

Distinctive features arising in maximally random jammed packings of superballsY. Jiao,¹ F. H. Stillinger,² and S. Torquato^{1,2,3,4,5}¹*Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544, USA*²*Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA*³*Department of Physics, Princeton University, Princeton, New Jersey 08544, USA*⁴*Princeton Center for Theoretical Physics, Princeton University, Princeton, New Jersey 08544, USA*⁵*School of Natural Sciences, Institute for Advanced Study, Princeton, New Jersey 08540, USA*

(Received 2 January 2010; published 15 April 2010)

Dense random packings of hard particles are useful models of granular media and are closely related to the structure of nonequilibrium low-temperature amorphous phases of matter. Most work has been done for random jammed packings of spheres and it is only recently that corresponding packings of nonspherical particles (e.g., ellipsoids) have received attention. Here we report a study of the maximally random jammed (MRJ) packings of binary superdisks and monodispersed superballs whose shapes are defined by $|x_1|^{2p} + \dots + |x_d|^{2p} \leq 1$ with $d=2$ and 3 , respectively, where p is the deformation parameter with values in the interval $(0, \infty)$. As p increases from zero, one can get a family of both concave ($0 < p < 0.5$) and convex ($p \geq 0.5$) particles with square symmetry ($d=2$), or octahedral and cubic symmetry ($d=3$). In particular, for $p=1$ the particle is a perfect sphere (circular disk) and for $p \rightarrow \infty$ the particle is a perfect cube (square). We find that the MRJ densities of such packings increase dramatically and nonanalytically as one moves away from the circular-disk and sphere point ($p=1$). Moreover, the disordered packings are hypostatic, i.e., the average number of contacting neighbors is less than twice the total number of degrees of freedom per particle, and yet the packings are mechanically stable. As a result, the local arrangements of particles are necessarily nontrivially correlated to achieve jamming. We term such correlated structures “nongeneric.” The degree of “nongenericity” of the packings is quantitatively characterized by determining the fraction of local coordination structures in which the central particles have fewer contacting neighbors than average. We also show that such seemingly “special” packing configurations are counterintuitively not rare. As the anisotropy of the particles increases, the fraction of rattlers decreases while the minimal orientational order as measured by the tetratic and cubatic order parameters increases. These characteristics result from the unique manner in which superballs break their rotational symmetry, which also makes the superdisk and superball packings distinctly different from other known nonspherical hard-particle packings.

DOI: [10.1103/PhysRevE.81.041304](https://doi.org/10.1103/PhysRevE.81.041304)

PACS number(s): 61.50.Ah, 05.20.Jj

I. INTRODUCTION

Particle packing problems, such as how to fill a volume with given solid objects as densely as possible, are among the most ancient and persistent problems in science and mathematics. A *packing* is a large collection of nonoverlapping solid objects (particles) in d -dimensional Euclidean space \mathbb{R}^d . The packing density ϕ is defined as the fraction of space \mathbb{R}^d covered by the particles. Dense ordered and random packings of nonoverlapping (hard) particles have been employed to understand the equilibrium and nonequilibrium structure of a variety many-particle systems, including crystals, glasses, heterogeneous materials and granular media [1–4]. Packing problems in dimensions higher than three attract current interest for retrieving stored data transmitted through a noisy channel [5–8].

The packings of congruent hard spheres in \mathbb{R}^3 have been intensively studied since despite the simplicity they exhibit rich packing characteristics. It is only recently that the densest packings with $\phi_{\max} = \pi/\sqrt{18} \approx 0.74$, realized by the face-centered cubic lattice and its stacking variants, have been proved [9]. In addition, three-dimensional random packings can be prepared both experimentally and numerically with a relatively robust density $\phi \approx 0.64$ [10,11]. The term *random close packing* (RCP) [12], widely used to designate the

“random” packing with the highest achievable density, is ill-defined since random packings can be obtained as the system becomes more ordered and a definition of randomness has been lacking. A more recent concept that has been suggested to replace RCP is that of the maximally random jammed (MRJ) state [11], corresponding to the most disordered among all jammed (mechanically stable) packings. A jammed packing is one in which the particle positions and orientations are fixed by the impenetrability constraints and boundary conditions [13]. It has been established that the MRJ state for spheres in \mathbb{R}^3 has a density of $\phi \approx 0.637$, as obtained by a variety of different order metrics [13,14]. This density value is consistent with what has traditionally been associated with RCP in three dimensions.

