Can a large packing be assembled from smaller ones?

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We consider zero temperature packings of soft spheres, that undergo a jamming to unjamming transition as a function of packing fraction. We compare differences in the structure, as measured from the contact statistics, of a finite subsystem of a large packing to a whole packing with periodic boundaries of an equivalent size and pressure. We find that the fluctuations of the ensemble of whole packings are smaller than those of the ensemble of subsystems. Convergence of these two quantities appears to occur at very large systems, which are usually not attainable in numerical simulations. Finding differences between packings in two dimensions and three dimensions, we also consider four dimensions and mean-field models, and find that they show similar system size dependence. Mean-field critical exponents appear to be consistent with the 3d and 4d packings, suggesting they are above the upper critical dimension. We also find that the convergence as a function of system size to the thermodynamic limit is characterized by two different length scales. We argue that this is the result of the system being above the upper critical dimension.

A starting point for characterizing the structure of ordered materials are their microscopic subunits, or building blocks. Crystalline materials, in their ground state, are defined by a single unit cells repeating throughout the system. Quasicrystalline materials, while aperiodic, still have a rather small number of building blocks, growing polynomially with the size of these subunits. In the case of disordered materials, each subsystems is different and the multiplicity of the different subsystems is huge [16]. Nonetheless, it is interesting to ask, how different is a subsystem from the whole packing it composes?

This question addresses, in part, the effect of boundaries, correlations in the structure, and multiplicity of ground states.

In this paper, we ask this aforementioned question in a commonly studied model for amorphous solids: disordered packings of soft spheres at zero temperature [14] [17] [25]. This model undergoes a rigidity transition, as a function of the packing fraction [20]. We compare the ensemble of subsystems cut out from large packing, to the ensemble of whole systems of the same volume with periodic boundary condition (Fig. [1]). Recently it has been found that the contact statistics possess unusual long range correlations near the transition [15]. We therefore focus on contact fluctuations as a metric to compare the two ensembles.

While we expect convergence of the two ensembles for large enough systems, the system size $V^*$ for which these converge appears to be in many cases well beyond the system size accessible via simulations. For system sizes smaller than $V^*$, fluctuations in contacts are significantly smaller in systems with periodic boundary conditions. When approaching the jamming transition this disparity grows, and $V^*$ appears to diverge, suggesting that it is associated with a diverging length scale. To study convergence to the thermodynamic limit we measure the contact fluctuations in whole systems as a function of the distance to the jamming transition. We perform finite size scaling to identify a length scale, and find that it differs from those previously measured in the contact statistics. Finding differences between 2d and 3d, we also consider 4d and mean-field variants of the jamming model. These appear to be consistent with results from 3d, suggesting that the the upper critical dimension is below three [13].

We interpret our additional length scale within the finite size scaling scenario above the upper critical dimension. Our measurements show that anomalous contact fluctuations survive in mean-field like models, which provides an avenue to measure the upper critical dimension.

We begin by defining the jamming model, in which overlapping particles of radius $R_i$ interact via a harmonic potential:

$$U_{ij} = \frac{1}{2k} \left( 1 - \frac{r_{ij}}{R_i + R_j} \right)^2 \Theta (R_i + R_j - r_{ij}).$$

(1)

Here, $r_{ij}$ is the distance between the centers of the particles and the Heaviside step function, $\Theta (x)$, insures that only overlapping particles interact. In 2d the radii are chosen to be polydisperse to avoid crystallization, while in higher dimension monodisperse particles lead to amorphous packings. The distribution of particle radii does not appear to affect our results. We begin with particles distributed randomly and uniformly throughout space, and minimize the energy at a constant pressure via FIRE algorithm [9] until the system reaches force balance.

An important quantity in understanding the geometry of the jamming transition is the average coordination number, $Z$. At the marginally rigid state at zero pressure, the average coordination number $Z$ attains a

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universal value that approaches \( Z_c = 2d \) for infinite system \([1, 2, 12, 13, 19]\). This amounts to the smallest number of contacts to maintain rigidity. The excess coordination number \( \Delta Z = Z - Z_c \), also characterizes the distance from the jamming transition. Recently, it has been realized that the coordination number possess subtle spatial correlations \([15, 25]\). Unlike equilibrium critical systems that have diverging fluctuations (associated with a diverging susceptibility), packings have anomalously small fluctuations. At the jamming transition the bulk contact fluctuations vanish, and the fluctuations inside a subsystem scale as its surface.

