Enumerating nonlinearly rigid sphere packings

Miranda Holmes-Cerfon
Courant Institute of Mathematical Sciences, New York University

We enumerate nonlinearly rigid clusters of identical, hard spheres for \( n \leq 14 \), and clusters with the maximum number of contacts for \( n \leq 18 \). A nonlinearly rigid cluster is one that cannot be continuously deformed while maintaining all contacts. These are the metastable states when the spheres interact with a short-range potential, so they model the geometry of a great many physical and chemical systems. We expect these lists are nearly complete, except for a small number of highly singular clusters (linearly floppy but nonlinearly rigid.) The data contained some major geometrical surprises, such as the prevalence of hypostatic clusters: those with less than the \( 3n - 6 \) contacts required for minimal rigidity. We discuss several other unusual clusters, whose geometries may shed insight into physical mechanisms, pose mathematical and computational problems, or bring inspiration for designing new materials.

What are all the possible ways to arrange \( n \) spheres in space, so they form a rigid cluster? This is a mathematical question whose solution would resolve conjectures in discrete and combinatorial geometry \([1, 2]\) and contribute to studies of structural rigidity \([3, 7]\), but it also has wide implications in several areas of science. In physics, the geometry of small clusters has brought insight into nucleation, gelation, and glass formation pathways \([8, 12]\), while the total number of clusters is argued to give rise to an extensive entropy in granular media \([13, 14]\). In chemistry, the set of hard-sphere clusters is conjectured to have the most “rugged” landscape, so molecules with smoother interactions may be derivable from these \([15, 16]\). Engineers and materials scientists have proposed to use clusters as the basis for new materials, but must know the possibilities and how to build them with high yield \([17, 19]\). Despite its simplicity, the question remains largely unanswered, because of both the conceptual difficulty of constructing an algorithm to enumerate all the possible packings, and the computational difficulty of implementing it when the number of packings is expected to increase very rapidly \([8, 14, 20]\).

In physics, a bar is set at clusters of \( n = 13 \) spheres \([15]\). This is the smallest number where one sphere becomes caged: completely surrounded by neighbouring spheres, so there is expected to be a richer variety of geometrical structures and thermodynamic behaviour. Previous work has listed clusters of \( n \leq 11 \) spheres \([21, 22]\) but these approaches are not easy to extend to higher \( n \), and they rely on a linear notion of “rigid” which is not the most physically natural.

We attack this question using a bottom-up, dynamical algorithm to list clusters of \( n \leq 14 \) spheres, and a subset for \( n \leq 18 \) that contains the ground states (clusters with the maximum number of contacts.) There is good evidence to believe these lists are nearly complete, save a very small number of clusters that are too singular (see below) for the algorithm to handle. Thus, for the first time, we produce data in a size regime where bulk behaviour may begin to play a role.

We aim to list clusters that are nonlinearly rigid: they cannot be deformed continuously by any finite amount and still maintain all contacts. This is different from previous studies, which look for minimally rigid clusters – those with at least \( 3n - 6 \) contacts – or linearly rigid clusters, those whose rigidity matrix has no zero eigenvalues except for translations and rotations (or dynamical matrix, when the contacts are harmonic springs.) A zero eigenvalue represents a linear degree of freedom, but is not always extendable to a higher order deformation, so linearly floppy clusters may still be nonlinearly rigid. We argue this is the most natural set of clusters to consider: first, because nonlinearly rigid clusters are topologically equivalent – they are all isolated solutions to the system of equations (see \((1)\)) – and second, because these clusters are the metastable states when the spheres interact with a short-range potential \([23]\).

The data contained several surprises – clusters that run counter to certain basic physical intuitions or assumptions – and the aim here is to highlight these. The biggest surprise was the prevalence of (i) Clusters with fewer than \( 3n - 6 \) contacts. This runs counter to the commonly-cited Maxwell’s criterion, which states that a rigid cluster should have at least \( 3n - 6 \) contacts \([24, 27]\). Other surprises include: (ii) Geometrically distinct clusters with the same adjacency matrices – i.e. clusters with the same set of contacts but which are not related by rotations, reflections, or permutations; (iii) Ground state clusters that are almost all fragments of a lattice (fcc, hcp, or random stacking) beyond \( n \geq 15 \). This occurs at much lower \( n \) than for a smoother potential such as Lennard-Jones; (iv) A sharply decreasing overall proportion of lattice fragments; (v) A roughly constant proportion of “singular” clusters \((\approx 2.5\%)\) – those that are linearly floppy but nonlinearly rigid; (vi) Clusters with localized, “circular” soft modes: when a single contact is broken, the cluster continuously deforms until it reforms exactly the same contact in exactly the same configuration; (vii) A rigid cluster that has no one-dimensional soft modes: if any single contact is broken, it acquires at least two modes of deformation.

These are more than geometrical curiosities – the bulk
behaviour of a material arises in part from geometrical arrangements of its most basic components, for which the set of clusters forms a catalogue of all possible motifs. Inventive new materials may be possible by changing the arrangements of a few localized components [28], and this catalogue can bring inspiration for unusual geometries that are hard to construct explicitly. Additionally, many of these clusters, particularly the singular and hypostatic ones, represent states of matter whose thermodynamics is not yet understood. Note that these are not surprising from a mathematical perspective – indeed, they are solutions to a system of nonlinear equations, so in principle any type of pathology could occur – yet, it is valuable to have concrete examples where they occur in a physically relevant system.

**PROBLEM AND METHODS**

Here is the problem we wish to solve: given $n$ spheres in three dimensional-space with unit diameters, what are all the possible ways to arrange them without overlap so they form a cluster that is nonlinearly rigid?

Mathematically, let a cluster be represented as a vector $\mathbf{x} = (x_1, x_2, \ldots, x_{3n}) \in \mathbb{R}^{3n}$ where $x_i = (x_{3i-2}, x_{3i-1}, x_{3i})$ is the center of the $i$th sphere, combined with a set of algebraic equations of the form

$$|x_i - x_j|^2 - 1 = 0$$

for each pair of spheres $(i, j)$ that are in contact. Additionally, we add six equations to remove the translational and rotational degrees of freedom, for example, by fixing one sphere at the origin, another on the $x$-axis, and a third on the $xy$-plane, as $x_s = 0$, $s \in \{1, 2, 3, 5, 6, 9\}$. The system (1) is often represented by an adjacency matrix $A$ by setting $A_{ij} = 1$ if spheres $i, j$ are in contact, and $A_{ij} = 0$ otherwise.

A cluster $\mathbf{x}$ with contacts (1) is **nonlinearly rigid** if $\mathbf{x}$ is an isolated solution to (1), i.e. the solution is a zero-dimensional point [4]. We consider only clusters that are **locally rigid**, which means the above holds in a small region near each solution $\mathbf{x}$; however there may be more than one solution for a given system of equations [5]. A cluster $\mathbf{x}$ is **floppy** if it lies on a positive-dimensional solution set.

This notion of rigidity differs from that more commonly considered of **minimal rigidity**, which denotes a cluster with at least $3n - 6$ contacts and comes from equating the number of variables $(3n)$ to the number of equations [24]. This condition is neither necessary nor sufficient for nonlinear rigidity.

