Maximally random jammed packings of Platonic solids: Hyperuniform long-range correlations and isostaticity

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Maximally Random Jammed Packings of Platonic Solids: Hyperuniform Long-Range Correlations and Isostaticity

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Abstract

We generate maximally random jammed (MRJ) packings of the four nontiling Platonic solids (tetrahedra, octahedra, dodecahedra and icosahedra) using the adaptive-shrinking-cell method [Torquato & Jiao, Phys. Rev. E 80, 041104 (2009)]. Such packings can be viewed as prototypical glasses in that they are maximally disordered while simultaneously being mechanically rigid. The MRJ packing fractions for tetrahedra, octahedra, dodecahedra and icosahedra are respectively 0.763 ± 0.005, 0.697 ± 0.005, 0.716 ± 0.002, and 0.707 ± 0.002. We find that as the number of facets of the particles increases, the translational order in the packings increases while the orientational order decreases. Moreover, we show that the MRJ packings are hyperuniform (i.e., infinite-wavelength local-number-density fluctuations vanish) and possess quasi-long-range pair correlations that decay asymptotically with scaling r^{-4}. This provides further evidence that hyperuniform quasi-long-range correlations are a universal feature of MRJ packings of frictionless particles of general shape. However, unlike MRJ packings of ellipsoids, superballs and superellipsoids, which are hypostatic, MRJ packings of the nontiling Platonic solids are isostatic. We provide a rationale for the organizing principle that the MRJ packing fractions for nonspherical particles with sufficiently small asphericities exceed the corresponding value for spheres (approximately 0.64). We also discuss how the shape and symmetry of a polyhedron particle affects its MRJ packing fraction.

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I. INTRODUCTION

A *packing* is a collection of nonoverlapping (hard) particles in d-dimensional Euclidean space $\mathbb{R}^d$. Dense particle packings have been widely employed to model crystals, glasses, heterogeneous materials, granular media and biological media [1–4]. The "geometric-structure" approach to characterizing jammed packings has revealed a great diversity of packing configurations attainable by frictionless particles [5]. A fundamental feature of that diversity is the necessity to classify individual jammed configurations according to whether they are locally, collectively, or strictly jammed [6, 7]. Each of these categories contains a multitude of jammed configurations spanning a wide range of intensive properties, including packing fraction ϕ [8], mean contact number Z, and several scalar order metrics ψ. Application of these analytical tools to frictionless spheres in three dimensions, an analog to the venerable Ising model [5], covers a myriad of jammed states, including maximally dense packings as Kepler conjectured [1], low-density strictly jammed tunnelled crystals [9], and a substantial family of disordered packings [10, 11].

A maximally random jammed (MRJ) packing of hard particles is the one that minimizes the degree of order (or maximizes disorder) as measured by certain scalar order metrics ψ, subject to the condition of jamming of a specific category [5, 10]. MRJ packings that meet the strict jamming condition can be viewed as prototypical glasses in that they are maximally disordered while simultaneously being mechanically rigid [5, 12]. Bernal first used disordered hard-sphere packings to describe the structure of liquids [12]. However, it is now known that three-dimensional (3D) MRJ hard-sphere packings possess quasi-long-range (QLR) pair correlations [13], a property markedly different from typical liquids, which possess pair correlations decaying exponentially fast [3]. In particular, such packings are *hyperuniform* [14], i.e., the infinite-wavelength local-number-density fluctuations are completely suppressed and the packings possess QLR correlations, which are manifested as a nonanalytic linear small k behavior in the structure factor, i.e., $S(k) \sim k$ for $k \to 0$. This implies that the corresponding pair correlation function decays to unity with scaling $1/r^4$. Moreover, it has been shown that such sphere packings are *isostatic* [15–18], meaning that the total number of inter-particle contacts (constraints) equals the total number of degrees of freedom (DOF) of the system. This implies that the average number of contacts per particle Z is equal to twice the number of DOF per particle f (i.e., $Z = 2f$) in the large-particle-number limit. It should be noted that disordered strictly jammed sphere packings exist in three dimensions with an anomalously low packing fraction of 0.6 [11].