We now briefly review the metrics and the results of Ref. \([15]\) for characterizing the fluctuations. Defining \( Z_i \) to be the number of particles in contact with particle \( i \), and the deviation from its average value, \( \delta Z_i = Z_i - \bar{Z} \), the fluctuations are characterized by measuring the variance in a hyper-cube of volume \( \ell^d \),

\[
\sigma^2_Z(\ell) = \frac{1}{\ell^d} \langle \left( \sum_{i \in \ell^d} \delta Z_i \right)^2 \rangle.
\]

(2)

Here the average is over many subsystems of a large packing, as well as many packings all at the same pressure. If \( \delta Z_i \) were uncorrelated random variables, then \( \sigma^2_Z(\ell) \) would not depend on \( \ell \), since the number of particles scales as the volume. At the jamming transition, \( \Delta Z = 0 \), the fluctuations scale in the smallest possible way, \( \sigma^2_Z(\ell) \propto \ell^{-1} \), implying that the sub-extensive fluctuations are dominated by the surface of the enclosure\([22]\). At a finite distance from jamming, \( \Delta Z > 0 \), the fluctuations are only suppressed up to a length scale \( \xi_f \propto \Delta Z^{-\nu_f} \); above \( \xi_f \), the lack of correlations imply that \( \sigma^2_Z(\ell) \) is independent of \( \ell \). We also remark that unlike typical critical systems, here there are two different diverging length scales. A second length scale, \( \xi_g \propto \Delta Z^{-\nu_g} \), can be measured from \( \langle \delta Z(r) \delta Z(0) \rangle \) and is different than \( \xi_f \), having different exponents \( \nu_f > \nu_g \).

In this paper, in addition to \( \sigma^2_Z(\ell) \), we characterize sample-to-sample fluctuations of many jamming configurations with periodic boundaries, at the same value of pressure. We define

\[
\delta^2 Z(N) \equiv N \left[ \langle Z^2 \rangle - \langle Z \rangle^2 \right],
\]

(3)

where the average is over realizations with different initial particle positions prior to the energy minimization. Here the coordination number of a given sample is defined by \( Z \equiv \frac{1}{N} \sum_{i=1}^N Z_i \), where \( N \) are the number of particles excluding the rattlers. The factor of \( N \) on the right hand side of Eq. (3) ensures convergence to a finite value in the limit of \( N \to \infty \). We also note that in the infinite size limit, where boundary condition are unimportant, \( \rho \delta^2 Z(N = \infty) = \sigma^2_Z(\ell = \infty) \), where \( \rho \) is the number density. To see how this is related to \( \xi_f \), we note that a sufficiently large system can decomposed into uncorrelated sub-regions of volume \( \xi_f^d \). In each such region the fluctuations scale as the surface, \( \ell^{-d-1} \). Because the number of uncorrelated regions is \( (L/\xi_f)^d \), we obtain

\[
\delta^2 Z(N \gg \xi_f^d) \propto \frac{1}{\rho} \xi_f^{-1} \propto \Delta Z^{\nu_f}.
\]

(4)

We now turn to show how \( \sigma^2_Z(\ell) \) and \( \delta^2 Z(N) \) compare on a finite length scale. To make this comparison, we express \( \sigma^2_Z(\ell) / \rho \) as a function of \( N = \rho \ell^d \), where the factor \( 1/\rho \) ensures that fluctuations are normalized by \( N \), instead \( V \). Results in 2d and in 3d (Fig. 2) show that sample-to-sample fluctuations, \( \delta^2 Z \), are smaller than \( \sigma^2_Z \) and have a fairly weak dependence on system size. The difference between the two ensembles grows dramatically upon approaching the jamming transition, \( \Delta Z \to 0 \). Because \( \sigma^2_Z(\ell) \) and \( \delta^2 Z(N) \) converge in the thermodynamic limit, one can define a length scale at which the two ensembles converge. This length scale is surprisingly large, especially in 3d. Even at \( \Delta Z \approx 1.22 \), which is usually considered to be far from the jamming transition, convergence occurs for \( N > 10^5 \). For \( \Delta Z \approx 0.12 \) convergence can be extrapolated to occur for system sizes of \( N > 10^8 \) which are currently not attainable numerically. The fact that convergence in 2d appears to occur at smaller \( N \) suggests that it is dominated by a correlation length.

It is interesting to speculate on why the sample-to-sample fluctuations are much smaller than the fluctuations in a subsystem. Subsystems, by definition, have boundaries, and these always entail a surface contribution that scales as \( \ell^{-1} \). This suggests that \( \delta^2 Z \), which lacks these surface fluctuations, measures the bulk contribution to the fluctuations, scaling as \( \Delta Z^{\nu_f} \), as noted in Eq. (4). We will demonstrate that this scaling holds on length scales smaller than \( \xi_d = \Delta Z^{-\nu_2} \), and above this length scale finite size effects are present. The length
Figure 2. Comparison of the fluctuations of contacts of entire packings, $\delta^2 Z$, to the contact fluctuations of a sub-system $\frac{1}{2} \sigma^2 d$ with the same number of particle in 2d (top) and 3d (bottom).