There is a good physical reason to consider nonlinear rigidity. Suppose the spheres interact with a very short-range potential, as is often the case for mesoscale particles such as colloids [12, 23, 29, 30]. Then, the energy of a cluster is basically proportional to the number of contacts, so a floppy cluster can lower its energy by moving along its degrees of freedom until it forms another contact. Once it reaches a nonlinearly rigid cluster it cannot rearrange without breaking a contact to overcome an energy barrier, so these clusters are metastable states where the system is expected to spend most of its time.

We test for nonlinear rigidity of a cluster $\mathbf{x}$ as follows. Suppose there is a deformation $p(t)$ depending analytically on parameter $t$, with $p(0) = \mathbf{x}$. Taking one derivative of (1) gives $R(\mathbf{x})p|_{t=0} = 0$, where $R(\mathbf{x})$ is the Jacobian of (1). If the right null space of $R(\mathbf{x})$ is empty, we cannot solve for $p'(0)$ so the cluster is linearly rigid, or **first-order rigid**. This is sufficient for nonlinear rigidity [4].

Otherwise, taking two derivatives of (1) gives $R(\mathbf{x})p''|_{t=0} = -R(p')p'|_{t=0}$. By the Fredholm alternative, we can solve for $p''(0)$ if and only if $w^T R(v)v = 0$ for all $w \in \mathcal{W}$, $v \in \mathcal{V}$, where $\mathcal{W}, \mathcal{V}$ are the left and right null spaces of $R(\mathbf{x})$. When this condition does not hold, the cluster is **second-order rigid** and this is also sufficient for nonlinear rigidity [4]. We test this by finding a single $w$ that blocks all $v$; this is called **pre-stress stability** and is slightly stronger than second-order rigidity. See Appendix for more details. We do not consider higher-order rigidity because there is no known method to test this.

We search for pre-stress stable clusters by following all the one-dimensional transition paths between clusters. We begin with a single rigid cluster of $n$ spheres. This is easy to obtain, for example by gluing a sphere with three contacts to a cluster of $n - 1$ spheres. Next we break a contact on this cluster, by deleting a single equation in (1). Typically, this makes a cluster with a single internal degree of freedom, i.e. the set of solutions of the reduced system of equations forms a one-dimensional manifold. We follow this one-dimensional path numerically until a new contact is formed. The new contact adds an equation to the system, so the resulting cluster is typically rigid. This cluster could be merely a permutation of the cluster we originally started with, but it could also be an entirely distinct cluster. In the latter case, we add it to our list of rigid clusters.

For each cluster in our list, we break all subsets of contacts that lead to a one-dimensional transition path, follow each path, and keep track of the clusters at the other end.

When we reach the end of the list, we stop: we have the entire set of pre-stress stable clusters that are connected to the starting cluster by one-dimensional paths.

**RESULTS**

We have implemented this algorithm for clusters of size $n \leq 14$. Table 1 shows the total number of nonlinearly
Table I. Number of clusters found for each $n$, organized by number of contacts in each cluster. For $n \geq 15$ only clusters with a minimum number of contacts were kept.

| $n$   | # of contacts |
|-------|---------------|
| $3n-9$| 1             |
| $3n-8$| 2             |
| $3n-7$| 5             |
| $3n-6$| 13            |
| $3n-5$| 52            |
| $3n-4$| 1,259         |
| $3n-3$| 18            |
| $3n-2$| 1618          |
| $3n-1$| 707           |
| $3n$  | 1,058         |
| $3n+1$| 7675          |
| $3n+2$| 798           |
| $3n+3$| 7895          |
| $3n+4$| 7796          |
| $3n+5$| 9629          |

| Total |               |
|-------|---------------|
|       | 1             |
|       | 2             |
|       | 5             |
|       | 13            |
|       | 52            |
|       | 263           |
|       | 1,659         |
|       | 11,980        |
|       | 98,529        |
|       | 895,478       |

The biggest surprise is the existence of clusters with fewer than $3n-6$ contacts: hypostatic clusters. The smallest has $n=10$ spheres and is “missing” one contact; it is shown in Figure 1 (left). To our knowledge this is the first known hypostatic cluster of spheres. (Hypostatic packings of ellipsoids have been observed, [33] but these arise because of the extra rotational degrees of freedom when the aspect ratio of the sphere is perturbed [34].) For $n=11$ there are 2 clusters missing two contacts, also shown in Figure 1 and 18 clusters missing one contact. Most clusters missing one contact are obtained from the $n=10$ hypostatic cluster by gluing a sphere, but the clusters missing two contacts cannot be formed this way. The smallest cluster missing 3 contacts occurs for $n=14$, see Figure 1.

Hypostatic clusters The biggest surprise is the existence of clusters with fewer than $3n-6$ contacts: hypostatic clusters. The smallest has $n=10$ spheres and is “missing” one contact; it is shown in Figure 1 (left). To our knowledge this is the first known hypostatic cluster of spheres. (Hypostatic packings of ellipsoids have been observed, [33] but these arise because of the extra rotational degrees of freedom when the aspect ratio of the sphere is perturbed [34].) For $n=11$ there are 2 clusters missing two contacts, also shown in Figure 1 and 18 clusters missing one contact. Most clusters missing one contact are obtained from the $n=10$ hypostatic cluster by gluing a sphere, but the clusters missing two contacts cannot be formed this way. The smallest cluster missing 3 contacts occurs for $n=14$, see Figure 1.

All of these are nonlinearly rigid, despite having several (often 2-3) linear degrees of freedom. A common feature is several spheres lie in a plane that is stabilized at its boundary. In this plane can move perpendicularly to it infinitesimally, but cannot move any finite amount without breaking a contact somewhere else. For example, the $n=10$ cluster is made of a rigid 6-cluster (dark+light blue) and a tetrahedron (green+light blue) that share a sphere (light blue) and two contacts to make a square face. Without the red sphere, these can twist along a single degree of freedom. When the red sphere is added exactly in the plane of the spheres it contacts, this stabilizes the twist and rigidifies the cluster.

Not all hypostatic clusters are planar; see for example the cluster in Figure 1 to be discussed later.
Clusters with the same adjacency matrices Another big surprise is that sometimes \(1\) has more than one physically realizable solution. In this case a single adjacency matrix corresponds to two or more distinct clusters. The smallest cluster for which this occurs is \(n = 11\) and the pair of solutions is shown in Figure 2. They differ by the location of a single sphere (red), which forms contacts with three spheres (light blue) either above or below the plane of the these spheres.

For \(n = 12, 13\) we find 23 and 474 pairs with the same adjacency matrix respectively. For \(n = 14\) there are 666,3,3 adjacency matrices with 2,3,4 solutions respectively. These multiple solutions do not all differ by a single sphere but can vary in more complicated ways. For example, Figure 2 shows a pair of solutions for which all spheres have at least four contacts. This solution is made of two rigid clusters of 6 (light blue / red) and 7 (green/red) spheres, glued together so they share a sphere (red) and form 3 other contacts. One can check this gluing condition is sufficient for minimal rigidity if the two rigid bodies are minimally rigid. The figure also shows a quadruple of solutions for \(n = 14\), which is hard to decompose into rigid body sub-components.

