Soft-Sphere Packings at Finite Pressure but Unstable to Shear

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When are athermal soft-sphere packings jammed? Any experimentally relevant definition must, at the very least, require a jammed packing to resist shear. We demonstrate that widely used (numerical) protocols, in which particles are compressed together, can and do produce packings that are unstable to shear—and that the probability of generating such packings reaches one near jamming. We introduce a new protocol which, by allowing the system to explore different box shapes as it equilibrates, generates truly jammed packings with strictly positive shear moduli $G$. For these packings, the scaling of the average of $G$ is consistent with earlier results, while the probability distribution $P(G)$ exhibits novel and rich scalings.

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Foams, emulsions, colloidal suspensions, granular media and other particulate media undergo a jamming transition when their constituent particles are packed densely enough [1–7]. This transition has been extensively studied in packings of deformable, athermal, frictionless spheres interacting through purely repulsive contact forces [8–12]. The limit where the particles just touch then plays the role of an unusual critical point, as a host of quantities, such as shear modulus, time and length scales, and contact number exhibit power law scaling with the distance to this critical point [8–17].

Numerically created particle packings play a central role in many fields of physics, in particular jamming. In all numerical jamming studies we are aware of, packings are created by compressing a collection of particles, either by inflating the particles or shrinking the simulation box [8–17]. It is then widely believed and tacitly assumed that, when compressed, the system simultaneously develops a finite pressure, a finite yield threshold [9,10] and a positive shear modulus $G$ [8–13]. Here we demonstrate that, to the contrary, algorithms that work solely by compression tend to produce packings that are unstable to shear, and hence have negative shear moduli. Nevertheless, such “improperly jammed” packings possess a positive pressure $P$ and a positive bulk modulus, and are in mechanical equilibrium—see Fig. 1(a).

In this Letter, we probe and explain this anomaly. The root problem is that compression-only (CO) algorithms ignore the global shear degrees of freedom. We find that this results in a fraction of improperly jammed CO packings which reaches one at the critical point. Hence, compression alone does not lead to jammed packings, and previous results on jamming have considered packings that, instead of being jammed, have been linearly unstable to shear—in particular near jamming.

Furthermore, we remedy this anomaly by introducing a shear stabilized (SS) packing algorithm that produces truly jammed packings with positive definite shear moduli [18], and probe the probability distribution of $G$, uncovering novel scaling with distance to jamming and system size.

Shear moduli in CO packings.—We have generated 2D packings of $N$ soft harmonic bidisperse disks (with unit spring constant [11]) by a standard CO packing generating algorithm, for pressures $P$ ranging from $10^{-6}$ to $10^{-1}$ and $16 \leq N \leq 1024$. Prior studies of the shear modulus have focused on ensemble averages at fixed distance to the jamming point ($P$), typically for large $N$, and without reference to the angular dependence of $G$.

As illustrated in Fig. 1(b), fluctuations and anisotropy are key: $G$ varies sinusoidally with $\theta$, and its angular average, $G_{DC}$, varies substantially with realization. We distinguish three types of packings. (I) Truly jammed...

FIG. 1 (color online). (a) Example of a well-equilibrated CO packing of $N =$ 32 particles which is unstable to shear (pressure $P = 10^{-2}$, bulk modulus $K = 0.385$, contact number $z \approx 4.26$). (b) Illustration of the sinusoidal angular dependence of $G$ on the principle direction of shear, $\theta$, for three different packings at the same $N$ and $P$—curve III corresponds to the packing shown in (a), and dashed lines indicate $G_{DC}$, the angular average of $G$. 

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packings for which \( G(\theta) > 0 \). (II) Improperly jammed packings for which \( G(\theta) < 0 \) (III) Improperly jammed packings for which \( G(\theta) \) becomes negative over an interval in \( \theta \). We stress that all these packings are in a mechanical equilibrium and have a positive bulk modulus.

It has been customary to measure \( G \) along a fixed direction [10,15,19–23], and the limited unstable range of type III packings, combined with the rare occurrence of type II packings, may explain why these instabilities have escaped attention to date. Since simulations often produce some “problematic” packings (for example due to issues with convergence), packings of types II and III have likely been treated as “bad apples” and thrown out of the ensemble [24,25].