It has been argued in the granular materials literature that large disordered jammed (MRJ) packings of hard frictionless spheres are *isostatic* [15,16], meaning that the total number of interparticle contacts (constraints) equals the total number of degrees of freedom of system and that all of the constraints are (linearly) independent. This implies that the average number of contacts per particle Z is equal to twice the number of degrees of freedom per particle f (i.e., $Z=2f$), in the limit as the number of particles gets large. This prediction has been verified computationally with very high accuracy [17,18]. On the other hand, a packing is *hypostatic* if it is mechanically stable (i.e., jammed) while the number of con-

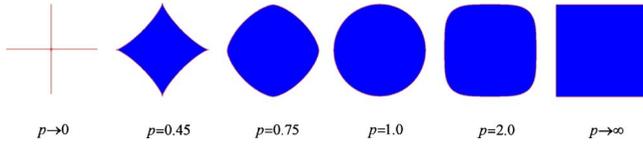


FIG. 1. (Color online) Superdisks with different values of the deformation parameter p .

straints is smaller than the number of degrees of freedom. For large packings, this is equivalent to the inequality $Z < 2f$. It has been shown that a jammed sphere packing cannot be hypostatic [17].

It is also of great practical and fundamental interest to understand the organizing principles of dense packings of nonspherical particles [19–28]. The effect of asphericity is an important feature to include on the way to characterizing more completely real dense granular media as well as low-temperature states of matter. Another important application relates to supramolecular chemistry [29] of organic compounds whose molecular constituents can possess many different types of symmetry groups [30]. Such systems can be approximated by nonspherical hard particles with the same symmetry groups.

Recently, MRJ packings of three-dimensional ellipsoids [31,32] have been studied. In particular, it was found that the density ϕ and the average coordination number Z (the average number of touching neighbors per particle) increase rapidly, in a cusplike manner, as asphericity is introduced from the sphere point. The density ϕ reaches a maximum at a critical aspect ratio α^* [33] and then begins to decrease; while Z increases monotonically until it attains a plateau value for all α beyond α^* . In addition, Z is always smaller than twice the number of degrees of freedom per particle f with its plateau value slightly below $2f$ (for an ellipse $f=3$ and for an ellipsoid $f=6$). In other words, the packings are *hypostatic* [32]. The characteristics of MRJ ellipsoid packings are distinctly different from their densest crystalline counterpart [21], in which ϕ increases smoothly as one moves away from the sphere point, and reaches a plateau value of 0.7707... for $\alpha > \sqrt{3}$ (oblate spheroids) and $\alpha < 1/\sqrt{3}$ (prolate spheroids).

In Refs. [25,26], we studied dense and maximally dense packings of *superballs*, a family of nonspherical particles with versatile shapes. In particular, a d -dimensional superball is a centrally symmetric body in \mathbb{R}^d occupying the region

$$|x_1|^{2p} + |x_2|^{2p} + \dots + |x_d|^{2p} \leq 1, \quad (1)$$

where x_i ($i=1, \dots, d$) are Cartesian coordinates and $p \geq 0$ is the *deformation parameter*, which indicates to what extent the particle shape has deformed from that of a d -dimensional sphere ($p=1$). Henceforth, the terms *superdisk* and *superball* will be our designations for the two-dimensional ($d=2$) and three-dimensional ($d=3$) cases, respectively. A superdisk possesses square symmetry, as p moves away from unity, two families of superdisks can be obtained, with the corresponding fourfold rotational symmetry axes rotated by 45° with respect to each other; when $p < 0.5$, the superdisk is concave (see Fig. 1). A superball can possess two types of

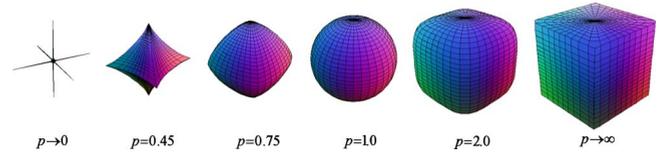


FIG. 2. (Color online) Superballs with different values of the deformation parameter p .

shape anisotropy: cubelike shapes (for $p > 1$) and octahedronlike shapes (for $0 < p < 1$) with a shape change from convexity to concavity as p passes downward through 0.5 (see Fig. 2).

Optimal packings of congruent superdisks and superballs apparently are realized by certain Bravais lattices possessing symmetries consistent with those of the particles [25,26,28]. Even these crystalline packings exhibit rich characteristics that are distinctly different from other known packings of nonspherical particles. For example, we found that the maximal density ϕ_{\max} as a function of p at $p=1$ (the sphere or circular-disk point) is nonanalytic and increases dramatically as p moves away from unity. In addition, we have discovered twofold degenerate maximal density states for squarelike superdisks, and both cubelike and octahedronlike superballs.

In this paper, we generate both packings of binary superdisks in \mathbb{R}^2 and monodispersed superballs in \mathbb{R}^3 that represent the MRJ state of these particles, using a novel event-driven molecular dynamics algorithm [34,35] and investigate their characteristics. For both superdisks and superballs, we find that the corresponding density ϕ and the average contact number Z increase rapidly, in a cusplike manner, as the particles deviate from perfect circular disks and spheres, respectively. In particular, we find that the MRJ packing density ϕ increases monotonically as p moves away from unity, and shows no signs of a plateau even for large p values. This is to be contrasted with the case of ellipsoids for which the packing density reaches a maximum as the aspect ratio increases from its sphere point value and then begins to decrease as the aspect ratio grows beyond that associated with the density-maximum value.