Hyperstatic clusters / Ground states At \(n = 10\) we begin to find clusters with greater than \(3n - 6\) contacts: hyperstatic clusters. This is expected, since the densest periodic sphere packing of \(\mathbb{R}^3\) has spheres arranged in a lattice with 6 contacts each \(25\).

The ground-state clusters: those with the maximum possible number \(M(n)\) of contacts, are shown for selected \(n\) in Figure 5. Lattice fragments are dark blue and defects are coloured. The ground states appear to converge rapidly to lattice fragments: for \(n = 15, 16\) there is one defect in a ground state, and for \(n = 17, 18\), there are none. This is in marked contrast to clusters with a smooth potential such as Lennard-Jones clusters, where non-lattice arrangements are found in ground states for \(n = O(100)\) \(20\).

A famous mathematical problem is the “kissing problem,” which asks how many spheres can touch a single sphere without overlap. The answer is 12 \(1\), and the two clusters that achieve this (one hcp, one fcc) are the left-most ground states for \(n = 13\). What is not commonly known is there are six other clusters with the same number of contacts, three of which have defects. As \(n\) increases, ground states more frequently contain caged spheres: 2/4, 5/6, 6/8, 6/6, 5/5 for \(n = 14-18\) respectively.

Lattice fragments Overall, the percentage of clusters which are lattice fragments decreases with \(n\), as 17%, 7.2%, 3.6%, 1.6%, 0.63% for \(n = 10-14\) respectively. A greater proportion of hyperstatic clusters are lattice fragments (see Appendix.) The ground states have slightly more hcp than fcc fragments, though we expect random stacking to dominate as \(n\) increases as it is combinatorially favoured. Note that even though the ground states may be lattice fragments, they could be thermodynamically dominated by the overwhelming number of clusters with defects.

Singular clusters The dataset contains a great many singular clusters: those which are linearly floppy, but nonlinearly rigid. \(30\) All hypostatic clusters are singular, but many others are as well including those with \(\geq 3n - 6\) contacts. The smallest occurs at \(n = 9\) and is shown in Figure 4 (left): this is a fragment of an fcc lattice. As \(n\) increases the fraction of singular clusters is nearly constant: 3%, 2.9%, 2.7%, 2.5% for \(n = 11, 12, 13, 14\) (see Appendix for more statistics.) Hyperstatic clusters can also be singular, as are two of the ground states for \(n = 13\).

The \(n = 9\) singular cluster was experimentally observed to occur in equilibrium with frequency 11% \(12\), which is much higher than if all 52 clusters occurred with equal probability. This is likely because the dynamical matrix acquires a zero eigenvalue so the vibrational partition function in the harmonic approximation diverges \(12\). Therefore, it could be that singular clusters dominate the free energy in a thermodynamic system. Since they are robust with \(n\), it is important to learn how to evaluate their free energies, and to determine how much depends on geometry and how much is due to the choice of interaction potential (for example as in \(24\)).

Localized (“circular”) transition paths The paths used to find rigid clusters are also relevant pieces of a cluster’s configuration space. For example, they are the minimum-energy paths between rigid clusters when the spheres interact with a short-range potential, so can be used to evaluate the leading-order transition rates \(23\). What are the topologies of the paths? Most are intervals connecting distinct clusters, as expected (Figure 5 (left).) Interestingly, we also find paths which are circles: we break a contact, move along the one-dimensional path, and re-form exactly the same contact in exactly the same configuration. This first happens for \(n = 11\) as shown in Figure 5 (right). For \(n = 13\) there are roughly 18,300 circular paths, and they occur for all types of clusters (regular/singular/hyperstatic/hypostatic.) This suggests there could be circular paths that do not eventually form another contact: the cluster may internally deform along a soft mode without ever becoming rigid. This would be analogous to the localized soft modes found in gels and networks \(25\,27\). Such a cluster would be metastable since it could not reach a lower-energy state without first breaking a contact, so for certain applications one should treat them on par with rigid clusters. How to find such circular metastable states is an open question.

A cluster with no one-dimensional deformation paths We found a cluster at \(n = 11\) that cannot be accessed from any other by one-dimensional paths, shown in Figure 6. We checked that breaking any single contact except two (in red) forms a regular cluster with two degrees
of freedom. When either or both of the red contacts is broken, the cluster is still nonlinearly rigid. Therefore there does not exist a subset of contacts that, when broken, forms a cluster with one degree of freedom.

We found this cluster by accident, by deleting a sphere (red) from an $n = 12$ cluster. This leads to an intriguing idea – perhaps other such highly singular clusters could be discovered through this method of catalysis?

**DISCUSSION**

**How to understand hypostaticity?**

How is it possible for a cluster to have fewer than $3n - 6$ contacts? To answer, it is helpful to have a low-dimensional analogy of system (1). Suppose the space of “clusters” is three-dimensional. Then each single contact equation in (1) is solved by points on a two-dimensional manifold: a surface. Two contacts make two surfaces that generically intersect in a one-dimensional manifold, or a curve, and three contacts make three surfaces that generically intersect at a point, as shown in Figure 7 (left).

Following this analogy, having extra contacts means there is one (or more) additional equation in (1) for which $x$ is already a solution. Figure 7 (middle) shows an example where four surfaces intersect at a point instead of three. Deleting one of the surfaces still leads to an isolated intersection point.

Having fewer contacts is also possible, as shown in Figure 8 (right). Here two surfaces intersect at a single point where they are exactly tangent. Linear analysis would predict a two-dimensional solution set, however we cannot move any small but finite distance away and remain on both surfaces, so this point is a nonlinearly rigid solution. Perturbing the surfaces slightly, for example by shifting one up or down, will either destroy the intersection point or turn it into a one-dimensional curve, so a hypostatic cluster is a special case that is extremely sensitive to the choice of parameters.

**Comparison with previous results**

Two previous studies sought to enumerate minimally rigid clusters, by listing all non-isomorphic adjacency matrices with $3n - 6$ contacts and trying to solve (1) for each. Arkus et al. [21] solved for the positions of the sphere centers analytically, or proved there is no solution, so this is guaranteed to be the complete set of minimally rigid clusters up to $n = 10$. Hoy et. al. [22] used Newton’s method with random initial conditions to solve for the positions of the sphere centers. Their method is not provably complete, partly because Newton’s method is not guaranteed to find a solution even if it exists, and partly because they incorrectly assumed a rigid cluster always contains a Hamiltonian path [38]. Nevertheless they produced a large dataset for $n \leq 11$ that can be used to test other methods. Our set of clusters is nearly identical to theirs, but with the following discrepancies for $n = 11$: (i) They list two clusters as rigid that our method identifies as floppy. (ii) They do not find the second solution for the adjacency matrix with two solutions. (iii) They do not find hypostatic clusters, because they do not look for these.

