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Two diverging length scales in the structure of jammed packings

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At densities higher than the jamming transition for athermal, frictionless repulsive spheres we find two distinct length scales, both of which diverge as a power law as the transition is approached. The first, ξ_Z , is associated with the two-point correlation function for the number of contacts on two particles as a function of the particle separation. The second, ξ_f , is associated with contact-number fluctuations in subsystems of different sizes. On scales below ξ_f the fluctuations are highly suppressed, similar to the phenomenon of hyperuniformity usually associated with density fluctuations. The exponents for the divergence of ξ_Z and ξ_f are different and appear to be different in two and three dimensions.

A key signature of a critical phase transition is the existence of a correlation length, ξ , which diverges at the critical point. On scales smaller than ξ the constituents act in a cooperative manner, while on large scales the system typically behaves as if it were non-interacting [1, 2]. The correlation length is defined by the second moment of the two-point correlation function for the local order parameter. For nonequilibrium disordered transitions, however, the local order parameter is not always known.

The jamming transition of a system of soft repulsive spheres is an example of such a transition. It occurs at temperature $T = 0$ as the applied pressure (or packing fraction) is increased driving the system from a floppy to a rigid state. While various length scales have been shown to diverge as the jamming critical point is approached, they do not characterize the structure itself but rather the normal modes, the mechanical stability, and the elastic response of the system [3–7].

In this paper, we show that the onset of rigidity is associated with the divergence of two distinct structural length scales, ξ_Z and ξ_f , both associated with the *contact number*. The contact number, Z_i , is the number of neighbors with which a particle i interacts and varies from one particle to the next. One of these lengths, ξ_Z , is associated with the decay of the two-point spatial correlation function for Z . Our finding that ξ_Z diverges at the jamming transition motivates us to examine the size of contact number fluctuations in subsystems of different sizes. In contrast to usual behavior of critical points, where the long-range correlations result in diverging fluctuations, here we find that the contact number fluctuations are highly suppressed on *large scales*. Namely, at the jamming transition the contact fluctuations in a volume of ℓ^d scale as its surface ℓ^{d-1} , which is the smallest

possible scaling consistent with local randomness in the contact network. Thus, a system at the jamming transition appears to have *contact hyperuniformity*, a term we introduce in analogy to the concept of density hyperuniformity [8], which was first observed in the mass distribution in the early universe and in plasmas [9–11]. We note that similar generalizations of hyperuniformity have been introduced, for example, in the study of foams [12], pattern formation [13] and random fields [13]. At a finite distance from the jamming transition the hyperuniform scaling persists up to a finite distance $\ell < \xi_f$, where ξ_f diverges at the jamming transition. We show how the exponents characterizing the divergence at the jamming transition of ξ_f and of ξ_Z are related; surprisingly, both exponents appear to depend on the dimension of the system, d in contrast to previously observed lengths that diverge with dimension-independent behavior [3–5].

Our analysis is based on numerically generated packings in either $d = 2$ spatial dimensions with $N = 128,000$ polydisperse, or $d = 3$ with $N = 10^6$ monodisperse frictionless soft repulsive particles in a volume, V . The harmonic repulsion between particles is given by:

$$U(r_{ij}) = \frac{1}{2}\epsilon \left(1 - \frac{r_{ij}}{\sigma_{ij}}\right)^2 \Theta\left(1 - \frac{r_{ij}}{\sigma_{ij}}\right), \quad (1)$$

where ϵ is the characteristic energy, $\Theta(x)$ is the Heaviside step function, and r_{ij} and σ_{ij} are respectively the separation between particles i and j and sum of their radii. Configurations are prepared by standard methods used for studies of jamming [14, 15]; spheres are distributed randomly in space and the system's energy is minimized using the FIRE [16] algorithm to produce a zero-temperature jammed configuration where force balance is maintained on every particle [17].