**Boundaries and shear stabilization.**—Improperly jammed packings are not caused by numerical artifacts but stem from the essence of compression-only (CO) algorithms. Consider the potential energy landscape as a function of the particle positions, \( |r| \), and shear deformations of the box, \( |\Delta L| \) (Fig. 2). CO algorithms fix the unit cell and generate packings at a minimum of \( U \) with respect to \( |r| \). Residual shear stresses and shear moduli correspond to the first and second derivatives, respectively, of \( U \) along a strain direction \( \Delta L \)—without permitting the strain degrees of freedom to equilibrate, both the residual stress and shear modulus are uncontrolled.

To create packings that are guaranteed to be stable against shear in all directions, we include shear deformations of the box and search for local energy minima of \( U \) (Fig. 2) [26]. We combine standard conjugate gradient techniques [25] with the FIRE algorithm [27], which improves the speed by an order of magnitude, and also precisely control the pressure of the resulting packings. Since the energy is at a minimum with respect to the shear degrees of freedom, these packings have strictly positive values of \( G \) and exhibit zero residual shear stress [26], unlike CO states. However, as a result of equilibrating the strain degrees of freedom, the unit cell is no longer square. For example, starting from a CO packing (minimum of \( U \) with respect to \( |r| \)), the box is deformed to find a minimum in the extended space spanned by \( |r| \) and the strain coordinates (Fig. 2). Such deformations are small for large systems [28].

A formal way of capturing the role of the boundaries is in terms of the stiffness matrices \( \hat{K}^0 \) and \( \hat{K} \), where \( \hat{K}^0 \) is the usual Hessian, while the “extended Hessian” \( \hat{K} \), introduced in a different context in Ref. [17], includes the dependence on the shear degrees of freedom—for details see the Supplemental Material [29]. It can then be shown that \( G(\theta) \) is positive definite for all \( \theta \) if all eigenvalues of \( \hat{K} \) are positive (excluding the trivial zero energy translational modes). Defining \( \lambda_{\text{min}} \) as the minimal eigenvalue of \( \hat{K} \), the sufficient condition for a packing to be stable against shear is \( \lambda_{\text{min}} > 0 \). In contrast, a positive spectrum for the usual Hessian \( \hat{K}^0 \) only guarantees stability in a box with fixed boundaries, but does not guarantee stability to all possible shear deformations (Figs. 1 and 2), contrary to the claim in Ref. [30].

Scatter plots of shear modulus and \( \lambda_{\text{min}} \) for CO and SS ensembles shown in Fig. 3 confirm our picture: (i) All SS packings have positive \( \lambda_{\text{min}} \) and \( G \). (ii) CO packings can have negative \( \lambda_{\text{min}} \). Although many of these \( \lambda_{\text{min}} < 0 \) packings are stable when sheared along a fixed direction (dots correspond to \( \theta = 0 \), they almost always have negative \( G \) when sheared along other directions.

**Fraction of improperly jammed CO packings.**—What fraction of CO packings is unstable to shear? What governs the scaling of this fraction? Fig. 4 shows that the probability that CO packings have shear directions along which \( G \) is negative, \( P_{G<0} \), reaches one near jamming, and that larger packings need lower pressures for these instabilities to become dominant. It is natural to expect that \( P_{G<0} \)

![FIG. 2 (color online). Energy landscape where \( |r| \) denotes the particle degrees of freedom, and \( \Delta L \) the box-shape. CO packings sit at a minimum of \( U \) with respect to \( |r| \); SS packings sit at a minimum with respect to both \( |r| \) and \( \Delta L \).](image-url)
isometric when the number of constraints, $Nz_{\text{iso}}:=z-z_{\text{iso}}=z-4+4/N$. Would collapse when plotted as a function of $L/l^*$, where $l^*$ is a characteristic length-scale which diverges as $1/\Delta z$ near jamming, and where $\Delta z$ is the difference between the contact number $z$ and its value at the jamming point $[11,12,15,31–33]$. Surprisingly, Fig. 4 shows that the number of excess contacts $\sim N\Delta z$, not the characteristic length scale $l^*$, governs the fraction of improperly jammed packings—note that we have included a finite size correction to $\Delta z$ (see below).

We conclude that the standard view of the jamming transition, in which rigidity is attained by simply compressing particles together $[10–12]$, needs a revision: when the pressure is lowered in finite CO packings, more and more packings will become unstable to shear, leading to a blurring of the (un)jamming transition. We stress that both the distance to jamming and the system size play a crucial role $[34]$.