**Completeness of the data**

The discovery of a cluster that has no one-dimensional deformation paths implies the algorithm cannot find all nonlinearly rigid clusters – there may be other single clusters or collections of clusters that are not accessible from the starting set by such paths. Additionally, we test only for pre-stress stability, and do not consider clusters that are rigid under weaker conditions. Nevertheless, the agreement with previous studies for lower $n$ makes it reasonable to expect it finds the vast majority of rigid sphere packings; we suspect the missing clusters or collections are rare. Perhaps it enumerates a complete subset of packings: for example, the set of non-singular clusters may be connected by one-dimensional transition paths. Proving such a statement or a variant (such as for non-identical spheres, or overlapping spheres), would be valuable because the algorithm is fast, so it could be applied to less-studied systems such as spheres of different sizes, or objects of different shapes.

**CONCLUSION**

We computed a set of nonlinearly rigid clusters of $n \leq 14$ hard spheres, using a dynamical algorithm that follows all possible transition paths between clusters. There is good evidence to believe this is the entire set of such clusters, minus a few rare clusters that are either too singular or cannot be reached by one-dimensional transition paths. This dataset is much larger and more complete than those produced before, so we expect it to be useful in addressing questions in statistical physics and chemistry, for example. Along the way we raise several issues that could usefully be addressed from a mathematical, geometrical, or computational perspective. The data contained several surprises, perhaps the biggest of which was clusters which are hypostatic. The thermodynamic importance of these is currently unknown, but experiments show that singular clusters – those which are linearly floppy but nonlinearly rigid – occur with high probability in a system of particles with a short-range interactions; quantitatively evaluating their thermodynamic properties is an important and open problem.
Thanks to Michael Brenner, Steven Gortler, and Vinothan Manoharan for many helpful discussions, and to Rob Hoy for sharing his data. This work was partially supported by the DOE Early Career Research Program de-sc0012296.

[1] J. H. Conway and N. J. A. Sloane, *Sphere Packings, Lattices, and Groups* (Springer, New York, 1999).
[2] K. Bezdek, A. Deza, and Y. Ye, in *Discrete geometry and optimization*, Fields Institute Communications, Vol. 69 (2013).
[3] L. Asimow and B. Roth, Trans. Amer. Math. Soc. 245, 279 (1978).
[4] R. Connelly and W. Whiteley, SIAM J. Disc. Math. 9, 453 (1996).
[5] S. J. Gortler, A. D. Healy, and D. P. Thurston, Am. J. Math. 132, 897 (2010).
[6] A. Ozkan and M. Sitharam, in *Proceedings of BiCoB* (New Orleans, 2011).
[7] C. W. Wampler and A. J. Sommese, Acta Numerica 20, 469 (2011).
[8] F. Stillinger and T. Weber, Science 225 (1984).
[9] D. R. Nelson and F. Spaepen, Solid State Physics 42, 1 (1989).
[10] S. Auer and D. Frenkel, Nature 409, 1020 (2001).
[11] C. P. Royall, S. R. Williams, T. Ohtsuka, and H. Tanaka, Nat. Mater. 7, 556 (2008).
[12] G. Meng, N. Arkus, M. Brenner, and V. Manoharan, Science 327, 560 (2010).
[13] S. Edwards and R. Oakeshott, Physica A 157, 1080 (1989).
[14] D. Asenjo, F. Paillusson, and D. Frenkel, Phys. Rev. Lett. 112, 098002 (2014).
[15] M. R. Hoare and J. A. McInnes, Advances in Physics 32, 791 (1983).
[16] D. J. Wales, Science 293, 2067 (2001).
[17] V. N. Manoharan and D. J. Pine, Mater. Res. Soc. Bull. 29, 91 (2004).
[18] J. A. Fan, C. Wu, K. Bao, J. Bao, R. Bardhan, N. J. Halas, V. N. Manoharan, P. Nordlander, G. Shvets, and F. Capasso, Science 328, 1135 (2010).
[19] N. B. Schade, M. Holmes-Cerfon, E. R. Chen, D. Aronzon, J. W. Collins, J. A. Fan, F. Capasso, and V. N. Manoharan, Phys. Rev. Lett. 110, 148303 (2013).
[20] D. J. Wales and J. P. K. Doye, J. Phys. Chem. A 101, 5111 (1997).
[21] N. Arkus, V. Manoharan, and M. Brenner, SIAM J. Disc. Math. 25, 1860 (2011).
[22] R. Hoy, J. Harwayne-Gidansky, and C. O’Hern, Phys. Rev. E 85 (2012).
[23] M. Holmes-Cerfon, S. J. Gortler, and M. P. Brenner, Proc. Natl. Acad. Sci. 110 (2013).
[24] J. C. Maxwell, Philos. Mag. 27, 294 (1864).
[25] J.-N. Roux, Phys. Rev. E 61, 6802 (2000).
[26] M. V. Hecke, J. Phys.: Condens. Matter 22, 033101 (2010).
[27] R. Sun, A. Souslov, X. Mao, and T. C. Lubensky, Proc. Natl. Acad. Sci. 109, 12369 (2012).
[28] J. Paulose, B. G. ge Chen, and V. Vitelli, arXiv:1406.3323 (2014).
[29] J. P. K. Doye and D. J. Wales, Chem. Phys. Lett. 262, 167 (1996).
[30] W. B. Rogers and J. C. Crocker, PNAS 108 (2011).
[31] R. Connelly and H. Servatius, Discrete Comput. Geom. 11, 193 (1994).
[32] M. Holmes-Cerfon, “http://cims.nyu.edu/~holmes/,”.
[33] A. Donev, I. Cisse, D. Sachs, E. A. Variano, F. H. Stillinger, R. Connelly, S. Torquato, and P. M. Chaikin, Science 303, 990 (2004).
[34] A. Donev, R. Connelly, R. H. Stillinger, and S. Torquato, Phys. Rev. E 75, 051304 (2007).
[35] T. C. Hales, Ann. Math. 162, 1065 (2005).
[36] This is slightly more restrictive than the usual definition, which also includes all clusters with extra contacts.
[37] C. L. Kane and T. C. Lubensky, Nature Phys. 10 (2014).
[38] B. Hayes, “Sphere packings and Hamiltonian paths,” http://bit-player.org/2013/sphere-packings-and-hamiltonian-paths (2013).
[39] K. Bezdek, Discrete Comput. Geom. 48, 298 (2012).
[40] K. Bezdek and S. Reid, J. Geom. 104, 57 (2013).
[41] G. Garcea, G. Formica, and R. Casciaro, In. J. Numer. Meth. Engng 62, 979 (2005).
[42] B. Dayton and Z. Zeng, in *ISSAC’05*, edited by N. Y. ACM (2005).
[43] A. Leykin, J. Verschelde, and A. Zhao, Theoretical Computer Science 359, 111 (2006).
[44] B. H. Dayton, T.-Y. Li, and Z. Zeng, Mathematics of Computation 80, 2143 (2011).
[45] B. McKay, Congressus Numerantium 30, 45 (1981).
[46] M. Wyart, L. E. Silbert, S. Nagel, and T. A. Witten, Phys. Rev. E 72, 051306 (2005).
[47] M. Wyart, Phys. Rev. Lett. 109, 125502 (2012).
FIG. 1. Selected hypostatic clusters. From left to right: \( n = 10 \) (smallest hypostatic cluster, missing 1 contact), \( n = 11 \) (missing 2 contacts), \( n = 11 \) (missing 2 contacts), \( n = 14 \) (missing 3 contacts; light blue spheres are \( n = 10 \) hypostatic cluster), \( n = 19 \) (missing 6 contacts; dark blue spheres are \( n = 11 \) hypostatic cluster).