The simplest measure of correlations is a two-point correlation function. To this end, we define $\delta Z_i \equiv Z_i - \bar{Z}$, measuring the deviation of Z_i from its average $\bar{Z} = \frac{1}{N} \sum_i Z_i$ and its two-point correlation function $h_Z(r_2, r_1) = \langle \delta Z(r_2) \delta Z(r_1) \rangle$. Here, $\delta Z(r) = \sum_i \delta Z_i \delta(r - r_i)$ where r_i denotes the location of the particles center and the average is over different realizations and all equidistant locations in the packing. Since, the packing are isotropic and homogeneous, $h_Z(r_2, r_1) = h_Z(r_2 - r_1, 0)$ and depends only the distance between two points; for brevity it is denoted by $h_Z(r_2 - r_1)$. For a finite number of realizations, N_0 , $h_Z(r)$ can be determined to an accuracy of $1/\sqrt{N_0}$. Since $h_Z(r)$ decays to zero as a function of distance, a growing number of realizations are needed to measure it when r is large. We therefore measure the contact-number structure factor

$$S_Z(q) = \frac{1}{N} \left\langle \left| \sum_{i=1}^N \delta Z_i e^{-iq \cdot r_i} \right|^2 \right\rangle. \quad (2)$$

Here the average is over different realizations and directions of the wave vector q and therefore $S_Z(q)$ depends only on the magnitude of q . The relation between $S_Z(q)$ and $h_Z(r)$ can be made apparent by using ρ , the particle density, and the definition of $\delta Z(r)$, which yields:

$$S_Z(q) = \left\langle (\delta Z_i)^2 \right\rangle + \frac{1}{\rho} \int d^d r h_Z(r) e^{-iq \cdot r}. \quad (3)$$

At the jamming transition in the thermodynamic limit, $\bar{Z} = Z_c = 2d$ (Here we do not include rattlers where Z_i is too small to confine a particle rigidly.). This corresponds to the minimal number of contacts needed for rigidity and $\Delta Z \equiv \bar{Z} - Z_c$ measures the distance from the critical point [15, 18, 19]. Correlations in ΔZ have been previously suggested [20, 21] but their nature was not studied.

Fig. 1a and c show $S_Z(q)$ in $d = 2$ and $d = 3$, for different values of ΔZ . As $q \rightarrow 0$, $S_Z(q)$ approaches a constant that depends on ΔZ . At intermediate values of q , this function rises steeply, approximately as a power-law, $S_Z(q) \propto q^\alpha$, where $\alpha_{2d} = 1.53 \pm 0.04$ and $\alpha_{3d} = 1.52 \pm 0.05$. The regime of $q \gtrsim 1$, corresponding to wavevectors greater than the inverse particle diameter, is not the focus of this paper. In the limit of $\Delta Z \rightarrow 0$, the power-law regime q^α , appears to extend to arbitrarily small q -values, implying that $S_Z(q \rightarrow 0) = 0$. Below we will argue that this has important consequences for large-scale contact fluctuations. In this limit, the real-space correlation function decays as a power-law with an exponent that is fairly large: $h_Z(r) \propto -r^{-d-\alpha}$. The negative sign can be inferred from the fact that the first term in Eq. 3 is positive and can only be reduced if $h_Z(r) < 0$ at large distances.

The transition between the first two regimes defines a length scale, $\xi_Z = 2\pi/q_c$ where q_c is the crossover wave-vector. This length scale diverges as $\Delta Z \rightarrow 0$, presumably in a power-law manner $\xi_Z = \Delta Z^{-\nu_Z}$. To measure this length scale it is convenient to write $S_Z(q)$ in the form of a scaling function:

$$S_Z(q) = \Delta Z^\beta f(q\xi_Z). \quad (4)$$

This implies that the data can be collapsed by rescaling the x-axis by $\Delta Z^{-\nu_Z}$ and the y-axis by $\Delta Z^{-\beta}$. To further constrain ν_Z and β we note that $f(x)$ has two limiting behaviors:

$$f(x) = \begin{cases} \text{const} & x \ll 1 \\ x^\alpha & x \gg 1 \end{cases}. \quad (5)$$

This scaling regime is cut off when q^{-1} becomes of the order of several particle diameters. In the limit of $q\xi_Z \gg 1$, $S_Z(q)$ is independent of ΔZ implying that

$$\beta = \alpha \nu_Z. \quad (6)$$

Thus by measuring α the data can be collapsed by varying a single exponent. Fig. 1b and d shows the collapse for both two and three dimensions, where the best collapse is found for $\nu_Z^{2d} = 0.7_{-0.1}^{+0.05}$ and $\nu_Z^{3d} = 0.85_{-0.1}^{+0.15}$. The errors arise from the uncertainty in α and the finite range of the data. Our results suggest that ν_Z may be different in two and three dimensions, in contrast to other critical exponents associated with jamming which do not appear to depend on dimension. We note that we cannot rule out that this apparent difference arises due to corrections to scaling near the upper-critical dimension, thought to be two dimensions in this case[22].