Over the past decade there has been increasing interest in the effects of particle shapes on the characteristics of disordered packings, since deviations from sphericity can lead to more realistic models for nanostructured materials and granular media. Nonspherical shapes that have been studied include ellipsoids [19, 20], superballs [21], superellipsoids [22] and polyhedra [23–25]. Unlike sphere packings, it has been found that disordered jammed packings of the aforementioned smoothly-shaped particles (not polyhedra) are hypostatic, i.e., $f < Z < 2f$ [19, 21, 22]. For disordered polyhedron packings, the flat facets of the particles enable one to determine the type of a contact (e.g., face-to-face, edge-to-face, etc.) and thus, the number of DOF constrained by each contact [24]. Using such analysis, Jaoshvili et al. [24] showed that experimentally produced disordered packings of plastic tetrahedron-like dice with $\phi = 0.76$ are virtually isostatic, i.e., each dice has on average 12 ± 1.6 constrains resulting from only 6.3 ± 0.5 contacts. Using an energy-minimization method, Smith, Alam and Fisher [25] numerically generated and studied disordered jammed packings of *soft* Platonic polyhedra (i.e., the repulsion between a pair of particles is proportional to their overlap volume).

Recently, it has been shown that MRJ packings of a class of $s$moothly-shaped nonspherical particles are hyperuniform and possess QLR pair correlations that decay asymptotically with scaling $r^{-(d+1)}$ (where d is the Euclidean space dimension) [26]. By contrast, polyhedral particles have geometrical singularities (e.g., sharp edges and corners), resulting in various types of contacts that can dramatically frustrate contacting neighbor distances. Therefore, it is not clear whether MRJ polyhedral packings still possess hyperuniform QLR pair correlations, especially for tetrahedra whose asphericity γ is very large [27, 29].

In this paper, using the adaptive-shrinking-cell (ASC) method [27], we generate and investigate via the "geometric-structure" approach strictly jammed maximally disordered packings of nontiling hard Platonic solids. Specifically, translational and orientational order are explicitly quantified by evaluating certain order metrics and correlation functions. We find that as the number of facets of the particles increases, the translational order in these packings increases while the orientational order decreases. Moreover, we find that the MRJ packings are hyperuniform (i.e., with infinite-wavelength local-number-density fluctuations that vanish) and possess QLR pair correlations, manifested in the structure factor as $S(k) \sim k$ and in the pair-correlation function as $g_2(r) \sim r^{-4}$. This provides further evidence that hyperuniform QLR are a universal signature of disordered jammed hard-particle packings. By directly determining the type and number of inter-particle contacts to a high accuracy, we show that the MRJ packings of the nontiling Platonic solids are isostatic. We provide a rationale for the organizing principle that the MRJ packing fractions for a class of nonspherical particles (including ellipsoids [19], superballs [21], superellipsoids [22] and the nontiling Platonic solids studied here) exceed the corresponding value for spheres (approximately 0.64). We also discuss how the MRJ packing fraction of a polyhedron particle is affected by its shape and symmetry.

II. GENERATION OF THE MRJ POLYHEDRON PACKINGS

We generate the MRJ polyhedron packings using the ASC method [27], which, in the current implementation, is equivalent to an isotension Monte-Carlo (MC) simulation [30] with a deformable periodic simulation box (fundamental cell). Specifically, starting from an unjammed initial packing configuration, the particles are randomly displaced and rotated sequentially. If a trial move (e.g., random displacement or rotation of a particle) causes overlap between a pair of particles, it is rejected; otherwise, the trial move is accepted and a new packing configuration is obtained. After a prescribed number of particle trial moves, small random deformations and compressions/dilations of the simulation box are applied such that the system is on average compressed. The compression rate Γ is defined as the inverse of the number of particle trial moves per simulation-box trial move. For large Γ, the system can not be sufficiently equilibrated after each compression and will eventually jam with a disordered configuration at a lower density than that of the corresponding maximally dense crystalline packing [5].

Two types of unjammed packings are used as initial configurations: dilute equilibrium hard polyhedron fluids with $\phi < 0.1$ and packings derived from MRJ hard-sphere packings. In the later case, a largest possible polyhedron with random orientation is inscribed into a sphere, which is to maximize both translational and orientational disordered in the initial packings. Initial configurations of both types are quickly compressed ($\Gamma \in [0.01, 0.1]$) to maximize disorder until the average interparticle gap is ~ 0.1 of the circumradius of the polyhedra. Then a much slower compression ($\Gamma \in [0.0002, 0.001]$) is employed to allow true contact network to be established which induces jamming [31]. The final packings are verified to be strictly jammed by shrinking the particles by a small amount (< 0.01 circumradius) and equilibrate the system with deformable boundary [7]. If there is no increasing of the interparticle gaps (decreasing of the pressure) for a sufficiently long period of time ($> 50\ 000$ MC moves per particle), the original packing is considered to be jammed [17, 21]. Translational and orientational order are explicitly quantified by evaluating certain order metrics and correlation functions, which then enables us to find those configurations with the minimal order metrics among a representative set of configurations. This analysis leads to reasonably close approximations to the MRJ states [28].