FIG. 2. (a) Smallest clusters with the same adjacency matrix \( (n = 11) \). The dark(light) blue spheres have identical coordinates on each, while the red sphere forms three contacts with the light blue spheres in two different ways. (b) Another pair with the same adjacency matrix \( (n = 12) \). The green+red spheres form a rigid cluster and have identical locations in each cluster, while the blue+red forms another rigid cluster. It shares three contacts and the red sphere with the green+red cluster, and there are two different ways to perform this gluing. (c) Four clusters with the same adjacency matrix \( (n = 14) \). The five dark blue spheres form a rigid cluster, while other spheres are colored to aid visualization.
FIG. 3. Clusters with the maximum number of contacts, for $13 \leq n \leq 17$. Dark blue spheres all lie on a lattice, while coloured spheres form defects. In some cases there is more than one natural way to group the spheres so the defects are given different colours, i.e. the lattice is either (dark blue + light blue), or (dark blue + green). The ground states for $n = 18$ are not shown as these are also all lattice fragments.
FIG. 4. Selected singular clusters, for \( n = 9, 10, 11 \) (left to right). Each has a linear degree of freedom, but is nonlinearly rigid. These are new seeds: they cannot be formed by gluing spheres to a smaller cluster. They all have \( 3n - 6 \) contacts.

FIG. 5. Left: a typical transition path. A contact is broken, and the cluster deforms into a geometrically distinct cluster. Right: a circular transition path (\( n = 11 \)). When the red contact breaks (top left), the light blue spheres twist to the right (top right), creating space for the red sphere to move down past the plane of the dark blue spheres, which are fixed in place. When the light blue spheres twist back to center all spheres return to their original positions except the red one (bottom right). The light blue spheres twist left (bottom left), allowing the red sphere to move back up through the plane and return to its original position.

FIG. 6. A cluster the algorithm cannot find (left) (\( n = 11 \)). This is a fragment of an fcc lattice that is missing 1 contact. Breaking either or both of the red contacts gives a nonlinearly rigid cluster. Breaking any other contact gives a cluster with two degrees of freedom. Therefore there are no one-dimensional transition paths leading to this cluster. Right: the cluster it came from (\( n = 12 \)), by deleting the red sphere.

FIG. 7. A low-dimensional analogy to understand nonlinear rigidity. Each contact is represented by a surface, and a nonlinearly rigid cluster is an isolated intersection point (in red). Left: a generically, three surfaces are required in \( \mathbb{R}^3 \) for an isolated intersection point; this is an analogy for a regular cluster. Middle: four surfaces intersecting at a single point, as for a hyperstatic cluster. Right: two surfaces that intersect at a single point, as for a hypostatic cluster.
TABLE II. Ratios of number of cluster of each type, to the number of the same type with one less sphere.

| n | # of contacts - 3n |
|---|-------------------|
| 6 | 2                 |
| 7 | 2.5               |
| 8 | 2.6               |
| 9 | 4                 |
| 10| 5.0              |
| 11| 6.2               |
| 12| 7.2               |
| 13| 7.8               |
| 14| 8.1               |
| 15| 8.7               |
| 16| 9.9               |
| 17| 10.1              |
| 18| 10.2              |

FIG. 8. Total number of clusters $N(n)$, and the best-fit curve $2.5(n-5)!$

This section contains more detailed statistical information about the set of clusters. The set of coordinates is listed on the author’s website [32].

Total number of clusters

Consider the ratios of total number of clusters $N(n + 1)/N(n)$. Table II shows this appears to be multiplied by nearly $n - 4.8$ for each $n$. Therefore the total number grows roughly as $(n - 5)!$. We fit the total number $y = b \cdot (n - 5)!$. Minimizing the mean-square error in linear space over $5 \leq n \leq 14$ gives $b = 2.46$. This does a very good job for the data computed, (see Figure 8), but will likely slightly underestimate for larger $n$.

Lattice fragments

We determined whether a cluster was a lattice fragment by choosing three mutually contacting spheres, and rotating this triangle to the seven triangles of a bipyramid (two tetrahedra in contact.) For each rotation we checked whether all the $z$-coordinates of the cluster were integer multiples of $\sqrt{2}/3$, and if they were we checked whether each plane of spheres at constant $z$ formed a hexagonal lattice. The data is shown in Table IV. This also identifies the lattice type of clusters in Figure (3).

Singular

We computed the number of rigid clusters for which the Jacobian of (1) had at least one element in the null space. This data is shown in Table V. We also show the numbers of clusters which are both singular, and lattice fragments.

Gaps

As $n$ increases, the smallest gap between spheres not in contact decreases. This is one major difference between sphere packings and clusters with a smooth potential, and may be part of the explanation for the combinatorial rather than exponential growth in the number of clusters.

We checked that we are resolving the smallest gap by computing the minimum gap size over all clusters, where the gap for each cluster is the minimum pairwise distance between non-contacting spheres minus 1. (Recall that for $n \geq 15$ not all clusters are computed.) The minimum gap decreases continually with $n$ as follows:

| n | minimum gap       |
|---|-------------------|
| 6 | 0.4142            |
| 7 | 0.05146           |
| 8 | 0.05146           |
| 9 | 0.05146           |
| 10| 0.03296           |
| 11| 0.02634           |
| 12| 2.129e-3          |
| 13| 5.768e-5          |
| 14| 1.296e-5          |
| 15| 0.004364          |
| 16| 0.006154          |
| 17| 0.006154          |
| 18| 0.006154          |

At $n = 13$ there are 23, 9 clusters with gaps less than $10^{-3}, 10^{-4}$ respectively. These are all regular clusters with $3n - 6$ contacts. The ten smallest gaps are $10^{-5} \times 10^{-4}$.
At \( n = 14 \) there are 929, 244, 34, 6 clusters with gaps less than \( 10^{-3}, 10^{-4}, 5 \times 10^{-5}, 2 \times 10^{-5} \) respectively. All have \( 3n - 6 \) contacts, and all are regular except three of the ones with the largest gaps. The ten smallest gaps are \( 10^{-5} \times (1.269, 1.377, 1.385, 1.387, 1.744, 2.536, 2.538, 2.538, 2.539) \).

The smallest gaps for \( n = 14 \) are close to our tolerance for adjacency (\( \text{tolA} = 10^{-5} \)), but the gaps appear to approach the minimum smoothly, with a jump to \( \text{tolA} \), so it is likely we have resolved the cutoff. However, applying the algorithm for larger \( n \) will require changing the numerical parameters to resolve smaller gaps.

The cumulative gap size distributions are shown in Figure 9. These are a fascinating mixture of smooth distributions, plus sharp jumps when many clusters have the same minimum gap size.