We turn next to consider what $S_Z(q)$ implies for the large-scale behavior of the contact fluctuations. We first note that previously-studied *density* hyperuniformity can be measured from the low- q behavior of the density structure factor, $S_\rho(q) = \frac{1}{N} \left| \sum_i e^{-iq \cdot r_i} \right|^2$. The low- q limit describes long length-scale density fluctuations[23]: $S_\rho(q \rightarrow 0) = \left(\langle N^2 \rangle - \langle N \rangle^2 \right) / \langle N \rangle$, where N is the number of particles in the system. Therefore, if $S_\rho(q \rightarrow 0) = 0$ the density fluctuations are sub-extensive and suppressed compared to typical equilibrium systems [8], on par with those of a perfect crystal. Our result that $S_Z(q) \rightarrow q^\alpha$ at low q at the jamming transition implies that at the transition, the system obeys contact hyperuniformity: the contact fluctuations are highly suppressed at long length scales despite the local randomness in Z_i .

To take a closer look at contact hyperuniformity, we measure contact fluctuations as a function of length scale. We consider a sub-region with linear dimension ℓ , specifically a hypercube of volume ℓ^d in d dimensions. The fluctuations of $\delta Z_i = Z_i - \bar{Z}$ in hypercubes of this size

are characterized by:

$$\sigma_Z^2(\ell) = \frac{1}{\ell^d} \left\langle \left(\sum_{i \in \ell^d} \delta Z_i \right)^2 \right\rangle. \quad (7)$$

where the angular brackets denote an average over different sub-regions (of size ℓ) in a given packing as well as different realizations.

If the δZ_i were uncorrelated random variables then $\sigma_Z^2(\ell) \propto \text{const}$ and any deviations from this would imply correlations. Figure 1e shows $\sigma_Z^2(\ell)$ in $d = 2$ for different values of ΔZ . Figure 1g shows the results are qualitatively similar in $d = 3$. At the smallest value of ΔZ , σ_Z^2 approaches ℓ^{-1} at large ℓ . This implies that fluctuations in the contact number are suppressed; there must be correlations in Z_i to insure this property as seen in $S_Z(q)$. Surface fluctuations are inevitable since translating slightly the measurement window varies which particles are within the measurement window, and as result also the contact number. Increasing ΔZ shows that the decay as a function of ℓ crossovers to what we will argue is a constant at $\ell = \infty$. This implies Poissonian fluctuations in this regime. The cross-over between these two behaviors defines a length scale, ξ_f , which diverges as $\Delta Z \rightarrow 0$. Strangely, this crossover appears to be very slow in comparison to the data presented for $S_Z(q)$. We will argue that ξ_f is indeed larger than ξ_Z , diverging faster than the latter.

We now argue that $\xi_f \propto \Delta Z^{-\nu_f}$ diverges with an exponent that is different from ξ_Z . To relate ξ_f to the measured exponents in $S_Z(q)$ it is useful to express $\sigma_Z^2(\ell)$ in terms of the two-point correlation function. Using, $h_Z(r_2, r_1) = \langle \delta Z(r_2) \delta Z(r_1) \rangle$ it straightforward to show that:

$$\sigma_Z^2(\ell) = \rho \langle (\delta Z_i)^2 \rangle + \frac{1}{\ell^d} \int_{\ell^d} d^d r_1 \int_{\ell^d} d^d r_2 h_Z(r_2, r_1), \quad (8)$$

where ρ is the density of particles and the integral is over the hyper-cube. In the limit of $\ell \rightarrow \infty$, surface terms can be neglected which leads to $\sigma_Z^2(\ell \rightarrow \infty) = \rho \langle (\delta Z_i)^2 \rangle + \int d^d r h_Z(r, 0)$. This is also equal to $S_Z(q \rightarrow 0) / \rho$ (see Eq. 3) such that if $S_Z(q) \propto q^\alpha$ on all length scales then fluctuations are sub-extensive, $\sigma_Z^2(\ell \rightarrow \infty) = 0$.