III. CHARACTERISTICS OF THE MRJ POLYHEDRON PACKINGS

A. Packing Fraction and Order Metrics

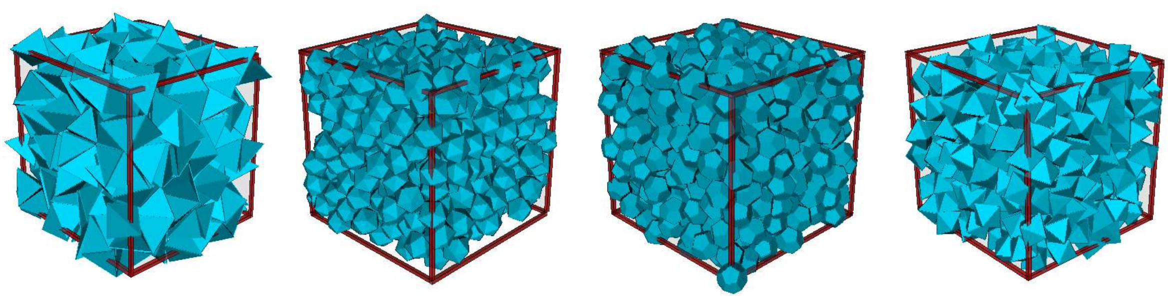

FIG. 1: (color online). Representative configurations of MRJ packings of the nontiling Platonic solids. From left to right: tetrahedra, icosahedra, dodecahedra, and octahedra. For purposes of visualization, each periodic simulation box only contains $N = 500$ particles. A much larger number ($N = 2500 \sim 5000$) has been used to obtain the packing characteristics reported in the paper.

For each shape, jammed final packings with similar ϕ and structural characteristics can be obtained from both types of initial configurations. Although larger Γ than employed here can lead to final packings with even lower ϕ and a higher degree of disorder, such packings are generally not jammed, i.e., they are "melt" upon small shrinkage and equilibration. We have used the largest possible initial compression rates ($\Gamma \in [0.01, 0.1]$) that lead to jammed packings. Both previous studies [17, 21] and the measured order metric (see below) indicate that the generated packings are representatives of the true MRJ states. Typically, a packing contains $N = 2000$ polyhedra but larger packings (with N upto 6000) are also studied to make sure that system size has no effects on our results. The packing fraction ϕ for MRJ packings of tetrahedra, icosahedra, dodecahedra, and octahedra are respectively 0.763 ± 0.005, 0.707 ± 0.002, 0.716 ± 0.002, and 0.697 ± 0.005. Representative configurations of MRJ polyhedron packings are shown in Fig. 1.