**Maximum number of contacts**

The “Combinatorial Kepler Problem” asks how \( M(n) \) behaves as \( n \to \infty \). We expect \( M(n) \sim 6n \) to leading order as the cluster approaches a lattice, but one can also include surface corrections, which scale as \( n^{2/3} \). Bezdek et al. [39,40] proved that \( 6n - 7.862n^{2/3} \leq M(n) \leq 6n - 0.926n^{2/3} \), where the upper bound holds for all \( n \) and the lower bound holds for \( n = 6, 19, \ldots, k(2k^2 + 1)/3, k \in \mathbb{N} \). We find that \( M(n) = \lfloor \text{lower bound} \rfloor + 1 \) for \( 6 \leq n \leq 16 \), (except \( n = 12 \) where the correction is 2), and the upper bound is more than double the maximum; this suggests the lower bound is closer to the correct scaling so the bounds could be strengthened. Table III shows this suggests the lower bound is closer to the correct scaling, plus sharp jumps when many clusters have the same minimum gap size.

**Numerical Algorithm**

The numerical algorithm consists of three components: one to determine the dimension of the solution set to equation (1), one to project onto the solution manifold, and one to walk along a one-dimensional manifold. We describe these in turn, as well as the algorithm to store and compare clusters.

**Determining the dimension of the solution set**

Suppose we have an adjacency matrix \( A \) representing a set of \( m \) contacts, and a solution \( \mathbf{x} \) to the corresponding system of equations (1). There is one equation for each pair of spheres \( (i,j) \) that are in contact, and the translational and rotational degrees of freedom are removed by fixing the first sphere at the origin, the second on the \( x \)-axis, and the third on the \( xy \)-plane. In practice, we choose the first three spheres that form a triangle of contacts. We wish to determine the dimension of the solution set near \( \mathbf{x} \), assuming that \( \mathbf{x} \) lies on a smooth manifold so this quantity is well-defined. In particular, we wish to determine whether the dimension is 0, 1, or \( > 1 \).

We do this in two ways. One is a semi-analytic method that determines the dimension via solvability conditions. This can be rigorously justified, but is not developed to handle every possible case that can appear in practice. The second is purely numerical, based on trying to move small distances in each of the candidate tangent directions. It produces an answer for all cases, and though it is not rigorous, it still worked extremely well in that it gave the correct dimension in cases we could verify with the semi-analytic method. However, it was orders of magnitude slower than the latter, which was necessary to apply our algorithm to larger values of \( n \).

Both methods require looking at derivatives of (1). Let us look for an analytic motion of the sphere centers \( \mathbf{p}(t) \) parameterized by \( t \in \mathbb{R} \) with \( \mathbf{p}(0) = \mathbf{x} \). Differentiating (1) gives

\[
R(\mathbf{x})\mathbf{p}' = 0 \tag{A.2}
\]

\[
R(\mathbf{x})\mathbf{p}'' = -R(\mathbf{p}')\mathbf{p}' \tag{A.3}
\]

\[
\vdots \vdots
\]

\[
R(\mathbf{x})\mathbf{p}^{(n+1)} - \sum_{k=1}^{n} \left( \binom{n}{k} R(\mathbf{p}(k))\mathbf{p}^{(n-k+1)} \right) \tag{A.4}
\]

where \( R(\mathbf{p}) \) is the “rigidity” matrix. It is constructed so that \( R(\mathbf{p})(\mathbf{y})_k = (\mathbf{p}_k - \mathbf{p}_{j_k}) \cdot (\mathbf{y}_i - \mathbf{y}_{j_k}) \) for any vector
TABLE III. Upper and lower bounds for the combinatorial Kepler problem, and our data. The upper bound is proven for all $n$ and the lower bound for $n = k(2k^2 + 1)/3, k \in \mathbb{N}$.

| $n$ | # of lattice fragments (total # of clusters) |
|-----|---------------------------------------------|
|     | $3n - 7$ | $3n - 8$ | $3n - 7$ | $3n - 6$ | $3n - 5$ | $3n - 4$ | $3n - 3$ | $3n - 2$ |
| 5   | 1 (1)   | 1 (1)   | 1 (1)   | 1 (1)   | 1 (1)   | 1 (1)   | 1 (1)   | 1 (1)   |
| 6   | 1 (2)   | 1 (2)   | 1 (2)   | 1 (2)   | 1 (2)   | 1 (2)   | 1 (2)   | 1 (2)   |
| 7   | 1 (5)   | 1 (5)   | 1 (5)   | 1 (5)   | 1 (5)   | 1 (5)   | 1 (5)   | 1 (5)   |
| 8   | 4 (13)  | 4 (13)  | 4 (13)  | 4 (13)  | 4 (13)  | 4 (13)  | 4 (13)  | 4 (13)  |
| 9   | 11 (52) | 11 (52) | 11 (52) | 11 (52) | 11 (52) | 11 (52) | 11 (52) | 11 (52) |
| 10  | 0 (1)   | 33 (259) | 3 (3)  | 3 (3)  | 3 (3)  | 3 (3)  | 3 (3)  | 3 (3)  |
| 11  | 0 (2)   | 4 (18)  | 103 (1618) | 12 (20) | 1 (1) |
| 12  | 0 (11)  | 13 (148) | 339 (11,638) | 77 (174) | 4 (8)  | 1 (1)  |
| 13  | 1 (87)  | 57 (1221) | 1079 (95,810) | 364 (1307) | 42 (96) | 5 (8)  |
| 14  | 0 (1)   | 6 (707)  | 242 (10,537) | 3451 (872,992) | 1622 (10,280) | 298 (878) | 35 (79) | 2 (4)  |
| 15  | 1748 (7675) | 265 (782) | 23 (55) | 5 (6)  |
| 16  | 1997 (7895) | 220 (664) | 29 (62) | 7 (8)  |
| 17  | 2036 (7796) | 267 (798) | 51 (85) | 6 (6)  |
| 18  | 2451 (9629) | 434 (1085) | 59 (91) | 5 (5)  |

TABLE IV. Lattice fragment data. Top: number of lattice fragments, organized by number of contacts. The total number of clusters of each type is shown in brackets. Middle: total number of lattice fragments for each $n$. Bottom: lattice fragment type for ground-state clusters, in the order they are shown in Figure 3 (if shown). Here fcc, hcp, rcp, 2d, none stand for face-centered cubic, hexagonal close packing, random-stacking, two-dimensional lattice fragment (undetermined), and defective respectively.

$y \in \mathbb{R}^{3n}$ and each contact $k, 1 \leq k \leq m$. From the final six equations we have $R_{m+j} = e^T_{s_j}$ for $1 \leq j \leq 6$, $s_j \in \{1, 2, 3, 5, 6, 9\}$ for the constrained vertices, where $e_s$ is the vector with 1 in the $s$th position and zeros elsewhere. Let the right and left null spaces of the rigidity matrix be $V, W$ respectively, with bases $\{v_i\}, \{w_i\}$ and sizes $n_v = |V|, n_w = |W|$.