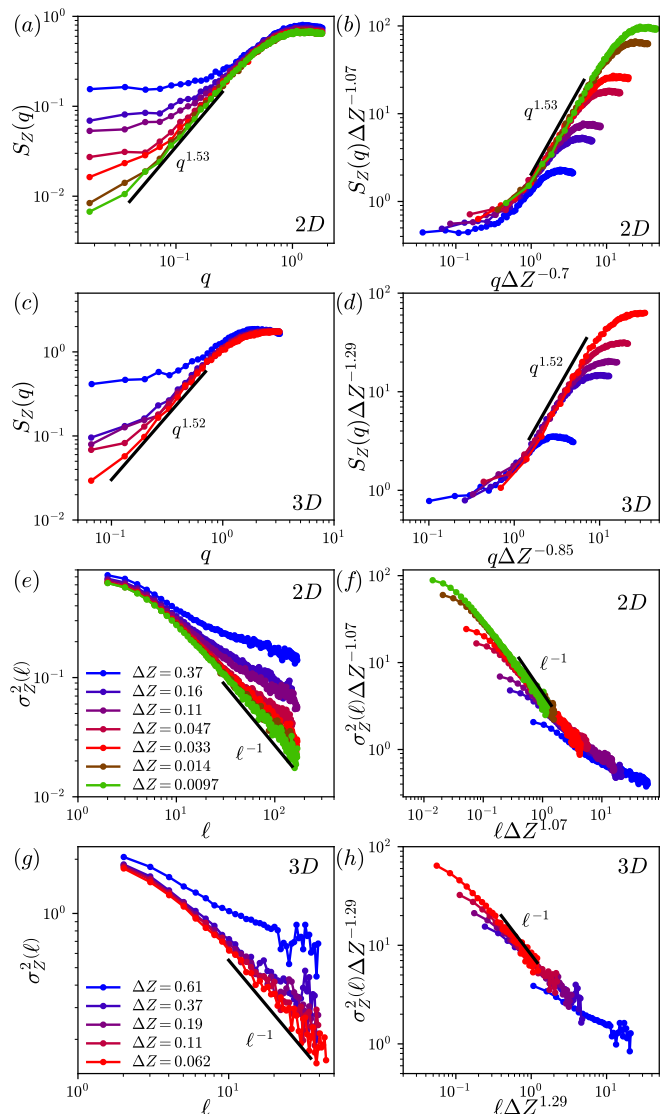


Figure 1. The length-dependent fluctuation of the contact number at different values of ΔZ . The real-space fluctuations are shown in (a) $d = 2$ and (c) $d = 3$ and the fluctuations in Fourier space in (e) $d = 2$ and (g) $d = 3$. The values of ΔZ are shown in the legend. (b), (d), (f) and (h) show the collapse of the data. The number of particles in 2d is $N = 128,000$ and in 3d is $N = 10^6$.

On finite scales the relation is more subtle, leading to two distinct length scales. Ref. [24] considers the relation between the structure factor and scaling of the density fluctuations as a function of scale. We apply their analysis here to the contact statistic, and find that if $S_Z(q) \propto q^\alpha$ then asymptotically $\sigma_Z^2(\ell) \propto \ell^{-\psi}$ where,

$$\psi = \begin{cases} \alpha & \alpha < 1 \\ 1 & \alpha > 1 \end{cases}. \quad (9)$$

This non-analytic relation arises because the fluctuations cannot decay faster than ℓ^{-1} – the contribution due to

fluctuations on the surface[25]. Since in our case $\alpha > 1$ we expect that near the jamming transition $\sigma_Z^2(\ell) \propto \ell^{-1}$ in agreement with the data in Figs. 1e and g. The exponent ν_f can be estimated by comparing ℓ^{-1} to the asymptotic behavior $\sigma_Z^2(\ell \rightarrow \infty) = S_Z(q \rightarrow 0)/\rho \propto \Delta Z^\beta$, yielding $\nu_f = \beta$. Using the values of β obtained in the collapse of $S_Z(q)$ we find that $\nu_f^{2d} = 1.07_{-0.18}^{+0.1}$ and $\nu_f^{3d} = 1.29_{-0.19}^{+0.27}$. Figure 1f and h show that these exponents provide a reasonable collapse of $\sigma_Z^2(\ell)$. Thus, as we asserted above, the fluctuation length scale diverges with an exponent different from that of the correlation length. We argue that generically for systems that have suppressed fluctuations there are two distinct length scales satisfying $\nu_f > \nu_Z$, when $\alpha > 1$, and a single length scale $\nu_f = \nu_Z$ when $\alpha < 1$.