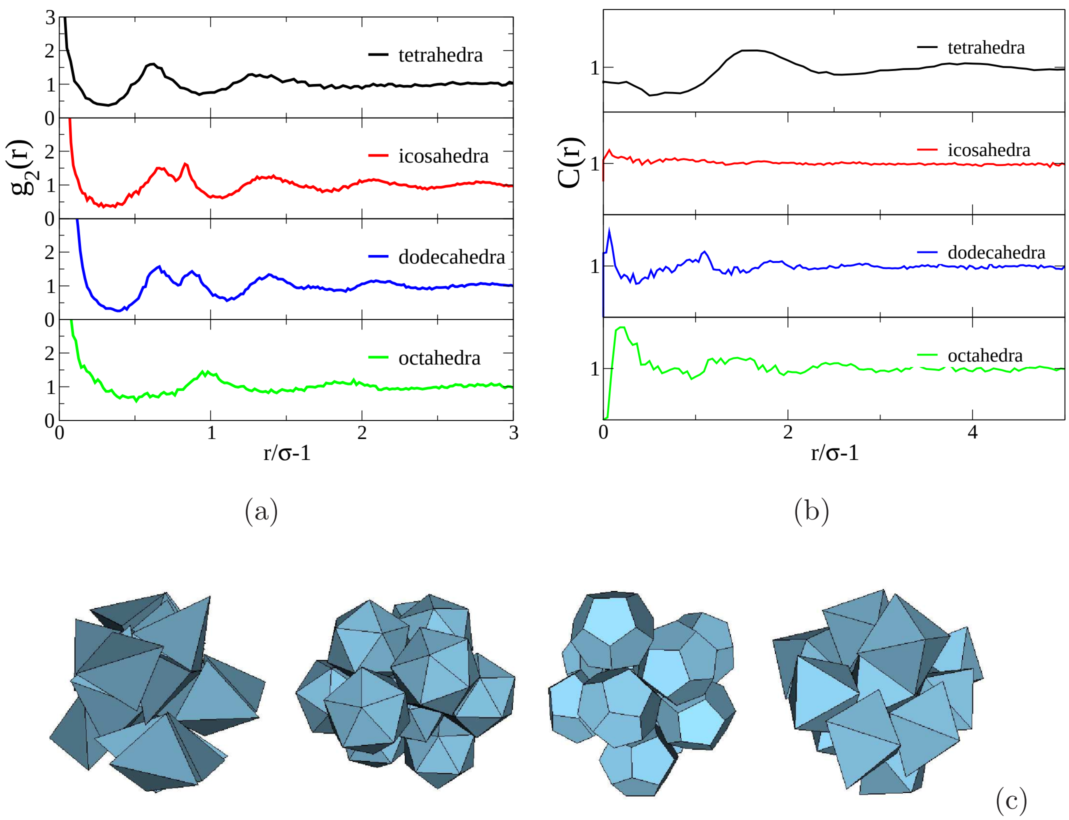

FIG. 2: (color online). Packing characteristics and local configurations of the nontiling Platonic polyhedra. (a) Pair-correlation function $g_2(r)$. Note that σ is the inradius of the polyhedra. (b) Orientational correlation function $C(r)$. (c) Local contacting configurations: from left to right, tetrahedra, icosahedra, dodecahedra, and octahedra.

Figure 2(a) shows the *pair-correlation function* $g_2(r)$ [1] for the polyhedron centroids in the MRJ packings. Specifically, $\rho g_2(r) 4\pi r^2 dr$ is the conditional probability of finding a particle in a spherical shell with differential volume $4\pi r^2 dr$ given that there is another particle at the origin, where ρ is number density (i.e., the number of particles per unit volume). For icosahedra and dodecahedra, whose asphericity value is relative small, the g_2 of their MRJ packings clearly resemble that of MRJ sphere packings, with the split second peak [17]. For octahedra and tetrahedra, their large asphericity strongly frustrates the contacting neighbor distances, but still possess many prominent oscillations than a typical hard-particle fluid.

The translational order in the packings is quantified using a crystal-independent metric $\mathfrak{T}$ [32]:

$$\mathfrak{T} = \frac{\int_{\sigma\rho^{1/3}}^{\eta_c} |h(\eta)| d\eta}{\eta_c - \sigma\rho^{1/3}}, \tag{1}$$

where $h(\eta) = g_2(\eta) - 1$ is the *total correlation function* [1], $\rho = N/V$ is the number density, σ is the inradius of the particles, $\eta = r\rho^{1/3}$ is the scaled radial distance and η_c is a cut-off value dependent on the system size (here $\eta_c = 4.5$). For MRJ sphere packings, $\mathfrak{T} = 0.39$ [32]. For MRJ packings of icosahedra, dodecahedra, octahedra and tetrahedra, the $\mathfrak{T}$ values are respectively 0.37, 0.36, 0.28 and 0.19, which are smaller than that for spheres, indicating a lower degree of translational order in these packings. This is because in MRJ sphere packings, the pair distances between contacting neighbors are exactly equal to the diameter of the spheres. However, for nonspherical particles, the pair distances between contacting neighbors in the associated MRJ packings can vary from the diameter of their insphere to that of their circumsphere, and thus, causing large fluctuations of pair distances between the particle centroids, which further diminishes translational order in the packings. Moreover, as the particle asphericity increases (the number of their facets decreases), the translational order in the packings as quantified by $\mathfrak{T}$ decreases.

The orientational correlation function $C(r)$, which measures the average alignment for two particles separated by r, is defined by [33]

$$C(r) =< C_{ql}(|\mathbf{r}^q - \mathbf{r}^l|) >=< \frac{1}{M}\sum_{i=1}^{M} \mathbf{n}_i^q \cdot \mathbf{n}_i^l >, \tag{2}$$

where $<,>$ denotes average over all particle pairs (q, l). For a tetrahedron q, $\mathbf{n}_i^q$ is the normal of its ith face, and $M = 4$ [33]. For the other three shapes, $\mathbf{n}_i^q$ is one of the three principal directions of a particle q, and $M = 3$ [27]. Figure 2(b) shows $C(r)$ for the MRJ packings of the four solids, which are properly shifted so that their long-range values are unity for purposes of comparison. The number of prominent oscillations in $C(r)$ and their magnitudes indicate the degree of orientational correlations in the packings, which decreases in the following order: tetrahedra, octahedra, dodecahedra and icosahedra. In other words, the orientational order in the MRJ polyhedron packings decreases as the particle asphericity increases. Note that in the limit of MRJ sphere packings, the orientation of a particular sphere is totally uncorrelated with the other spheres.

