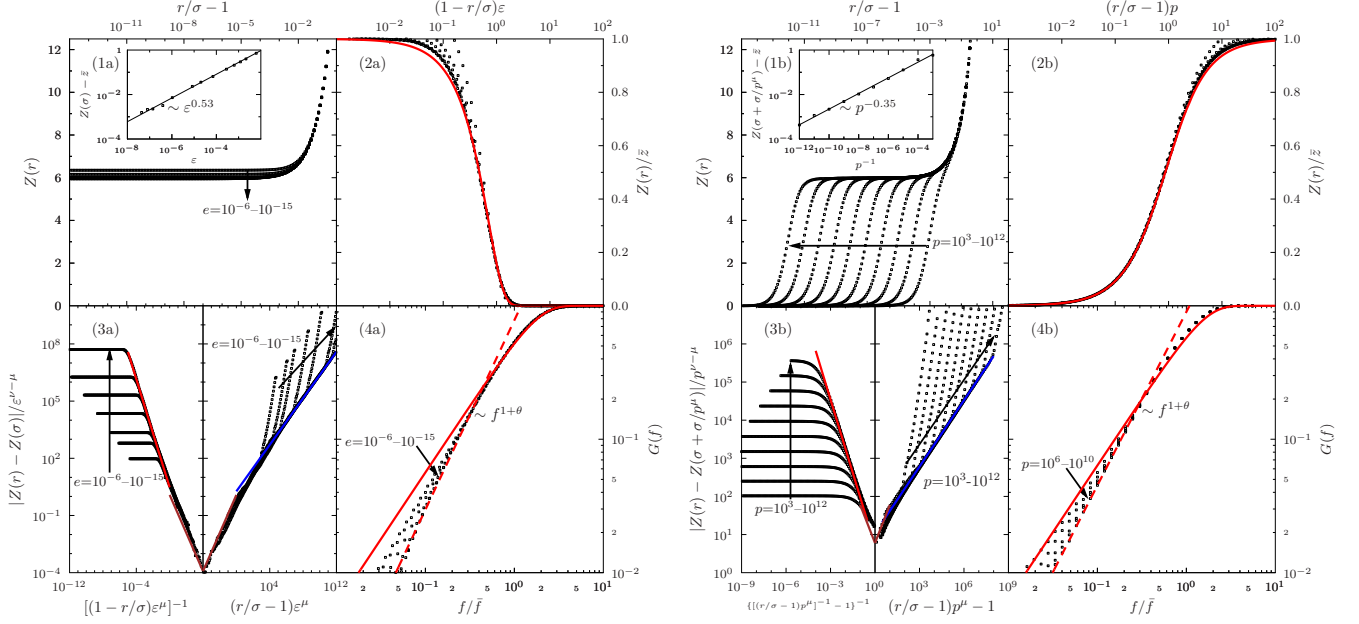


FIG. 3. Scaling of the cumulative structure function $Z(r)$ and the cumulative force distribution $G(f)$ in $d = 3$ upon approaching jamming from above **(a)** by SS energy minimization (where $e \propto |\Delta\varphi|^2 \rightarrow 0$ and $\varepsilon = \sqrt{ed/2}$), and from below **(b)** by HS compression (where $p \propto |\Delta\varphi|^{-1} \rightarrow \infty$). **(1a)** For diminishing e , the height of the plateau (inset) converges to the isostatic value with $\zeta=0.53(3)$. **(2a)** The small $r < \sigma$ regime shows the “contact” scaling function $Z_+(x)$, which agrees well with the G-RT prediction (red line). **(3a)** Rescaling $Z(r)$ using $\mu = (1 + \theta)/(2 + \theta - \alpha)$ and $\nu = \alpha\mu$ highlights the behavior of the scaling function $|\mathcal{H}_-(x) - \mathcal{H}_-(1)| \sim 1.2x$ (brown lines – middle) along with the $\theta = 0.42(2)$ (red line – left) and the $\alpha = 0.39(1)$ (blue line – right) power-law regimes. **(4a)** $G(f)$, with power-law tail exponent $\theta = 0.42(2)$ (dashed line). **(1b)** For increasing p , $Z(r)$ grows on an earlier scale $r - \sigma \sim p^{-1}$ to a plateau at the isostatic value, whose height (inset) decays with $\zeta = 0.36(1)$. **(2b)** The small $r - \sigma$ regime shows the “contacts” scaling function $Z_-(x)$, which agrees well with the G-RT prediction (red line). **(3b)** Rescaling $Z(r)$ using $\mu = (1 + \theta)/(2 + \theta - \alpha)$ and $\nu = \alpha\mu$ highlights the behavior of the scaling function $|\mathcal{H}_-(x) - \mathcal{H}_-(1)| \sim 6x$ (brown lines – middle) along with the $\theta = 0.28(3)$ (red line – left) and the $\alpha = 0.42(2)$ (blue line – right) power-law regimes. **(4b)** $G(f)$, with power-law tail exponent $\theta = 0.28(3)$ (dashed line), compared with the G-RT prediction (solid line).

Comparison with microscopic theory – G-RT, the only available first-principle theory of jammed packings, provides predictions for the contact regime scaling function $\mathcal{Z}_\pm(x)$ [10, 13] (Appendix). We find the form of $\mathcal{Z}_\pm(x)$ to be extremely accurate when x is of order 1, but G-RT fails to capture the ensuing power-law regimes (Fig. 3). G-RT indeed predicts an exponent $\theta = 0$ for both protocols, and completely misses the power-law divergence related to α , predicting $\alpha = 0$. A similar deviation is observed at weak forces. We attribute these discrepancies to the Gaussian assumption for the cage form of G-RT, which has recently been found to be erroneous in dense disordered fluids [33, 34]. This non-Gaussian structure also naturally suggests a microscopic explanation for the breakdown of the normal-mode decomposition of jammed states [35, 36]. Including a non-Gaussian cage to RT ought to provide a better mean-field understanding of the jamming phenomenology.

Conclusions – Our results show that the jamming terminology controversy should be resolved by replacing the j-point [5] with the j-line [9, 13], and by distinguishing a *range* of maximally random jammed packings from their partially crystallized counterparts [6, 17, 21].

They also reveal that the contacts’ complex microstructure in jammed packings is characterized by universal, well-defined scaling regimes and by their corresponding scaling functions. We give precise numerical predictions for the scaling exponents, and show that the scaling functions are related to the force probability distribution. These specific predictions can be tested in soft matter and granular experiments. A preliminary investigation indeed examined the scaling of the peak of the pair correlation function [3], but our comprehensive predictions can help experimentalists access the full scaling of $Z(r)$ and $G(f)$. This feat should be possible once a force resolution of $\sim 5\%\bar{f}$ is experimentally achieved [26].

Finally, it is worth noting that the present study was limited to zero temperature T in the sense that no thermal motion is allowed in SS and that for HS the energy interaction scale is infinite compared to T . At finite T , the jamming transition is blurred [10], but vestiges of the scaling relations should remain visible [3]. Future work will detail how temperature and its associated anharmonicities affect the $T = 0$ scaling relations identified here [10, 35].

Acknowledgments – We acknowledge discussions with S. Torquato and S. Nagel. The European Research Council has provided financial support through ERC grant agreement no. 247328. P.C. acknowledges National Science Foundation support no. DMR-1055586.

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