Isostaticity of constraints in amorphous jammed systems of soft frictionless Platonic solids

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Isostaticity of constraints in amorphous jammed systems of soft frictionless Platonic solids

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The average number of constraints per particle \(\langle C_{\text{total}} \rangle\) in mechanically stable amorphous systems of Platonic solids approaches the isostatic limit at the jamming point \(\langle C_{\text{total}} \rangle \rightarrow 12\), though average number of contacts are hypostatic. By introducing angular alignment metrics to classify the degree of constraint imposed by each contact, constraints are shown to arise as a direct result of local orientational order reflected in edge-face and face-face alignment angle distributions. With approximately one face-face contact per particle at jamming, chainlike face-face clusters form with finite extent—a signature of amorphous jammed systems.

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Following Maxwell’s approach [1], jammed assemblies of frictionless spheres exhibit an average number of contacts per particle \(\langle Z_{\text{total}} \rangle\) equal to the isostatic value \(2n_f\) [2], where \(n_f\) is the degrees of freedom per particle. In contrast, ellipses [3,4], ellipsoids [4], tetrahedra [5,6], and the remaining Platonic solids [6] exhibit hypostatic behavior \(\langle Z_{\text{total}} \rangle < 2n_f\). The isostatic condition has been linked to the mechanical stability of soft sphere systems [7], and the hypostaticity of ellipses has been attributed to the presence of floppy vibrational modes, which provide vanishing restoring force [3]. Jaoshvili et al. [5] recently asserted that the average constraint number \(\langle C_{\text{total}} \rangle\), which incorporates topology-dependent contact constraint (e.g., through vertex-face, edge-edge, edge-face, and face-face contact topologies), is isostatic for tetrahedral dice even though \(\langle Z_{\text{total}} \rangle < 2n_f\). Similar approaches incorporating variable contact constraint have been utilized in the prediction of mechanism mobility as early as 1890 (see Ref. [8]). The presupposition underlying constraint counting as a valid means of predicting net degrees of freedom is the mechanical independence of constraints. As a result, such constraint counting approaches fail to predict the true mobility of mechanisms when kinematic redundancy is present (see Ref. [8]), and isostatic \(\langle C_{\text{total}} \rangle\) is not guaranteed at the jamming point. Though constraint counting may yield an isostatic result, the validity of this conclusion depends on the methods used to estimate \(\langle C_{\text{total}} \rangle\) as we show in this Rapid Communication.

Additionally, packing density and structure of Platonic solids have been the focus of recent studies. All Platonic solids except for tetrahedra pack optimally in Bravais lattices [9]. In contrast, tetrahedra pack optimally in a highly ordered double-dimer configuration [10–12]. “Random close-packed” tetrahedral dice [5,13], athermally jammed tetrahedra [6], and tetrahedroids [14] have exhibited dramatically lower densities [5,6,13] and only short-range translational order [5,6]. Also, athermally jammed tetrahedra exhibit a radial distribution function and face-face orientational correlation function consistent with densely packed experimental tetrahedral dice [6].

The main goal of this Rapid Communication is to assess the validity of generalized isostaticity [5] for amorphous jammed systems of Platonic solids through energy-based structural optimization and objective topological classification. We also present jamming threshold density and show that these packings are vibrationally stable. The ill-conditioned vibrational spectrum is a direct result of topological heterogeneity in the contact network, and we therefore identify and highlight the orientational order of contacts by introducing angular alignment metrics. Topology classification via angular alignment metric distributions is thereby used to assess the isostaticity of constraints.

Contact model and jamming protocol. Structural optimization coupled with controlled consolidative and expansive strain is used to probe the jamming point as in Ref. [6]. The conservative model employed assumes that contact between particles \(\alpha\) and \(\beta\) results in energy \(E_{\alpha\beta} = YV^2/4V_p\) after a Hookian contact model applied to uniaxially compressed bars, where \(V\) is the intersection volume between the particles, \(V_p\) is the volume of a single particle, and \(Y\) is the elastic modulus. Conjugate gradient minimization with line searching is utilized with a relative energy change convergence tolerance of less than \(10^{-12}\) at each strain step to simulate static equilibrium (see Ref. [6]). Density is defined as \(\phi = N V_p / V_{\text{cell}}\), where \(V_{\text{cell}}\) and \(N\) are the volume and the number of particles in the primary periodic cell.