Scaling of contact number and $G$—Do the same scaling laws for, e.g., $z$ or $G$ $[11,12]$, govern both CO and SS packings? To answer this question, we have performed a finite size scaling analysis of both SS and CO packings: both the distance to jamming and the system size play a crucial role $[34]$.

We first consider the contact number $z$ $[9–12,35]$. A packing is called isometric when the number of constraints, $C$, equals $N_{\text{DOF}}-N_0$, the number of degrees of freedom $N_{\text{DOF}}$ minus the number of rigid body modes $N_0$. There is one constraint for each of the $N_c = Nz/2$ force bearing contacts $[36]$. In two dimensions, $N_0 = 2$, corresponding to two rigid body translations (rotation is incompatible with periodic boundary conditions). Hence,

$$z_{\text{iso}} \geq \frac{2}{N}(N_{\text{DOF}} - N_0).$$

(1)

For CO states in two dimensions, $N_{\text{DOF}} = 2N$ (the particle displacements), so that $z_{\text{iso}}^{\text{CO}} = 4 - 4/N$. For SS states the particle displacements are augmented by two shear degrees of freedom, leading to $z_{\text{iso}}^{\text{SS}} = 4$.

Is the isostatic bound reached at unjamming? We have found that both CO and SS packings have one contact in excess of their respective isostatic values when approaching the jamming point (see Supplemental Material $[29]$). Goodrich et al. have argued that this extra contact reflects the requirement that jammed states have positive bulk modulus, which puts an additional constraint on the box size $[37]$.

We now turn our attention to the scaling of $G$, and first investigate the scaling of the angle-averaged shear modulus $G$ in ensembles of finite sized CO and SS packings. In Fig. 5(a) we show that in the CO ensemble, $G$ is proportional to $z-z_{\text{iso}}$, consistent with prior results $[10,15,17,23,37]$. In Fig. 5(b) we show that in the SS ensemble, the average shear modulus is proportional to $z-(z_{\text{iso}} - 8/N)$. So, although the SS shear modulus is also linear in $z$, its vanishing point extrapolates to a state with four contacts less than the isostatic state. We note that in both ensembles $G$ is of order $1/N$ in the zero pressure limit.

The amount of scatter in $G$ observed in our new CO packings is surprisingly large. We note that previous work did not consider the value of $G$ over all angles and discarded negative values of $G$, which leads to a smaller scatter $[24,25]$. Recent work by Goodrich et al. shows that this scatter can be further suppressed by using exceptionally accurate equilibration and larger ensembles $[37]$. Nevertheless, the observation that SS data exhibits far lower scatter than CO data, while both packings were obtained with the same numerical accuracy, suggests that remnants of the unstable modes present in the CO ensemble hinder accurate equilibration.

With few exceptions $[10,15,16,38–42]$, studies of jamming have focused on ensemble averages. Here we consider the probability distribution $P(G)$ for both ensembles, sampling both $\theta$ and realizations. Figure 6(a) illustrates that for CO packings, $P(G)$ often peaks at negative $G$, and can possess an extended tail towards negative $G$. In con-
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[18] The distinction between CO and SS packings is comparable to the difference between what Torquato and F. Stillinger refer to as collectively and strictly jammed packings, although these concepts are defined for hard particles [46].
[26] To obtain positive \( G \), in principle one only requires the sign of the curvature of \( U \), \( \partial^2 U / \partial y^2 \), to be positive. At a minimum of \( U \), \( \partial U / \partial y = 0 \) as well, leading to states with zero residual shear stress.

FIG. 6 (color online). (a) The probability distributions for \( G \) of CO and SS packings differ qualitatively. (b) Scaling of the variance \( \langle (G - \langle G \rangle)^2 \rangle \) for SS packings reveals novel scaling. (c) \( P(G/\langle G \rangle) \) shows a systematic variation with \( L \Delta \tilde{z} \).
[28] We stress here that these anisotropies pertain to individual packings—ensembles of CO or SS packings are isotropic.
[31] For harmonic particles, $\Delta z \sim P^{1/2}$ [11,12].
[34] S. Dagois-Bohy, B. P. Tighe, and M. van Hecke (to be published).
[36] Here, $N$ denotes the number of particles after a small fraction of non-force-bearing particles, or “rattlers,” have been removed.