B. Hyperuniform Quasi-Long-Range Correlations

It is very difficult to ascertain the large-r asymptotic behavior of g_2 (long-range correlations) by direct sampling in real space. Therefore, we compute the associated structure factor $S(k)$, formally defined as the Fourier transform of the total correlation function $h(r)$, i.e., $S(k) = \mathfrak{F}\{g_2(r) - 1\} = \mathfrak{F}\{h(r)\}$, where $\mathfrak{F}$ is the Fourier transform of a radial function [1]. Here $S(k)$ is directly computed from the distributions of the particle centroids,

$$S(\mathbf{k}) = \frac{|\rho(\mathbf{k})|^2}{N} = \frac{1}{N}|\sum_{j=1}^{N} \exp(i\mathbf{k}\cdot\mathbf{r}_j)|^2, \tag{3}$$

where N is the number of particles in the packing and $\rho(\mathbf{k})$ defined by

$$\rho(\mathbf{k}) = \sum_{j=1}^{N} \exp(i\mathbf{k}\cdot\mathbf{r}_j) \tag{4}$$

are the collective coordinates and $\mathbf{r}_j$ denotes the location of the centroid of particle j. Note the forward scattering (associated with $\mathbf{k} = 0$) is excluded. The radial function $S(k)$ can be obtained by angularly

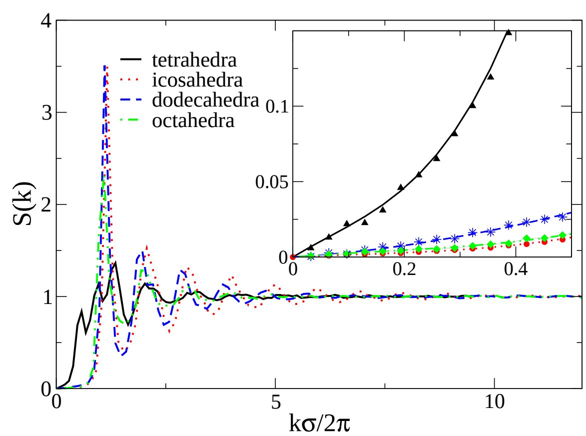

FIG. 3: (color online). Structure factor $S(k)$ for MRJ polyhedron packings. Insert: the small-k behavior and the polynomial approximation $a_0 + a_1k + a_2k^2 + a_3k^3$.

Figure 3 shows $S(k)$ of the MRJ polyhedron packings. Importantly, we find that $S(k) \to 0$ as $k \to 0$, i.e., the infinite-wavelength local-number-density fluctuations are completely suppressed in these packings, which indicates they are hyperuniform [13, 26]. We employ a third-order polynomial to approximate the small-k behavior of $S(k)$, i.e., $S(k) = a_0 + a_1 k + a_2 k^2 + a_3 k^3$, and use it to fit computed $S(k)$. We find that for all four solids, $a_0 \approx 0$ ($< 10^{-5}$) [34], which is also verified by directly computing number-density fluctuations in larger packings ($N = 6000$). These observations indicate that the MRJ polyhedron packings possess hyperuniform quasi-long-range pair correlations that decay asymptotically with scaling r^{-4}. Moreover, we find that the slopes a_1 of the linear portions of $S(k)$ for small k for icosahedra, dodecahedra, octahedra and tetrahedra are respectively 0.015, 0.023, 0.029 and 0.21. In other words, as the polyhedral shape deviates more from that of a sphere, the value of the slope a_1 increases, which is consistent with recent studies on MRJ packings of various nonspherical shapes in two dimensions [26]. Larger asphericities induce larger local number density fluctuations at fixed long wavelengths (i.e., small k values) due to the QLR correlations.

This is a very surprising result, since one might have expected that due to the large fluctuations in pair distances caused by particle asphericity, the hyperuniform QLR which exists in MRJ sphere packings would be lost in MRJ polyhedron packings, especially for tetrahedra. Indeed, $\mathfrak{T}$ of the MRJ polyhedron packings is similar to that of hard-sphere liquids with no long-range order. The existence of QLR in MRJ polyhedron packings implies that strict jamming imposes strong constraints on particle positions and orientations, which is consistent with a recent study on MRJ packings of certain smoothly shaped particles with a size distribution [26]. This also suggests that analysis based on local statistics alone can be misleading and insufficient to completely characterize MRJ packings [5].