Assemblies of monodisperse Platonic solids with periodic cubic lattice boundary conditions were consolidated with an average energy per particle near \(3.2 \times 10^{-5}Y V_p\), from low-density random configurations at \(\phi = 0.05\). Cubes have been excluded from the present study because such systems exhibit long-range orientational order [6] and hence are not amorphous. Estimates of the jamming threshold density \(\phi_j\) (Table I) were obtained by expansion toward the jamming point as in Ref. [6]. \(\phi_j\) converges well at \(N = 100\), but the results differ somewhat from the “random close-packed” densities measured by Ref. [13] for finite systems of rounded dice. Unless otherwise stated, hereafter the results presented are for \(N = 400\).

Mechanical stability. We computed the low-energy vibrational spectra of these monodisperse systems as \(\omega_i = \sqrt{\lambda_i^2/m}\)
TABLE I. Jamming threshold $\phi_J$ estimated for each system with 95% confidence intervals.

<table>
<thead>
<tr>
<th>System</th>
<th>$N = 100$</th>
<th>$N = 400$</th>
<th>Expt.$^a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tetrahedra</td>
<td>0.629 ± 0.001</td>
<td>0.634 ± 0.011</td>
<td>0.64 ± 0.01</td>
</tr>
<tr>
<td>Octahedra</td>
<td>0.6796 ± 0.0003</td>
<td>0.686 ± 0.001</td>
<td>0.64 ± 0.01</td>
</tr>
<tr>
<td>Icosahedra</td>
<td>0.6953 ± 0.0003</td>
<td>0.7008 ± 0.0003</td>
<td>0.59 ± 0.01</td>
</tr>
<tr>
<td>Dodecahedra</td>
<td>0.7065 ± 0.0002</td>
<td>0.7085 ± 0.0003</td>
<td>0.63 ± 0.01</td>
</tr>
</tbody>
</table>


As in Ref. [3], where $\lambda_i$ is the $i$th eigenvalue of the dynamical matrix $D_{\alpha\beta} = \partial^2 E/\partial r_\alpha \partial r_\beta$, $m$ is the particle mass. Frequency $\omega_i$ is presented in units of $V_p^{1/3} \sqrt{V/\rho}$, where $\rho$ is the mass density of the solid phase. Coordinates $r_\alpha$ of particle $\alpha$ are composed of translational $x_\alpha$ and rotational $\theta_{\alpha,\alpha}$ components $r_\alpha = \{x_\alpha, x_\alpha, x_\alpha, R_\alpha \theta_{\alpha,\alpha}, R_\alpha \theta_{\alpha,\alpha}, R_\alpha \theta_{\alpha,\alpha}\}$, where $R_\alpha$ is the radius of gyration. We calculate $D_{\alpha\beta}$ through central differences of forces and moments, considering only its symmetric part. The resulting spectra of static equilibrium systems with density nearest $\phi_J$ are displayed in Fig. 1(a).

For static equilibrium systems at all densities we find $6N - 3$ stable modes with three trivial (rigid-body) translational modes, confirming that our soft packings are indeed stably stable modes with three trivial (rigid-body) translational modes, respectively, where $\delta e_i$ is the unit edge vector of edge $i$ on particle $q$.

Randomly oriented faces and edges provide a starting point for understanding alignment angle distributions in jammed systems. Three-dimensional (3D) random edges and faces possess a probability density of edge-face alignment with $p(\theta_{e,f}) \propto \cos(\theta_{e,f})$. Edge-face contacts are therefore expected to be ubiquitous in jammed systems, because probability is weighted toward small $0 < \theta_{e,f} < \pi$. In contrast, face-face contacts are expected to be less common, because 3D random faces possess an alignment probability density that vanishes in the face-face limit. Cumulative distribution functions (CDFs) are plotted in Fig. 2 for all the contacts in one realization of each system in addition to CDFs of ideal random systems. Simulated CDFs exhibit critical angles plotted in Fig. 2 and listed in Table II that bound the possible alignment angles for face-vertex, edge-edge, and edge-face contact topologies; we denote critical edge-face and face-face alignment angles as $\theta_{e,f,ci}$ and $\theta_{f,f,ci}$, respectively, where $i$ denotes the particular contact topology. These angles correspond to pairs of particles contacting with a particular topology oriented with the highest possible symmetry. The angular breadth of $c(\theta_{e,f})$ spans proportional