Moreover, we find that Z for superdisk and superball packings reaches its associated plateau value at relatively small asphericity deviations (i.e., $|p-1|$) and the packings remain *highly hypostatic* for all values of p examined. By “highly hypostatic,” we mean that Z is much smaller than twice the number of degrees of freedom per particle. This is to be contrasted with random ellipsoid packings in which the asymptotic value of Z for large aspect ratios (i.e., the plateau value) is only *slightly* below $2f$. Therefore, to achieve jamming, the local particle arrangements are necessarily correlated in a nontrivial way. We call such correlated structures “nongeneric” [36]. We quantify the degree of “nongenericity” of the packings by determining the fraction of local coordination configurations in which the central particles have fewer contacting neighbors than average Z . We also show that such “nongeneric” configurations are not rare, which is a rather counterintuitive conclusion. In addition, we find that although the rapid increase of density is unrelated to any observable translational order, the orientational order (e.g., the tetratic and cubatic order parameters [37]) increases as p

moves away from unity. These packing characteristics, which are distinctly different from that of the MRJ packings of ellipsoids, are due to the unique way in which rotational symmetry is broken in superdisk and superball packings.

The rest of the paper is organized as follows: in Sec. II, we briefly describe the simulation techniques and the obtained packings. In Sec. III, we provide a detailed analysis of the novel packing characteristics. In Sec. IV, we make concluding remarks.

II. MAXIMALLY RANDOM JAMMED PACKINGS VIA COMPUTER SIMULATION

We use an event-driven molecular dynamics packing algorithm recently developed by Donev, Torquato, and Stillinger [34,35] (henceforth, referred to as the DTS algorithm) to generate MRJ packings of convex superdisks in two dimensions and superballs in three dimensions. The DTS algorithm generalizes the Lubachevsky-Stillinger (LS) sphere-packing algorithm [38] to the case of other centrally symmetric convex bodies (e.g., ellipsoids and superballs). Initially, small particles are randomly distributed and randomly oriented in the simulation box (fundamental cell) with periodic boundary conditions and without any overlap. The particles are then given translational and rotational velocities randomly and their motion followed as they collide elastically and also expand uniformly with an expansion rate γ , while the fundamental cell deforms to better accommodate the configuration. After some time, a jammed state with a diverging collision rate is reached and the density reaches a local maximum value. To generate random jammed packings, initially large γ are employed to prevent the system following the equilibrium branch of the phase diagram that leads to crystallization. Near the jamming point, sufficiently small expansion rate is necessary for the particles to establish contacting neighbor networks and to form a truly jammed packing. On the basis of our experience with spheres [17] and ellipsoids [31], we believe that our algorithm with rapid particle expansion produces final states that represent the MRJ state well. Here we use the largest possible initial $\gamma \in (0.1-0.5)$ that is numerically feasible to ensure the generated superdisk and superball packings are maximally jammed. We mainly focus on superdisks and superballs with deformation parameters p within the range 0.85–3.0, since extreme values of p associated with polyhedronlike shapes present numerical difficulties.

All of the generated packings used in the subsequent analyses are verified to be at least collectively jammed using an “infinitesimal shrinkage” method [13], i.e., the particles in the packing are shrunk by a very small amount [39] and given random velocities. If no significant structural changes and no decrease in pressure occur after the system “relaxes” after a sufficiently long enough time, the packing is considered to be collectively jammed. It is well established that the “infinitesimal shrinkage” method is robust, i.e., it always gives the same results for sphere packings as those obtained from a rigorous linear programming jamming test algorithm provided the amount of shrinkage from the jammed state is sufficiently small for a given number of particles within the periodic cell [40].

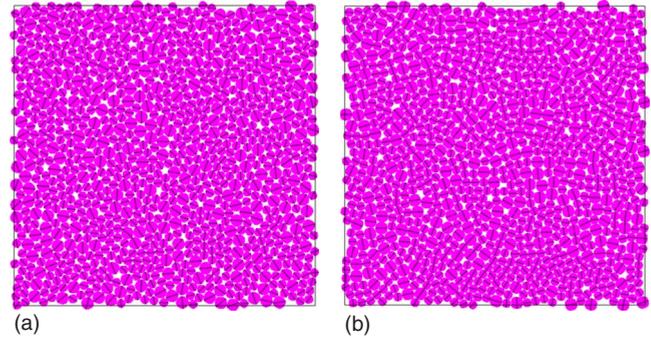


FIG. 3. (Color online) Typical configurations of MRJ packings of binary superdisks for two different values of the deformation parameter p . The chords show one of the symmetry axes of the superdisks: (a) $p=0.85$, (b) $p=1.5$.