In summary, we have shown that there are two diverging length scales which characterize the contact fluctuations near the jamming transition. Unlike traditional equilibrium critical phenomena, the diverging length scale in the two-point correlations of ΔZ is not accompanied with large fluctuations but rather with the suppression of contact fluctuations on large scales. Indeed it is precisely this *smallness* of fluctuations that make this structural “order” elusive, as there are no large scale features seen to the naked eye.

The small fluctuations in Z_i suggest that it should be considered a control parameter, analogous to temperature in the Ising model, rather than as an order parameter. If we adopt this view, the Harris criterion compares the average of the control parameter, ΔZ inside a volume ξ_f^d to its fluctuations. Stability requires that the average must vanish faster than the fluctuations. The average coordination number scales as ΔZ while contact hyperuniformity implies that the fluctuations scale as the surface area of the region of size ξ_f , as our simulations suggest. The magnitude of the fluctuations scale as the square root of the variance, namely $\xi_f^{-(d+1)/2}$. Comparing these, we obtain the inequality

$$\nu_f > \frac{2}{d+1}. \quad (10)$$

The fact that our observed values obey this inequality in $d = 2$ and $d = 3$ suggests that ΔZ should indeed be viewed as the control variable rather than an order parameter. We note that while the Harris criterion is usually employed in disordered systems in which fluctuations in the control parameter are quenched, here the fluctuations Z_i emerge from many-body interactions.

This conclusion is consistent with the choice made in the scaling ansatz for the jamming transition [26], which suggests that packing fraction and shear strain should be considered the order parameters. However, there are no apparent diverging length scales in the two-point correlations of the packing fraction [27]. A single contact connects two particles and is therefore related to the two-point density correlation function. Therefore, the

two-point contact correlations studied here correspond to four-point density correlations. Our results demonstrate that while “order” can sometimes be found in plain sight, its identification, especially in disordered systems, may require a carefully tailored higher-order correlation function, as has been proposed for glasses [28, 29].

Our results on contact hyperuniformity should be compared to recent studies of density fluctuations at or above the jamming transition. It has been suggested that systems at and above the jamming transition are hyperuniform in density[30–35], but this is controversial. The findings of references [27, 36–38] support the absence of density hyperuniformity above the jamming transition; states prepared upon approach to jamming from below appear to be even less hyperuniform with better equilibration [39]. However, studies of very large systems that explicitly identify a crossover length ξ_ρ below which the system is uniform[40] suggest that ξ_ρ might increase somewhat in the dual limit as the pressure is decreased towards the jamming transition and the equilibration time increases[40]. Density hyperuniformity has also been predicted for sedimentation[41] and periodically sheared suspensions[42, 43].

Our findings open the door to studying several aspects of the jamming transition. *Dynamics*: In studying jamming dynamics, our spatial metrics could be used study how spatial “order” evolves as the spheres approach the jammed state. This is characterized by a dynamical exponent relating relaxation time to the correlation length, $\tau \propto (\xi_Z)^\mu$. Such an exponent was identified in the first study of the jamming transition by Durian [18]. *Interplay of structure and elasticity*: We expect that ξ_Z and ξ_f should be reflected in the diverging length scales found in elasticity [3, 5, 44, 45]. We note that Ref. [45] finds a length scale that diverges as $\Delta Z^{-0.66}$ in two dimensions, consistent with the length scale found in $S_Z(q)$ [46]. *Role of dimensionality*: Our results suggest that some of the exponents depend on dimension, in contrast to previous findings. This suggests that contact hyperuniformity has a non-mean-field flavor in low dimension. It would be interesting to examine this length scale in mean-field calculations.

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