FIG. 1. (Color online) (a) Vibrational spectra for stable systems nearest the jamming threshold. (b) The power-law scaling of $\langle \omega_0 \rangle$ (lower curve set) and the asymptotically constant scaling of $\langle \omega_0 \rangle$ (upper curve set).

FIG. 2. (Color online) CDFs of (a) $\theta_{e,f}$ and (b) $\theta_{f,f}$ for stable systems nearest $\phi_J$. Points plotted on the simulated curves correspond to $c(\theta_{e,f,ci})$ and $c(\theta_{f,f,ci})$. Region 1 of $c(\theta_{e,f})$ is masked in gray, while region 2 extends from the edge of region 1 to $\theta_{e,f,ci,\min}$ the minimum critical face-face alignment angle. Ideal random CDFs for edge-face constrained (open squares) and unconstrained (open circles) contacts are displayed as well.
TABLE II. Critical edge-face $\theta_{e,f,c,i}$ and face-face $\theta_{f,f,c,i}$ alignment angles for each topology $i$ in degrees.

<table>
<thead>
<tr>
<th>Topology, $i$</th>
<th>$\theta_{e,f,c,i}$</th>
<th>$\theta_{f,f,c,i}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Vertex-face</td>
<td>Edge-edge</td>
</tr>
<tr>
<td>Tetrahedra</td>
<td>54.7</td>
<td>54.7</td>
</tr>
<tr>
<td>Octahedra</td>
<td>45.0</td>
<td>35.3</td>
</tr>
<tr>
<td>Dodecahedra</td>
<td>20.9</td>
<td>31.7</td>
</tr>
<tr>
<td>Icosahedra</td>
<td>31.7</td>
<td>20.9</td>
</tr>
</tbody>
</table>

Figure 2(b) shows that $c(\theta_{f,f})$ for all systems possess three regions of descending probability density (i.e., the CDF slope): (1) ultralow-angle ($<1^\circ$) face-face contact region, (2) intermediate uniform probability region, and (3) high-angle region. Region 2 contains the largest portion of total contacts and exhibits $c(\theta_{f,f})$ similar to that of random edge-face constrained contacts [open squares, Fig. 2(b)] rather than unconstrained contacts [open circles, Fig. 2(a)]. This results from the abundance of contacts with small $\theta_{f,f}$ that exhibit CDFs approaching that of edge-face constrained contacts [open squares, Fig. 2(a)] rather than unconstrained contacts [open circles, Fig. 2(a)]. Region 2 possesses approximately $\langle Z_{f,f} \rangle = \langle Z_{f,c} \rangle$ similar to that of random edge-face contacts [open squares, Fig. 2(c)] rather than unconstrained contacts [open circles, Fig. 2(b)]. The emergence of region 1 [gray mask, Fig. 2(b)] can be understood by considering the constrained rotation of an ideal edge-face contact. During consolidation such a contact will rotate randomly about its edge through a range of $\theta_{f,f}$. Repulsion between opposing faces at $\theta_{f,f} = 0$ will prevent the contact from rotating further. We observe the evolution of $c(\theta_{e,f})$ and $c(\theta_{f,f})$ as $\phi \to \phi_f$, qualitatively consistent with this idealized picture—region 1 of $c(\theta_{f,f})$ emerges only after $c(\theta_{f,c})$ becomes hyper-random.