A. Binary mixtures of MRJ superdisks

In two dimensions, we study MRJ packings of a specific family of binary superdisk mixtures. We do not use mono-dispersed superdisk systems here because they easily crystallize into ordered packings [25]. The size ratio κ of the two superdisk species is defined as the ratio of the diameter of a large superdisk over that of a small superdisk and we choose $\kappa=1.4$. The molar ratio β of the two superdisk species is defined as the number large superdisks over the number of small superdisks and we choose $\beta=1/3$. Let N denote the total number of particles within the periodic simulation box. For $p=1$, one obtains the binary circular-disk system which has been intensively studied as a prototypical glass former [41]. Typical jammed packing configurations for two different values of the deformation parameter ($p=0.85$ and $p=1.5$) are shown in Fig. 3, in which $N=1000$. We have also generated MRJ packings with $N=250, 500, 625,$ and 2500 , and we find that statistical fluctuations associated with the packing characteristics are sufficiently diminished when $N > 500$. For very large systems (e.g., $N=2500$), it is numerically very expensive to produce truly jammed packings. Therefore, the characteristics reported here are obtained from MRJ packings with $N=1000$ in both two and three dimensions. The density ϕ and the average contact number per particle Z as a function of p are shown in Fig. 4, which reveals that the initial rapid increases of ϕ and Z are linear in $|p-1|$ [42]. The density ϕ increases monotonically as p moves away from unity and shows no signs of a plateau, even for relatively large p . In addition, ϕ quickly surpasses the density of the optimal binary circular-disk packing associated with the size and molar ratios employed here, which contains phase-separate regions of triangular lattice packings of different sized circular disks [41]. The quantity Z quickly reaches its plateau value $Z^* \approx 4.7$ at $p \approx 1.3$, which is smaller than $2f=6$, indicating the packings are hypostatic. The tetratic order parameter S_4 in two dimensions is defined as $S_4 = \frac{1}{2} \langle \cos(4\theta) \rangle$, where θ is the angle between the particle axis and the director, along which the principle axes of the particles have maximum mutual alignment [37]. The measured tetratic order parameter is $S_4 \approx 0.06$ to 0.48 with the tendency to increase as $|p-1|$ grows.

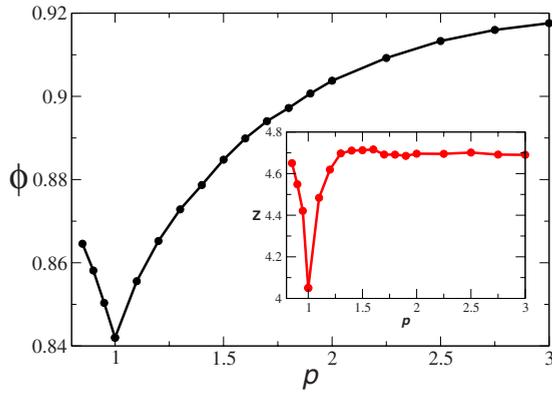


FIG. 4. (Color online) The density of MRJ packings of binary superdisks as a function of p . Insert: the average contact number Z as a function of p .

B. MRJ packings of monodisperse superballs

In three dimensions, monodispersed superballs can be easily compressed into a jammed random packing due to geometrical frustration (i.e., the densest local particle arrangement cannot tile space). Typical jammed packing configurations for two different values of the deformation parameter ($p=0.85$ and $p=1.5$) are shown in Fig. 5, in which $N=1000$. The quantities ϕ and Z as a function of p are shown in Fig. 6, respectively. As in two dimensions, ϕ and Z increase rapidly, in a cusplike manner [43], as the particles deviate from perfect sphere. ϕ increases monotonically as p moves away from unity, quickly goes beyond the optimal sphere packing density and shows no signs of plateau, even for relatively large p values. The contact number per particle Z reaches its plateau value $Z^* \approx 8.15$ at $p \approx 1.4$, which is significantly smaller than $2f=12$, indicating that the packings are hypostatic. The cubatic order parameter P_4 in three dimensions is defined as $P_4 = \frac{3}{14} \langle (35 \cos^4 \theta - 30 \cos^2 \theta + 3) \rangle$, where θ is the angle between the particle axis and the director, along which the principle axes of the particles have maximum mutual alignment [37]. The measured cubatic order parameter is $P_4 \approx 0.03$ to 0.32 , which increases with $|p-1|$.