$\xi_d$ is smaller than both $\xi_Z$ and $\xi_f$ in $d > 2$, so that $\nu_d < \nu_z < \nu_f$.

In order to measure $\nu_z$ and $\nu_f$, in Fig. 3 we plot the fluctuation $\delta^2 Z$ as a function of $\Delta Z$, for different system sizes, in $d = 2, 3, 4$. In all cases there is a dependence on system size, mostly observed at small values of $\Delta Z$, where $\delta^2 Z$ decreases with system size. This effect seems to be smaller in 2d than in 3d and 4d. For large enough systems the curves appear to converge, and for these we measure $\nu_f$, from Eq. (4). The values of $\nu_f$ are consistent with Ref. 15, where $\nu_f^a \approx 1.25$ and $\nu_f^a \approx 1.0$. The variation between 2d and 3d is also manifest in the qualitative shape of the curves: unlike the 3d curves, the 2d results taper off at large values of $\Delta Z$. The behavior in 4d is consistent with the three dimensional case, $\nu_f^d \approx 1.25$.

To characterize the system size dependence, we collapse the different curves by assuming a scaling form,

$$\delta^2 Z = N^{-\alpha_f} (\Delta Z N^\alpha) .$$  \hspace{1cm} (5)

Requiring that in the limit of $N \to \infty$, $\delta^2 Z \propto \Delta Z^{\nu_f}$ is independent of the system size, yields $\beta = \alpha \nu_f$. Hence, given $\nu_f$, the curves can be collapsed by varying a single exponent. Because the number of particles is proportional to the volume, $L^d$, the argument of Eq. (3) can be rewritten as $\Delta Z N^\alpha \propto \left(\frac{L}{\xi_d}\right)^{\alpha_d}$, with $\xi_d \equiv \Delta Z^{-\nu_d}$ and $\nu_d \equiv 1/(\alpha d)$. The collapse shown in Fig. 3 yields approximately $\alpha \approx 0.6$ both in 3d and 4d, implying that $\nu_d$ depends on dimension. In 3d the exponent $\nu_d$ is smaller than $\nu_z$ and $\nu_f$, measured in Ref. 15. In 2d it is difficult to determine $\alpha$; because $\nu_f^d \approx 1.0$ there is a range of exponents $\alpha = \beta$ which collapse the data reasonably well.

To explore the dependence on dimension, we also consider the mean-field limit of the jamming model, by simulating the Mari-Kurchan (MK) model 18. This model retains most of the details of jamming model, including the interaction potential in Eq. (1), but aims at disrupting the spatial correlations by varying the spatial metric. A given particle $i$ sees particle $j$ at a location shifted by a random value, $d_{ij}$, which is uniformly distributed through space. The potential between particle $i$ and $j$ is thus given by $U_{ij} = U(|r_i - r_j - d_{ij}|)$, and the interaction between particles does not depend on the actual Euclidean distance between them.

Figure 4 shows the results of the simulations of the
MK model in 2d and 3d, which overall appear very similar to the 3d and 4d non-mean field variant. In the large system size limit, the MK curves appear to converge to $\Delta Z^{\nu_{MK}}$ and $\nu_{MK} \approx 1.25$ independently of dimension. The exponent is also very similar to the 3d and 4d result, suggesting that the upper critical dimension is less than three [13]. Figure 4a) we also collapse the curves using the scaling form in Eq. (5). Within error, the resulting exponents agree with those of the 3d and 4d jamming model. Hence, the collapse of $\delta^2 Z$ does not depend on the length of the system but rather its volume, or number of particles. Because $\alpha$ is independent of dimension (for 3d and above), the scaling of the length scale $\xi_d \propto \Delta Z^{-\nu_d}$, with $\nu_d = 1/(\alpha d)$, does depend on dimension. This is contrasted by the collapse of the fluctuations in a subsystem with $\ell/\xi_f$, the length $\xi_f$ scaling independently of dimensions.