**Constraint isostaticity and topological distributions.** To classify topologies we fit $c(\theta_{e,f})$ and $c(\theta_{f,f})$ independently with a piecewise continuous distribution function basis $c_f(\theta) = H(\theta - \alpha)[a_0 + \sum_{n=1}^{3} a_n(\theta - \alpha)^n]$, where $a_n$ are fitted coefficients, $H$ is the Heaviside step function, and $\alpha$ is the fitted CDF discontinuity. All empirical CDFs have been fitted by minimizing $\int_0^{\theta_{e,f,c,i}} c_f(\theta) - c(\theta) d\theta$, where $i$ corresponds to the particular alignment angle. With the fitted parameter $a_0$ the angular alignment cutoffs for topological classification $\theta_{cut}$ are determined such that $c(\theta_{cut}) = a_0$. Edge-face contacts are classified as those with $\theta_{e,f} < \theta_{e,f,cut}$ and $\theta_{f,f} \geq \theta_{f,f,cut}$ and face-face contacts as those with $\theta_{f,f} < \theta_{f,f,cut}$.

The variation of average contact number $\langle Z_{total} \rangle$ with respect to $\Delta \phi$ [Fig. 3(a)] confirms the generally hypostatic nature of $\langle Z_{total} \rangle$, consistent with our previous findings for smaller systems [6]. We determine the average contact number for face-face $\langle Z_{f,f} \rangle$, edge-face $\langle Z_{e,f} \rangle$, and lower order contacts $\langle Z_i \rangle$. The average constraint number $\langle C_{total} \rangle$ is thereby calculated as $\langle C_{total} \rangle = 3\langle Z_{f,f} \rangle + 2\langle Z_{e,f} \rangle + \langle Z_i \rangle$ [5]. Importantly, $\langle C_{total} \rangle$ of each system approaches values near the isostatic limit [Fig. 3(b)], in contrast with $\langle Z_{total} \rangle$ [Fig. 3(a)]. Amorphous jammed systems therefore possess contacts that independently constrain motion. They also possess $\langle Z_{f,f} \rangle \lesssim 1$ [Fig. 3(c)]. We attribute this effect to a twofold rotational constraint induced on a given particle once a single face-face contact is formed. Such a rotational constraint appears to hinder the formation of additional face-face contacts. In contrast, optimal Bravais lattices of octahedra, dodecahedra, and icosahedra (that are implicitly jammed) exhibit 14, 12, and 12 contacts per particle [9], respectively, with all such contacts being face-face. Therefore, such ordered systems exhibit ultrahyperstatic average constraint numbers of 42, 36, and 36, respectively. Thus, ordered systems differ drastically from amorphous jammed systems in terms of average constraint number and face-face contact number.

Note that the low $\langle Z_{f,f} \rangle$ of tetrahedra clearly contrasts with the value of 2.3 recently reported for tetrahedral dice [5]. The practical importance of this finding is very significant, for if two to three face-face contacts per particle were present, as reported by Ref. [5], we expect such systems to readily
TABLE III. Distributions of average contact and constraint numbers for the present work and prior work.

<table>
<thead>
<tr>
<th></th>
<th>Present work\textsuperscript{a}</th>
<th>Various $\theta_{\text{cut}}$\textsuperscript{b}</th>
<th>Expt.\textsuperscript{c}</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\langle Z_{\text{total}} \rangle$</td>
<td>11.1</td>
<td>11.1</td>
<td>6.3</td>
</tr>
<tr>
<td>$\langle Z_{f} \rangle$</td>
<td>0.9</td>
<td>5.4</td>
<td>2.3</td>
</tr>
<tr>
<td>$\langle Z_{r,f} \rangle$</td>
<td>1.5</td>
<td>3.7</td>
<td>1.2</td>
</tr>
<tr>
<td>$\langle Z_{l} \rangle$</td>
<td>8.6</td>
<td>2.0</td>
<td>2.8</td>
</tr>
<tr>
<td>$\langle C_{\text{total}} \rangle$</td>
<td>14.5</td>
<td>25.5</td>
<td>12.1</td>
</tr>
</tbody>
</table>

\textsuperscript{a}100 tetrahedra at $\Delta \phi = 0.04$.
\textsuperscript{b}Values are computed by averaging over results obtained with $\theta_{\text{cut}} = \{5, 15, 25, 35, 45, 55\}$ as in Refs. \cite{5} and \cite{15}.
\textsuperscript{c}Values presented in Ref. \cite{5} for tetrahedral dice.