III. PACKING CHARACTERISTICS

A. Rattlers

MRJ packings generated in both two and three dimensions contain a small fraction of rattlers, i.e., particles that

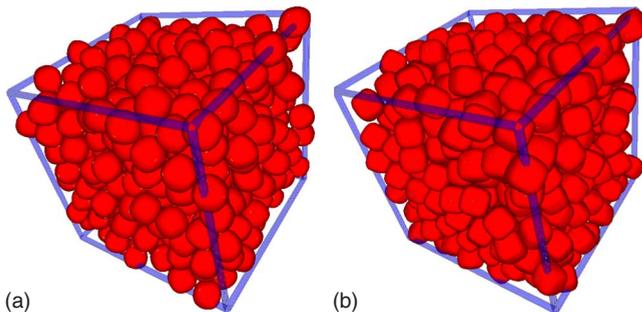


FIG. 5. (Color online) Typical configurations of MRJ packings of superballs for two different values of the deformation parameter: (a) $p=0.85$, (b) $p=1.5$.

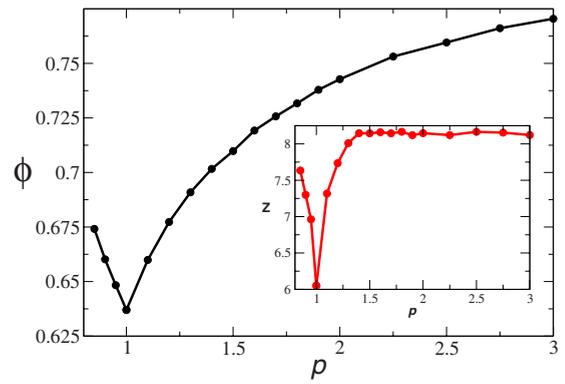


FIG. 6. (Color online) The density of MRJ packings of superballs as a function of p . Insert: the average contact number Z as a function of p .

can wander freely within cages formed by their jammed non-rattling neighbors. When p is close to unity, the fraction of rattlers is approximately 2.6% and 1.2% for two and three dimensions, respectively. As p moves away from unity, the fraction of rattlers decreases quickly and practically vanishes for large p (e.g., $p > 2.75$). This behavior results from the increasing protuberance of the particle shape, which makes it more difficult to form isotropic cages and also requires more average contacts per particle to achieve jamming. Note that rattlers are excluded when reporting average contact numbers in the following discussion.

B. Packing density

The rapid increase in the density is mainly due to the broken rotational symmetry of the particles. In particular, the cubiclike (squarelike) and octahedral-like particles are more efficient to cover the space than spheres (circular disks), i.e., near the jamming point the particles can rotate to accommodate the neighbors by orienting the “far corners” to fill the available gaps and thus cover more space. For small values of p , the increase in ϕ is also attributed to the expected increase in the number of contacting neighbors per particle, which means locally more particles can be packed in a given volume. The manner in which rotational symmetry is broken in superball packings is distinctly different from that in ellipsoid packings. For example, the asphericity [27,28], defined as the ratio of the radii of circumsphere and insphere of a nonspherical particle, is always bounded and close to unity for all values of p for superballs, while it can increase without limit as the largest aspect ratio α grows for ellipsoids. For very elongated or flakelike ellipsoids with large aspect ratios, the effect of a very anisotropic exclusion volume becomes dominant and causes the density of random ellipsoid packings to decrease. By contrast, the shape of superballs becomes more efficient in filling space as the deformation parameter deviates more from unity and thus results in a monotonically increasing density. The nonanalyticity of ϕ at $p=1$ is also associated with the broken symmetry of superdisks and superballs. This nonanalytical behavior has also been observed in the optimal packings of these particles realized by various Bravais lattices [25,26]. This stands in con-

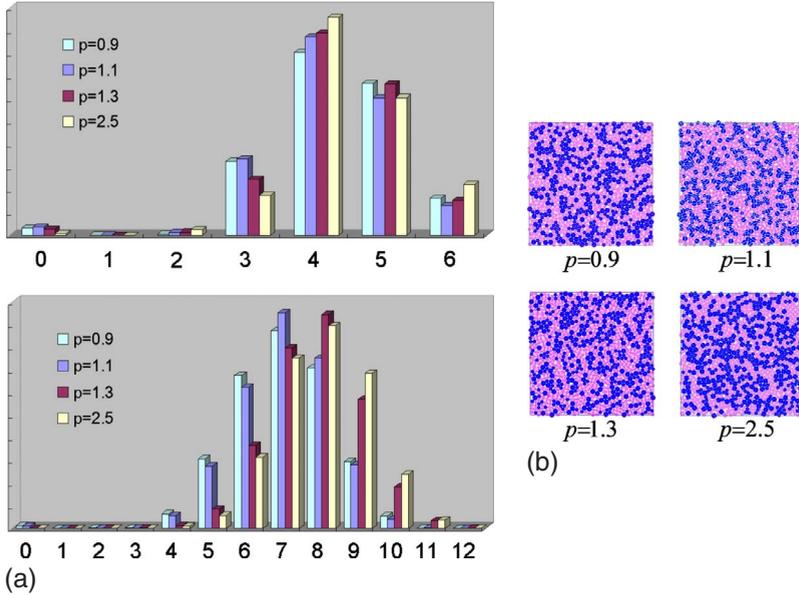


FIG. 7. (Color online) (a) Distribution of contact numbers for different p values for MRJ packings of superdisks (upper panel) and superballs (lower panel). (b) Local packing structures with more contacts than average (shown in dark gray, or blue online) and those with less contacts than average (shown in light gray, or pink online) in two-dimensional superdisk packings for different p values.