We now discuss the finite size scaling of $\delta^2 Z$. The theory of finite size scaling above the upper critical dimension $d_u$ has emerged from work on the Ising model [2, 23] predicts two types of scalings, depending on the quantities considered. Finite size scaling of fluctuations of whole systems collapse as a function of the system size (number of particles). The intuitive reason is that some mean-field models cannot be embedded in Euclidean space, and are thus defined by system size alone. Nonetheless, there is a correlation length, whose exponent is given by its mean-field value. The scaling of quantities associated to a finite wavelength, on the other hand, depend on the ratio of a length and the correlation length. Hence, quite generally one can define two diverging length scales for systems above $d_u$, in contrast to dimension below $d_u$ where only one correlation scale is relevant. In the jamming model this scenario is realized by a different collapse of $\sigma_Z^2$ and $\delta^2 Z$. One can exploit these different collapses to measure $d_u$, by estimating the dimension where the two length scales coincide. Extrapolating $\nu_d = 1/(\alpha d)$ to the dimension where it is equal to the mean field exponent yields $d_u$. However, as mentioned above, in the jamming transition there are two length scales that characterize contact statistics [13]: $\xi_Z$, which characterizes the two point correlation function, and $\xi_f$, which characterizes the cross-over of the hyperuniform fluctuations to the normal fluctuations. We argue that the first is a more fundamental quantity, and using the exponent $\nu_Z^d \approx 0.85$ measured in [14] we obtain that $\nu_d = \nu_Z$ when $d_u \approx 2$.

This estimate of $d_u \approx 2$ is consistent with our findings that 2d appears somewhat different. Differences can arise either due to logarithmic corrections at $d_u$, or because $d_u$ is slightly different than two. In the latter case, then $\delta^2 Z$ would collapse with the two dimensional correlation length, implying that $\alpha_{2d} = 1/2\nu_{2d}^d$. The collapse in Fig. 4 shows reasonable agreement, but the finite range of our data allows other values as well. Note that it has long been thought that the upper critical dimension is two [17, 24]. This is mostly based on observations that exponents appear to be independent of dimension, for $d \geq 2$ [6, 8, 9, 21].

We also consider a different class of jamming models, which are not isostatic at the jamming transition [5]. This model is thought to be associated with packings of non-spherical particles [4, 19, 11]. The inter-particle interactions are given by Eq. (1), but the particle radii are also considered as degrees of freedom. To ensure that particles do not shrink to zero, a confining potential is assigned to the radii:

$$U_r = \sum_i k_r \left( R_i - R_i^0 \right)^2. \quad (6)$$

To avoid crystallization, in 2d we consider a bidisperse particle distribution, where the diameter $R_i^0$ of half of the particles is larger by a factor 1.4 than that of the others. An important feature of this model is the scaling of the stiffness $k_r$. To achieve a radii distribution with finite width at jamming, $k_r = P k_0$, where $P$ is the pressure and $k_0$ sets the overall magnitude of the stiffness. In the limit of $k_0 \rightarrow \infty$, the behavior of the usual jamming transition is recovered.

Unlike the usual jamming transition, in the limit of $P \rightarrow 0$, the system is not isostatic, $\Delta Z > 0$. In Fig. 5a) we show that our simulations are consistent with the results of Ref. [5]. In Fig. 5b) we plot the contact fluctuations as a function of pressure. In the limit of $P \rightarrow 0$, the contact fluctuations $\delta^2 Z$ remain finite, in contrast to the vanishing fluctuations of the conventional jamming transition. This suggests that isostaticity is important for the suppression of fluctuations and the divergence of correlation lengths.

We conclude by reiterating our main results. Fluctuations in whole systems are smaller than in subsystems.
This is most significant at the jamming transition where the $\delta^2 Z \to 0$, while the fluctuations in a subsystem scale as $\ell^{-1}$, which is the fastest possible decay. Moreover, $\delta^2 Z$ and $\sigma_2^2$ converge to their thermodynamic value with different exponents for 3d and above. The sample-to-sample fluctuations, $\delta Z$, approach their asymptotic value at system sizes $N \sim \Delta Z^{-1/\alpha}$, where $\alpha \approx 0.6$ is independent of dimension. Fluctuations in a subsystem only reach their asymptotic values at a system length $\ell \sim \Delta Z^{-\nu_f}$, where $\nu_f \approx 1.25$ is also independent of dimension. Under typical system sizes and values of $\Delta Z$, usually considered in simulations, the system is well below $\xi_f$. It is therefore, interesting to explore if new behaviors arise for large systems and how $\xi_f$ and $\xi_Z$ affect the behavior of the packings. As a byproduct of this analysis, we obtain an estimate of the upper critical dimension $d_u \approx 2$, as the dimension where the distinction between $\xi_d$ and $\xi_Z$ disappears. Our results also show that a signature of suppressed fluctuations survive in mean-field variants of the jamming model. The exact solution of these models enables, in principle, the calculation of $\nu_f$, although the calculation is technically involved. The exponent $\nu_z$ that characterizes the spatial decay of $\langle \delta Z(r) \delta Z(0) \rangle$ still remain inaccessible to present theory.

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