If $R(x)$ is of full rank and the number of rows does not exceed the number of columns, then the solution set is regular, the Implicit Function Theorem applies, and the dimension of the solution set is $n_v$. Otherwise, the solution set is singular, and in general there is no algorithm to determine its dimension that is guaranteed to terminate in finite time. Nevertheless, in certain cases we can determine the dimension, and this is the basis of our semi-analytic method.
| $n$ | $3n - 9$ | $3n - 8$ | $3n - 7$ | $3n - 6$ | $3n - 5$ | $3n - 4$ | $3n - 3$ | $3n - 2$ |
|-----|---------|---------|---------|---------|---------|---------|---------|---------|
| 9   |         |         | 1 (52)  |         |         |         |         |         |
| 10  |         | 1 (1)   | 4 (259) |         | 0 (3)   |         |         |         |
| 11  | 2 (2)   | 18 (18) | 28 (1618)| 1 (20) | 0 (1)   |         |         |         |
| 12  | 11 (11) | 148 (148)| 175 (11,638) | 7 (174)| 8 (8)   |         |         |         |
| 13  | 87 (87)| 1221 (1221)| 1311 (95,810)| 50 (1307)| 1 (96)| 2 (8)   |         |         |
| 14  | 1(1)   | 707(707)| 10,537 (10,537)| 10,390 (872,992)| 416 (10,280)| 4 (878)| 3 (79)| 0 (4) |

| $n$ | Total singular (Total clusters) | % Singular |
|-----|--------------------------------|-----------|
| 9   | 1 (52)                         | 1.9%      |
| 10  | 5 (263)                        | 1.9%      |
| 11  | 49 (1659)                      | 2.95%     |
| 12  | 341 (11,980)                   | 2.85%     |
| 13  | 2672 (98,529)                  | 2.71%     |
| 14  | 22,058 (895,478)               | 2.46%     |

| $n$ | lattice&singular (total singular) | % |
|-----|----------------------------------|---|
| 9   | 1 (1)                           | 100% |
| 10  | 2 (5)                           | 40%  |
| 11  | 13 (49)                         | 26.5%|
| 12  | 40 (341)                        | 11.7%|
| 13  | 174 (2672)                      | 6.5%  |
| 14  | 791 (22,058)                    | 0.088%|

| $n$ | # of singular clusters (total # of clusters) |
|-----|---------------------------------------------|
| 9   | 11.7%                                        |
| 10  | 1 (52)                                       |
| 11  | 87 (87)                                      |
| 12  | 1311 (95,810)                                |
| 13  | 50 (1307)                                    |
| 14  | 416 (10,280)                                 |

**Semi-analytic determination of dimension** Let the tangent space to the solution to (1) have orthogonal basis $B$, and let $D = |B|$ be its dimension. This method proceeds as follows:

1. If $|V| = 0$: the cluster is first-order rigid. Return $D = 0$.

2. If $|W| = 0$: there are no solvability conditions on $\sum_{a,j} a_j v_j$, so this system can be solved up to any order. Proceed to numerical method, or return $D = n_v$.

3. Test for second-order rigidity. To solve (A.3) for $p' \in V'$, where $V' \subset V$ is a linear subspace, the Fredholm Alternative requires that $w^T R(v) v = 0$ for all $w \in V, v \in V'$. When this does not hold for any subspace $V'$, the cluster is second-order rigid [4].

An arbitrary right and left null vector can be written as $v = \sum_j a_j v_j$, $w = \sum_j b_j w_j$, with $a = (a_1, \ldots, a_n)$, $b = (b_1, \ldots, b_n)$. The RHS of (A.3) can be written as $-\sum_{i,j} a_i b_j R(v_i) v_j$. Taking the inner product with $w$ yields the following:

$$a^T \left( \sum b_k Q^{(k)} \right) a = 0, \quad \text{where} \quad Q^{(k)}_{ij} = w_i^T R(v_i) v_j.$$

If we can find a linear subspace of $a$-values such that this holds for all $b \in \mathbb{R}^{n_w}$, then we can solve (A.3), and the tangent space is contained in the space $V'$ spanned by $\sum a_j v_j$. The negation requires showing that for every $a \in \mathbb{R}^{n_v}$, there is a $b \in \mathbb{R}^{n_w}$ such that (A.5) is non-zero, and then the cluster is second-order rigid. This is hard to show in general, but what is possible is to find a $b$ such that $\sum b_k Q^{(k)}$ is sign-definite. The left null vector $w = \sum_j b_j w_j$ “blocks” all right null vectors and the cluster is called pre-stress stable. It is possible to find such a $b$ using semi-definite programming methods, for example.

In practice, we only check the vectors $b_k = e_k$. If any matrix formed from these is sign-definite, return $D = 0$. Otherwise, continue to the next step. We do this because we got lucky: this test always agreed with our numerical algorithm. Enumerating larger $n$ where unusual cases are more likely to occur will require considering the full set of possibilities.

4. If the dimension is still undetermined, continue to the numerical method.

It was shown in [4] that if the cluster is either first-order-rigid or second-order rigid as described in the tests
(1, 3.) above, then it is nonlinearly rigid, so these tests are sufficient to prove nonlinear rigidity (up to numerical tolerance.) Unfortunately there is no equivalent notion of higher-order rigidity, because it could be that every analytic parameterization of cluster motion has \( p'(0) = 0 \), i.e. the cluster corresponds to a “cusp,” in which case there is a different system of equations to solve [31, 41]. It would be useful to extend these solvability conditions to higher orders and cusps, even if they do not prove nonlinear rigidity, because this would still provide useful information about a cluster’s stability.

**Numerical determination of dimension.** This method tries to estimate an orthogonal basis \( B \) for the tangent space by doing the following for each information about a cluster’s stability.

1. Take a step of size \( \Delta s_0 \) in directions \( \pm v_j \) to obtain \( x_\pm = x \pm \Delta s_0 v_j \)
2. Project back onto the manifold of constraints to obtain \( x'_\pm = \text{Proj}(x_\pm) \). Initially we also require \( (x'_\pm - x_\pm) \perp v_j \) to prevent the projection from going back to the starting point, but if this fails we relax the condition.
3. Let \( v_i = x'_\pm - x \) be the estimated tangent vector. If \( |v_i| > x\text{TolMax} \) or \( |v_i| < x\text{TolMin} \), reject the vector. Otherwise, project \( v_i \) onto our current estimate of \( B \), and let \( v_i^\perp/|v_i| \) be orthogonal to the projection.
4. If \( |v_i^\perp| > \sqrt{Tol} \), then add \( v_i^\perp \) to the basis \( B \).

We use both methods to determine whether to follow a path or not, but only use the semi-analytic method to decide whether or not a cluster is rigid. Therefore all clusters we list are pre-stress stable up to numerical tolerance.

**Projecting onto a manifold**

If we have an approximate solution \( x' \) to (1), we obtain a more accurate solution by solving (1) using Newton’s method with a given tolerance Tol. This is not an orthogonal projection, but we compared it with the orthogonal projection described in [23] which works for regular clusters, and found the two to be very close. We imposed a maximum step size of \( \Delta x_{max} \) in each Newton’s iteration to avoid moving too far away from the solution.