trast to the densest known ellipsoid packings, which are periodic packings with a two-particle basis possessing a smooth initial increase of ϕ_{\max} as the aspect ratio moves away from unity [21].

C. Hypostaticity and nongeneric local structures

There have been conjectures [15,16] that frictionless random packings have just enough constraints to completely statically define the system (i.e., it is *isostatic*), i.e., for large packings, one has $Z=2f$. It has been shown both experimentally and computationally that although the isostatic conjecture [15] holds for large sphere packings [40,44], it is generally not applicable to nonspherical particles, such as ellipsoids [31,32]. It was found that even for ellipsoids with large aspect ratios, Z is still slightly below $2f$ [31].

Here we observe that in MRJ packings of superdisks and superballs Z is significantly smaller than $2f$ for all values of p examined, i.e., the packings are significantly *hypostatic*. The hypostatic packings result from the competition between f_T translational and f_R rotational degrees of freedom of the particles ($f=f_R+f_T$) in developing the contacting networks close to the jamming point. In particular, although it is true that to constrain the translational degrees of freedom each particle needs at least $2f_T$ contacts, rotational degrees of freedom can be blocked with less than $2f_R$ additional contacts per particle if the curvatures at the contacting points are sufficiently small [32]. In addition, due to the relatively small asphericity of superdisks and superballs, there is little reason to expect the rotational motions of these particles (especially those with p close to unity) would be frozen even when they are translational trapped and may only rattle inside small “cages” formed by their neighbors. Near the jamming point, it is expected that the particles can rotate significantly [45] until the actual jamming point is reached, at which rotational jamming will also come into play, and rotational degrees of freedom are frozen with the number of additional contacts much less than $2f_R$. This is in contrast to hypostatic MRJ

packings of ellipsoids with large aspect ratios, for which the translational and rotational degrees of freedom are on the same footing and, thus, the average contact number per particle is only slightly below twice the number of total degrees of freedom.

Furthermore, the local geometry of the MRJ packings is necessarily nontrivially correlated (nongeneric), i.e., all the normal vectors at the points of contact for a particle should intersect at a common point to achieve torque balance and block rotations. In light of the isostatic conjecture, the local packing structures are less nongeneric when they possess larger contact numbers so that the constraining neighbors are less correlated. The truly generic local packing structures should have $Z=2f$ per particle, for which the constraining neighbors could be completely uncorrelated. To characterize the nongenericity of the packings, we compute G_{ng} , the fraction of local structures composed of particles with fewer contacts Z_{local} than average $Z_{average}$, i.e.,

$$G_{ng} = \frac{N(Z_{local} \leq Z_{average})}{N_{total}}. \quad (2)$$

A larger G_{ng} indicates a larger degree of nongenericity. We find G_{ng} is approximately 0.65 in two dimensions and 0.78 in three dimensions when p is close to unity, which quickly decreases and plateaus at 0.6 and 0.68, respectively as p increases. Figure 7 shows the distribution of contact numbers for different p values and the topology of the local structures contributing to G_{ng} . It can be seen that as p moves away from unity, the distributions become more skewed as the means shift to larger Z . Moreover, the subset of particles associated with the nongeneric structures percolate. We do not observe any tendency of increasing Z even for the largest p values that are computationally feasible and we expect that MRJ packings in the cubic limit are also hypostatic. It is noteworthy that isostatic random packings of superdisks and superballs are difficult to construct, since achieving isostaticity requires $Z=2f=12$ which is necessarily associated with translational crystallization [46].

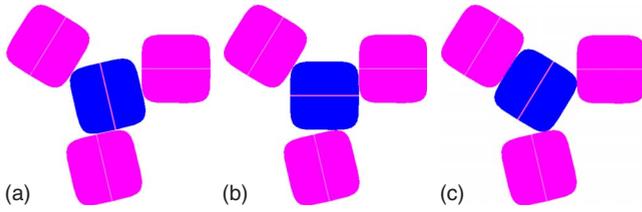


FIG. 8. (Color online) Nongeneric locally jammed configurations associated with three fixed superdisks shown in light gray (pink online) and the trapped one shown in dark gray (blue online). In each configuration, the central superdisk is approximately aligned with one of its fixed neighbors to form at least one contact such that each face has small curvature in order to block the rotation of the central particle.