C. Isostaticity

We determine the type of an interparticle contact by projecting the vertices of the polyhedra onto their separation axis [27]. If the distance between the projected faces/edges/vertices is smaller than a prescribed tolerance (< 0.001 of the circumradius of the particle) and the projected faces/edges/vertices overlap each other, we consider the particles contact each other. The flat facets of polyhedra allow one to determine the DOF constrained by a particular contact. Following Ref. [24], a face-to-face (f-f), edge-to-face (e-f), edge-to-edge (e-e) and vertex-to-face (v-f) contact respectively provides 3, 2, 1 and 1 constraint(s). In Table

I, we provide the average number of contacts per particle for each contact type and the total DOF constrained, which is virtually equal to the number of DOF ($f = 12$) for the polyhedra. Therefore, these MRJ polyhedron packings are isostatic, in contrast to MRJ packings of ellipsoids [19], superballs [21] and superellipsoids [22], which are hypostatic.

TABLE I: Average number of contacts per particle and the total DOF constrained in MRJ polyhedron packings.

	f-f	e-f	v-f	e-e	DOF
Tetrahedron	2.21 ± 0.01	0.98 ± 0.01	1.54 ± 0.02	1.91 ± 0.03	12.04
Icosahedron	2.35 ± 0.01	0.85 ± 0.01	0.64 ± 0.02	2.69 ± 0.01	12.08
Dodecahedron	2.28 ± 0.01	1.71 ± 0.02	0.74 ± 0.02	1.06 ± 0.01	12.06
Octahedron	1.44 ± 0.01	1.38 ± 0.01	2.24 ± 0.01	2.74 ± 0.02	12.06

We note that our MRJ packings are denser than the packings of soft Platonic polyhedra in Ref. [25] that were generated within a cubic simulation box. It has been established that for polyhedra, an increasing number of face-to-face contacts leads to higher packing fraction ϕ, since such contacts reduce the distances between the particle centroids [27]. Indeed, Table I shows that the MRJ polyhedron packings possess a relatively large number of face-to-face contacts [see Fig.2(c) for local contacting configurations]. We note that face-to-face contacts are also necessary for strict jamming. Since edges and vertices are local extremes on a polyhedron, it is clear that edge- and vertex-type contacts cannot efficiently block particle rotations. With a deformable box, collective particle rotations that break edge- and vertex-type contacts are facilitated by macroscopic shearing, until a sufficient number of face-to-face contacts are formed. Since a fixed-shape simulation box is used in Ref. [25], it is likely that the soft-polyhedron packings, which should be collectively but not strictly jammed, possess a larger number of edge- and vertex-type contacts, leading to lower ϕ than we obtain here. In contrast, the disordered tetrahedron-like dice packings in Ref. [24] were stabilized by vibration, which reduced the number of floppy local contacting configurations resulting in a packing fraction ϕ similar in value that we have found for our MRJ tetrahedron packings.

IV. CONCLUSIONS AND DISCUSSION

Using the ASC method, we have generated and studied maximally random strictly jammed packings of hard nontiling Platonic solids. We found that these MRJ packings are hyperuniform (with infinite-wavelength local-number-density fluctuations completely suppressed) and possess hyperuniform QLR pair correlations that decay asymptotically with scaling r^{-4}, implying that MRJ packings are intrinsically non-local. Moreover, the MRJ polyhedron packings are isostatic, which results from the particle shapes and the requirement of strict jamming. Granular materials made from sintering MRJ polyhedron packings would have stronger interparticle bounding and a higher packing fraction. Such materials could also possess interesting novel dynamical properties.

TABLE II: Characteristics of MRJ packings of hard particles with different shapes. For ellipsoids [19], superballs [21] and superellipsoids [22], the range of MRJ packing fractions reported here are for the cases where the asphericity of the particle is close to unity ($\gamma < 1.2$).

Particle Shape	Isostatic	Hyperuniform QLR	MRJ Packing Fraction
Sphere	Yes	Yes	0.642
Ellipsoid	No (hypostatic)	Yes	0.642 – 0.720
Superball	No (hypostatic)	Yes	0.642 – 0.674
Superellipsoid	No (hypostatic)	Yes	0.642 – 0.758
Octahedron	Yes	Yes	0.697
Icosahedron	Yes	Yes	0.707
Dodecahedron	Yes	Yes	0.716
Tetrahedron	Yes	Yes	0.763

Table II summarizes the characteristics of MRJ packings of hard particles with different shapes. We note that the MRJ polyhedron packings behave like MRJ sphere packings in that they all possess hyperuniform QLR and are isostatic; while the MRJ packings of ellipsoids, superballs and superellipsoids are hypostatic (i.e., the total number of constraints is smaller than the total number of degrees of freedom). We also find that for these smoothly-shaped particles, at least when the asphericity is close to unity ($\gamma < 1.2$), their MRJ packings also possess hyperuniform QLR, which provides further evidence that hyperuniform QLR are a universal signature of disordered jammed hard-particle packings.