This method suffers several drawbacks for singular clusters. First, Newton’s method loses its quadratic order of convergence, so it typically took an order of magnitude more iterations to converge, and for certain types of singularities it may never converge (this happened only very rarely – there were 1548 total projection errors of all types for \( n = 13 \).) Second, even though the constraints are satisfied to tolerance Tol, the actual solution is less accurate if it is singular. For example, if the equation \( x^2 = 0 \) is satisfied to order \( \epsilon \), then we expect \( x \approx \sqrt{\epsilon} \).

In practice, all clusters we encountered appeared to be accurate to within \( \sqrt{Tol} \).

These concerns can be mitigated through the use of deflation techniques, see e.g. [7, 42–44]. We tried these, but found them not as useful for our study because they require doubling the number of variables at each deflation step. For many singular clusters we had to apply several deflation steps before we obtained quadratic convergence and linear accuracies, however for these clusters we achieved accuracies of \( \sqrt{Tol} \) anyways so the huge slowdown due to the extra variables was not worth the computational effort.

**Moving along a one-dimensional manifold**

Once we determine that a solution set to (1) is one-dimensional, we move along it as follows: first, we extract the direction(s) that make the broken contacts increase in length. For each direction, we alternate between taking a step of size \( \Delta s \) along the manifold in the tangent direction \( v_k \), and projecting back onto the manifold. After each projection we form the rigidity matrix in (A.2), compute its null space \( V \), and find the next tangent direction \( v_{k+1} \) by the least-squares projection of \( v_k \) onto \( V \). This ensures that we keep going in the same direction, i.e. we don’t accidentally start moving backwards along the manifold, and it provides an estimate of the single tangent direction when the path is singular.

After the first step, we check the dimension as in section 1 and stop moving if this dimension has increased or decreased. For \( n = 13 \) it increased for 3851 paths and decreased for 23. We do not check the dimension after the first step, as this is very time-consuming.

At each step we check whether two spheres initially not in contact are within some tolerance \( 1 + \text{tolA} \). The first time this happens we back up one step and repeat the continuation with a smaller step size \( \Delta s_0 \), and again stop when spheres are within \( 1 + \text{tolA} \). Then, we project onto this new set of constraints and check if the cluster is rigid, using a new tolerance \( \text{tolA} \) to determine whether two spheres are adjacent. If, as happens very occasionally, this projection fails (for example because \( \text{tolA} \) is deliberately chosen too big initially, to “catch” more pairs than are actually adjacent), we delete subsets of the new constraints until the projection succeeds. If it never succeeds we abandon the cluster. Note that \( \text{tolA} \) should be chosen comparable in magnitude to \( \Delta s \) because sometimes spheres can come into contact tangentially.

**Cluster isomorphism**

We keep track of clusters through their adjacency matrices in a hash table. Each adjacency matrix has a canonical form that we compute using nauty [45]. This
is converted to a binary vector \( a \in \{0, 1\}^n \) and we define an ordering by setting \( a < b \) if \( a_k < b_k \) where \( k \) is the first entry where they differ.

Adjacency vectors are stored as a binary tree. Each leaf contains the indices of the clusters with that adjacency matrix, and the indices of the child adjacency vectors that are larger or smaller. To add an adjacency vector \( a \) we compare it to a leaf \( b \) on the tree, and move to the larger or smaller child depending on whether \( a > b \) or \( a < b \). We add \( a \) as a child to the leaf at the end of the tree.

When we find a new cluster, we compute the canonical form of the adjacency matrix and coordinates. If this adjacency matrix is already in the list, we compare the cluster and its reflection to those with the same adjacency matrices, by rotating so the same spheres on each are at the vertices of a given equilateral triangle. We use a tolerance \( \text{tolD} \) to determine if the coordinates are the same.

| Parameter      | Value       | Description                                           |
|----------------|-------------|-------------------------------------------------------|
| \( \Delta s \) | 5e-3        | step size along path, in endgame                      |
| \( \Delta s_0 \) | 5e-2        | step size along path, initially                       |
| Tol            | 9e-16       | tolerance for Newton’s method when projecting / sharpening cluster coordinates |
| TolN           | 1e-6        | tolerance on singular values for null space of rigidity matrix |
| \( \Delta x_{\text{max}} \) | 0.02        | maximum step size in Newton’s method                  |
| tolA           | 1e-5        | tolerance for spheres being adjacent                   |
| tolA0          | 1e-3        | initial tolerance for spheres being adjacent, used to stop following path |
| tolD           | 1e-5        | tolerance for coordinates of a cluster being identical |
| xTolMax        | 10\( \Delta s \) | upper bound on cluster displacement, to determine if a cluster has moved along tangent space |
| xTolMin        | \( \Delta s/8 \) | lower bound on cluster displacement, to determine if a cluster has moved along tangent space |
| vTol           | 2\( \Delta s \) | tolerance for determining whether a unit vector is orthogonal to the estimated tangent space: the part orthogonal to the projection must have at least this magnitude. Depends on step size \( \Delta s \) used to move in tangent space, because of curvature of manifold. |

The value of \( \text{tolA} \) was chosen to stay well away from the resolution of \( \sqrt{\text{tol}} \approx 3e-8 \) of the coordinates of the singular clusters, to avoid computing junk clusters. For \( n \geq 15 \) it will be unable to resolve the gaps of certain regular, non-hyperstatic clusters. These gaps may be resolvable in double precision for a few more values of \( n \) because \( \text{tolA} \) can be increased and still be larger than the numerical precision of the cluster coordinates. However, as \( n \) increases further the distances between non-contacting spheres are expected to become arbitrarily close to 1, so higher precision will be necessary.

**Bottleneck**

The computational bottleneck is not only the factorial growth in the number of clusters, but also the polynomial growth in the number of subsets of contacts that must be broken to find transition paths leading out of hyperstatic clusters. For example, for a cluster of \( n = 13 \) with 3 extra contacts, we have to break 4 contacts generically to find a transition path, so we have to check roughly \( (3n-6)^4 \) sets, which is the equivalent of \( (3n-6)^3 \approx 10^9 \) regular clusters. Therefore one ground state takes roughly the same computational time as all the regular clusters combined. This worsens at the number of extra bonds grows: for \( n = 16 \), breaking all subsets of up to 7 contacts for a ground-state cluster is the equivalent of roughly \( (3 \times 16 - 6)^5 \approx 10^{10} \)

**Numerical parameters**

Here are the values of the numerical parameters used in most of the simulations. For \( n = 11–13 \) we ran several simulations with different choices of parameters, and combined data if necessary. Typically the datasets for \( n = 12, 13 \) differed by an \( O(1) \) number of clusters, while for \( n = 11 \) they were typically identical. All numerical computations were performed in double precision.
regular clusters. Higher $n$ may be feasible by developing new methods to avoid checking all possible subsets, e.g. by predicting in advance which subsets are likely to lead to valid transition paths. Ideas from physics may be useful, for example those which study the “soft” modes of interacting particle systems and show these give rise to catastrophic deformations [46, 47].