We note that the aforementioned nongeneric structures [see Fig. 7(b)] are not rare. In particular, a nonspherical particle can be rotationally jammed if it has neighbors that can translationally jam the particle [32]. To illustrate this point, we will consider a small packing composed of four superdisks in two dimensions. Now we show that one can locally jam a superdisk by three contacting neighbor superdisks. Translational jamming requires that the centroids of the neighbors cannot lie in the same semicircle around the centroid of the central superdisk. Suppose a superdisk is translationally trapped (not jammed) by its three neighbors, whose positions and orientations are fixed. This four-particle configuration has four degrees of freedom: two translational and one rotational degrees of freedom of the trapped particle as well as the expansion of the particles. To obtain a jammed configuration, the four degrees of freedom need to be completely constrained. This can be achieved by the three contact conditions for the jammed particle and its neighbors and the requirement that the three inward normal vectors at the contacting points meet at a common point, a sufficient condition for torque balance [32]. Thus, one has four independent equations for the four degrees of freedom; see the Appendix for details.

Figure 8 shows the nongeneric jammed configurations associated with three specific fixed trapping superdisks. The multiplicity of the configurations is due to the multiple solutions of the equations. The jamming configurations can be also obtained using the DTS algorithm, which allows the trapped particle to translate and rotate and allows all the particles to grow. Although the above analysis is for local jamming (i.e., the neighbors of the central particle are fixed), it is reasonable to expect that collective particle rearrangements further facilitate the formation of nontrivial orientational correlations and thus, enable a larger number of nongeneric jamming configurations. Indeed, the numerous hypostatic jammed packings that we found from our simulations strengthen our argument that nongeneric structures are not rare.

D. Nonvanishing orientational order

We also observe the increase in the orientational order (measured by S_4 and P_4) associated with the increasing p values, although the largest possible expansion rate γ has

been used to suppress the formation of orders (i.e., to maintain the maximal degree of randomness) [47]. As p deviates from unity, the particle shape develops “edges” and “corners” with large curvatures, which may not be able to block rotational unjamming motions if contacts occur at significantly curved regions of the particle surface. On the other hand, low-curvature contacts are more favorable, which is associated with partial alignments of the particles. The tendency of particle alignments to form low-curvature surface contacts required by jamming becomes stronger as the particle moves further away from the sphere point. Thus, there is also a competition between orientational disorder and jamming for packings of superdisks and superballs, resulting from their unique symmetry-breaking manner, which has not been observed in random packings of ellipsoids. Due to numerical difficulties, we could not use the DTS algorithm to study the random jammed packings of particles with extreme shapes, i.e., in the limit $p \rightarrow 0.5$ and $p \rightarrow \infty$. However, it is reasonable to expect considerable orientational ordering in such packings.

IV. CONCLUSIONS

In this paper, we studied the maximally random jammed packings of superdisks and superballs. The packing densities increase dramatically and nonanalytically as one moves away from the circular-disk and sphere point ($p=1$) and the packings are hypostatic. To achieve jamming, the local arrangements of particles are necessarily nontrivially correlated and we term these structures nongeneric in light of the correlations. The degree of nongenericity of the packings is quantitatively characterized by the fraction of local structures composed of particles with fewer contacts than average. Moreover, we showed that such seemingly “special” packing configurations are not rare. As the anisotropy of the particles increases, the fraction of rattlers decreases while the minimal orientational order increases. The novel features arising in MRJ packings of superdisks and superballs result from the unique manner in which rotational symmetry is broken. This makes such packings distinctly different from other known MRJ packings of nonspherical particles such as ellipsoids and ellipses.

The ability to produce dense random packings using superballs casts lights on several industrial processes such as sintering and ceramic formation, where interest exists in increasing the density of powder particles to be fused. If superball-like particles instead of spherical particles are used, the packing density of a randomly poured and compacted powder could be increased to a value surpassing that of the maximal sphere-packing density. We note that superdisks and superballs can be experimentally mass produced using current lithography techniques. Recently, inorganic nanocrystals possessing similar shapes and symmetry with superdisks and superballs have been produced through nonhydrolytic chemical routes [48], which make it possible to prepare and study the behavior of colloidal systems composed of such nanocrystals and compare them with our simulation results. The experimental analog of the nongeneric local configurations as shown in Fig. 8 could be detected using a

combination of polarized and depolarized dynamic light scattering [49].

Understanding the statistical thermodynamics of the jamming transition of superdisks and superballs, especially the role of rotational and translational degrees of freedom for different deformation parameters is a subject that merits future investigation. Such studies could deepen our understanding of the nature of glass transitions, since the preponderance of previous investigations has focused on spherical particles. Superellipsoids generalize the ellipsoidal shape in the way that superballs generalize the spherical shape [50]. Not surprisingly, MRJ-like packings of superellipsoids have been shown to possess similar packing characteristics as those of superball packings when the aspect ratio is small [51]. However, MRJ superellipsoid packings may exhibit distinctly different features from the analogous superball packings for larger aspect ratios. We will focus on the packing properties of such shapes in our future research.