It should not go unnoticed that the MRJ packings of nonspherical particles listed in Table II generally possess a higher packing fraction than that of spheres $\phi_{\rm MRJ}^{\rm sphere} = 0.642$. In general, provided that the asphericity value γ of a convex nonspherical particle is sufficiently close to unity (e.g., $\gamma < 1.2$), we argue that the associated MRJ packing fraction $\phi_{\rm MRJ}$ is always above $\phi_{\rm MRJ}^{\rm sphere}$ [35]. This is a natural consequence of the asphericity and the requirement of jamming. It has been shown that the flat faces of polyhedra [27] and the small-curvature regions on the surface of smoothly-shaped particles [19, 21] are more effective in blocking the relative rotations between the particles as opposed to either the edges and vertices of polyhedra or the large-curvature regions (such as rounded corners) of smoothly-shaped particles. Therefore, contacts through flat faces of polyhedra or small-curvature regions of smoothly-shaped particles are more favored in jammed configurations [19, 21]. It has been shown that such contacts lead to smaller separations between the centroids of particle pairs, and thus, result in a higher packing fraction. The principle that $\phi_{\rm MRJ}$ of convex nonspherical particles with γ sufficiently close to unity is always above the sphere value $\phi_{\rm MRJ}^{\rm sphere}$ can be considered to be the analog of Ulam's conjecture for ordered packings stating that the optimal packing of spheres possess the lowest packing fraction among all convex shapes in three dimensions [36].

A natural question is whether or not one can estimate from the aforementioned organizing principle the MRJ packing fraction of nontiling polyhedra. This is a very difficult question to answer rigorously, since $\phi_{\rm MRJ}$ is generally related to the unknown relative importance associated with different types of contacts (e.g., face-to-face, edge-to-face, edge-to-face, vertex-to-face). However, we can provide qualitative trends for the MRJ packing fraction relative to the sphere value. We define two polyhedra to be *similar* if they possess the same symmetry and asphericity value. In addition, a polyhedron satisfies the semi-regularity condition if its faces are polygons with similar areas (e.g., the ratio of the largest area over the smallest area is smaller than 1.2) and small ratios (e.g., < 1.2) of circumradius over inradius of the polygons. Then, for two similar polyhedra satisfying the semi-regularity condition, the one with the larger number of faces should possess a smaller MRJ packing fraction. In general, the more faces a nontiling polyhedron satisfying the semi-regularity condition has, the closer its MRJ packing fraction will be to the sphere value of about 0.64. This principle can be very well seen in the case of dodecahedra and icosahedra as listed in Table II. One might naively have guessed that the MRJ packing fraction should be inversely proportional to the number of faces, but we see that the MRJ packing fraction of the octahedron is slightly above that for the dodecahedron. However, this inverse proportionality should be true when a polyhedron that is semiregular possess a very large number of faces.

Finally, we note that cubes are not considered here because the jammed packings of cubes produced via our ASC algorithm generally possess a very high degree of order due to the cubic symmetry of the solid and its ability to fill all of the space. This could be a deficiency of our ASC algorithm or any known hard-particle-packing algorithm in not being able to generate MRJ cube packings or it is possible that the MRJ packings of hard cubes are intrinsically highly ordered. These issues will be examined in future work as well as carrying out analogous investigations of the MRJ packings of the Archimedean solids. An interesting question is whether or not one could devise a quantitative formula of the MRJ packing fraction of a nonspherical particle whose asphericity is sufficiently close to unity.

Acknowledgments

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[1] S. Torquato, *Random Heterogeneous Materials: Microstructure and Macroscopic Properties* (Springer-Verlag, New York, 2002).

[2] R. Zallen, *The Physics of Amorphous Solids* (Wiley, New York, 1983).

[3] P. M. Chaikin and T. C. Lubensky, *Principles of Condensed Matter Physics* (Cambridge UP, New York, 2000).

[4] S. F. Edwards, *Granular Matter*, edited by A. Mehta (Springer-Verlag, New York, 1994).

[5] S. Torquato and F. H. Stillinger, Rev. Mod. Phys. **82**, 2633 (2010).

[6] A locally jammed packing is one in which the particles are locally trapped by fixed neighbors. A collectively jammed packing is one in which no collective motions with fixed boundary can unjam the packing. A strictly jammed packing is one in which no collective motions with deformable boundary can unjam the packing. The readers are refered to Refs. [5] and [7] for

details.

[7] S. Torquato and F.H. Stillinger, J. Phys. Chem. B **105**, 11859 (2001).

[8] The packing fraction ϕ is defined to be the fraction of space covered by the particles in the packing.