exhibit cluster percolation and radically different structures and mechanical behavior than those with near unity $\langle Z_{r,f} \rangle$. In Table III we compare the contact and constraint numbers of the present work (column 1) with that of Ref. \cite{5} (column 3). Indeed, all contact numbers are markedly different (except $\langle Z_{r,f} \rangle$) from that of Ref. \cite{5}. We also utilize a topological classification procedure similar to that in Refs. \cite{5} and \cite{15} by averaging the contact numbers obtained for various values of $\theta_{\text{cut}}$ (column 2 in Table III). The resulting constraint number is twice as large as the isostatic value. Thus, an arbitrary choice of $\theta_{\text{cut}}$, as employed in Refs. \cite{5} and \cite{15}, can yield a geometrically infeasible range of contact numbers and generally nonisostatic $\langle C_{\text{total}} \rangle$.

We have analyzed the structure of clusters formed by face-face contacts (Table IV). The topological connectivity of clusters was considered under periodic boundary conditions. The average size of clusters $S$ is defined in terms of the number of particles $s$ in each cluster as $S = \sum s^2 / \sum s$; we find that $S$ increases with $\langle Z_{r,f} \rangle$ as the particle shape is changed. We also find that all clusters in systems of $N = 400$ particles do not percolate according to topological connectivity. Such a requirement for periodic percolating networks is stricter than the requirement that a cluster spans the system boundaries \cite{16}. Therefore, we have also considered the less restrictive percolation requirement that a cluster spans system boundaries. Clusters in the respective systems exhibit maximal extent along Cartesian axes $l_{\text{max}}$ smaller than the length of the finite cubic cell. Clusters with maximal linear extent exhibit chainlike structures [Fig. 3(d)] with fractal dimension $D_{\text{max}} \gtrsim 1$ (Table IV). Considering the fractal dimension of $\sim 2.5$ for a percolating cluster at the threshold in a simple cubic lattice \cite{17}, these chains are substantially of lower dimension and appear to be far from percolation.

The lack of cluster percolation is a direct consequence of near unity $\langle Z_{r,f} \rangle$, and is a signature of amorphous jammed systems. These results suggest that face-face cluster formation is a bond percolation process with respect to $\langle Z_{r,f} \rangle$. Therefore, we expect that systems of particles with shapes conducive to ordering (e.g., cubes) or with attractive interactions could increase $\langle Z_{r,f} \rangle$, forming larger clusters that percolate.

In summary, we have established that the average constraint number of amorphous jammed systems of Platonic solids approaches the isostatic limit near the jamming point, and have linked this condition to their mechanical stability. The structure and extent of face-face clusters is found to be a consequence of few face-face contacts in these systems. Our results therefore suggest that $\langle Z_{r,f} \rangle$ or other integral functions of $p(\theta_{r,f})$ are suitable order parameters to determine the maximally random jammed state of faceted particle systems according to the approach described in Ref. \cite{18}. Future work will focus on identifying the means by which the face-face contact number may increase and on studying the critical behavior of such systems with ensuing face-face contact percolation.

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\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|}
\hline
\multicolumn{5}{|c|}{TABLE IV. Face-face contact number $\langle Z_{r,f} \rangle$, average cluster size $S$, maximal extent along Cartesian axes $l_{\text{max}}$, and the fractal dimension of clusters with maximal linear extent $D_{\text{max}}$ for stable $N = 400$ systems nearest $\phi_J$.} \\
\hline
& Octahedra & Icosahedra & Tetrahedra & Dodecahedra \\
\hline
$\langle Z_{r,f} \rangle$ & 0.59 & 0.77 & 0.94 & 1.02 \\
$S$ & 1.88 & 2.45 & 3.18 & 4.13 \\
$l_{\text{max}}/(V_{\text{cell}})^{1/3}$ & 0.665 & 0.795 & 0.741 & 0.776 \\
$D_{\text{max}}$ & 1.01 ± 0.10 & 1.23 ± 0.08 & 1.37 ± 0.09 & 1.32 ± 0.14 \\
\hline
\end{tabular}
\end{table}

\textsuperscript{[1]} J. C. Maxwell, Philos. Mag. 27, 294 (1864).