ACKNOWLEDGMENTS

The authors thank Robert Batten and Aleksandar Donev for valuable discussions. S.T. thanks the Institute for Advanced Study for its hospitality during his stay there. This work was supported by the Division of Mathematical Sciences at the National Science Foundation under Award Number DMS-0804431 and by the MRSEC Program of the National Science Foundation under Award Number DMR-0820341.

APPENDIX: EQUATIONS FOR LOCALLY JAMMED FOUR-SUPERDISK CONFIGURATIONS

In this section, we provide the equations that determine locally jammed four-superdisk configurations composed of a trapped central particle and three fixed contacting neighbors (see Fig. 8). In particular, the boundary of a superdisk with radius R is define by

$$\left| \frac{x_1}{R} \right|^{2p} + \left| \frac{x_2}{R} \right|^{2p} = 1, \quad (\text{A1})$$

which can be also expressed by the parametric equations

$$\begin{aligned} x_1(\theta) &= |\cos \theta|^{1/p} R \operatorname{sgn}(\cos \theta), \\ x_2(\theta) &= |\sin \theta|^{1/p} R \operatorname{sgn}(\sin \theta), \end{aligned} \quad (\text{A2})$$

where $\operatorname{sgn}(x)$ gives the sign of argument x . Let the centroids of the three fixed neighbors be (a_i, b_i) ($i=1,2,3$), and the orientations be θ_i . Their boundaries are then given by

$$\begin{aligned} x_1^{(i)}(\theta) &= a_i + \cos \theta_i |\cos \theta|^{1/p} R \operatorname{sgn}(\cos \theta) \\ &\quad + \sin \theta_i |\sin \theta|^{1/p} R \operatorname{sgn}(\sin \theta), \\ x_2^{(i)}(\theta) &= b_i - \sin \theta_i |\cos \theta|^{1/p} R \operatorname{sgn}(\cos \theta) \\ &\quad + \cos \theta_i |\sin \theta|^{1/p} R \operatorname{sgn}(\sin \theta). \end{aligned} \quad (\text{A3})$$

Similarly, if the centroid of the central particle is at (a_o, b_o) and its orientation is characterized by θ_o , its boundary is specified by

$$\begin{aligned} x_1^o(\theta) &= a_o + \cos \theta_o |\cos \theta|^{1/p} R \operatorname{sgn}(\cos \theta) \\ &\quad + \sin \theta_o |\sin \theta|^{1/p} R \operatorname{sgn}(\sin \theta), \\ x_2^o(\theta) &= b_o - \sin \theta_o |\cos \theta|^{1/p} R \operatorname{sgn}(\cos \theta) \\ &\quad + \cos \theta_o |\sin \theta|^{1/p} R \operatorname{sgn}(\sin \theta). \end{aligned} \quad (\text{A4})$$

Since the positions and orientations of the three neighbors are fixed, the four-particle system has four degrees of freedom, namely the position (a_o, b_o) and orientation θ_o of the central particle, as well as the radius R of all particles, as discussed in Sec. III C.

In the jammed configuration, the central particle contacts all its three neighbors. From Eqs. (A1) and (A4), the contact point $(x_{1c}^{(i)}, x_{2c}^{(i)})$ between neighbor particle i and the central particle can be expressed in terms of (a_o, b_o, θ_o, R) , which must also lie on the boundary of the neighboring particle i , i.e.,

$$\left| \frac{x_{1c}^{(i)}(a_o, b_o, \theta_o, R) - a_i}{R} \right|^{2p} + \left| \frac{x_{2c}^{(i)}(a_o, b_o, \theta_o, R) - b_i}{R} \right|^{2p} = 1, \quad (\text{A5})$$

for $i=1,2,3$. This leads to three equations in the variables a_o, b_o, θ_o , and R . In addition, to achieve jamming the three normals at contacts must meet at a common point, which guarantees torque balance. The normals at contacts are along the lines

$$(x_2 - x_{2c}^{(i)}) = - \frac{dx_1^{(i)}/d\theta}{dx_2^{(i)}/d\theta} \Big|_{(x_{1c}^{(i)}, x_{2c}^{(i)})} (x_1 - x_{1c}^{(i)}). \quad (\text{A6})$$

The aforementioned torque balance condition requires that the three lines given by Eq. (A6) must intersect at a common point. This leads to another equation in the variables a_o, b_o, θ_o , and R . Thus, there are four independent equations for the four degrees of freedom and (a_o, b_o, θ_o, R) can be completely determined for a locally jammed four-particle configuration.

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