[9] S. Torquato and F.H. Stillinger, J. Appl. Phys. **102**, 093511 (2007). The tunneled crystals constitutes an uncountably infinite number of strictly jammed crystal sphere packings that are subpackings of the densest crystal packings and are characterized by a high concentration of self-avoiding "tunnels" (chains of vacancies) that permeate the structures with $\phi = \sqrt{2}\pi/9 = 0.49365\ldots$ and $Z = 7$.

[10] S. Torquato, T. M. Truskett, and P. G. Debenedetti, Phys. Rev. Lett. **84**, 2064 (2000).

[11] Y. Jiao, F. H. Stillinger and S. Torquato, J. Appl. Phys. **109**, 013508 (2011).

[12] J. D. Bernal, In *Liquids: Structure, Properties, Solid Interactions*. Hughel, T. J., Ed. (Elsevier, New York, 1965) pp. 25-50.

[13] A. Donev, F. H. Stillinger, and S. Torquato, Phys. Rev. Lett. **95**, 090604 (2005).

[14] S. Torquato and F.H. Stillinger, Phys. Rev. E **68** 041113 (2003).

[15] S. Alexander, Phys. Rep. **296**, 65 (1998).

[16] S.F. Edwards and D.V. Grinev, Phys. Rev. Lett. **82**, 5397 (1999).

[17] A. Donev, S. Torquato and F. H. Stillinger, Phys. Rev. E **71**, 011105 (2005).

[18] C.S. O'Hern, L.E. Silbert, A.J. Liu, and S. R. Nagel, Phys. Rev. E **68**, 011306 (2003).

[19] A. Donev, *et. al.* Science **303**, 990 (2004).

[20] M. Mailman, C. F. Schreck, B. Chakraborty, and C. S. O'Hern, Phys. Rev. Lett. **102** 255501 (2009).

[21] Y. Jiao, F. H. Stillinger, and S. Torquato, Phys. Rev. E **81**, 041304 (2010).

[22] G.W. Delaney and P.W. Cleary, EPL **89**, 34002 (2010).

[23] SX Li, J Zhao and X Zhou, Chinese Phys. Lett. **25**, 4034 (2008); A. Haji-Akbari, *et. al.* Nature **462**, 773 (2009); J. Baker and A. kudrolli, Phys. Rev. E **82**, 061304 (2010).

[24] A. Jaoshvili, A Esakia, M. Porrati and P.M. Chaikin, Phys. Rev. Lett. **104**, 185501 (2010).

[25] K.C. Smith, M. Alam and T. Fisher, Phys. Rev. E **82**, 051304 (2010).

[26] C. Zachary, Y. Jiao and S. Torquato, Phys. Rev. Lett. **106**, 178001 (2011); C. Zachary, Y. Jiao and S. Torquato, Phys. Rev. E **83**, 051308 (2011); *ibid* 051309 (2011).

[27] S. Torquato and Y. Jiao, Nature **460**, 876 (2009); S. Torquato and Y. Jiao, Phys. Rev. E **80**,

041104 (2009).

[28] Studies of different order metrics for three-dimensional frictionless spheres have consistently led to a minimum at approximately the same density 0.64 [10, 32] for collectively and strictly jammed packings. This consistency among the different order metrics speaks to the utility of the order-metric concept, even if a perfect order metric has not yet been identified. See Refs. [1] and [5] for detailed discussions on order metrics.

[29] The asphericity of a particle is defined as the ratio of its circumsphere radius over its insphere radius.

[30] L. Filion et al., Phys. Rev. Lett. **103**, 188302 (2009).

[31] This procedure is similar to those used in Refs. [17, 19, 21] to produce MRJ packings of various smooth-shaped particles. Two polyhedra are considered to be contacting each other if their gap is < 0.001 of the circumradius of the particles.

[32] T.M. Truskett, S. Torquato and P.G. Debenedetti, Phys. Rev. E **62**, 993 (2000).

[33] This definition of $C(r)$ closely follows the definition of the angular correlation function $S(r)$ defined by Jaoshvili et al. in Ref. [24]. For tetrahedra, $C(r)$ and $S(r)$ are equivalent.

[34] Due to computational cost, the system size N used here is much smaller than that for spheres in Ref. [13]. However, our system-size study shows that a_0 decreases with increasing N. For MRJ sphere packings of same size, a_0 is of the same magnitude as here.

[35] MRJ packing fractions $\phi_{\rm MRJ}$ for very elongated ellipsoids and superellipsoids are smaller than $\phi_{\rm MRJ}^{\rm sphere}$. When the asphericity of a particle is close to unity ($\gamma < 1.2$), its MRJ packing fraction is always above the corresponding value for a sphere; see Refs. [19] and [22].

[36] J.H. Conway and S. Torquato, PNAS **103**, 10612 (2006).