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Dionysian Hard Sphere Packings are Mechanically Stable at Vanishingly Low Densities

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High strength-to-weight ratio materials can be constructed by either maximizing strength or minimizing weight. Tensegrity structures and aerogels take very different paths to achieving high strength-to-weight ratios but both rely on internal tensile forces. In the absence of tensile forces, removing material eventually destabilizes a structure. Attempts to maximize the strength-to-weight ratio with purely repulsive spheres have proceeded by removing spheres from already stable crystalline structures. This results in a modestly low density and a strength-to-weight ratio much worse than can be achieved with tensile materials. Here, we demonstrate the existence of a packing of hard spheres that has asymptotically zero density and yet maintains finite strength, thus achieving an unbounded strength-to-weight ratio. This construction, which we term Dionysian, is the diametric opposite to the Apollonian sphere packing which completely and stably fills space. We create tools to evaluate the stability and strength of compressive sphere packings. Using these we find that our structures have asymptotically finite bulk and shear moduli and are linearly resistant to every applied deformation, both internal and external. By demonstrating that there is no lower bound on the density of stable structures, this work allows for the construction of arbitrarily lightweight high-strength materials.

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When sand is densely packed, it is strong enough to support the weight of an elephant. But how loosely can one pack sand before this rigidity is lost? The answer is as loosely as one would like. That is, it is possible to rigidly pack hard spheres at any density, from filling all of space to filling none. In this manuscript we show a method for creating the sparsest possible hard sphere packings and demonstrate their impressive stability. Hard sphere packings are of particular interest because unlike other materials with a high strength-to-weight ratio such as tensegrity structures [1] and aerogels [2], hard spheres are purely compressive and do not rely on internal tensile forces.

There exist mechanically rigid packings with a density arbitrarily close to unity, such as the Apollonian gasket [3,4]. We wish to find the foil to such a packing, that is, one with the smallest possible packing fraction that remains mechanically stable. As Dionysus is the nadir to the zenith that is Apollo [5], we refer to the sparsest possible mechanically stable packings as *Dionysian* packings. We present in this Letter a construction for a Dionysian packing which has vanishingly low density in two and three dimensions.

Rigidity [6] describes a state in which no motion is possible. In the context of sphere packings, this is termed *strictly jammed* [7–11]. A strictly jammed packing is resistant to all possible volume preserving deformations of the particles and boundaries.

Demonstrating that a packing is mechanically stable is commonly done using a linear programming algorithm [8–10]. In addition to demonstrating that our packings are stable through this same linear programming approach, we also compute the elastic moduli for the underlying spring network.

Finding a Dionysian packing is the same as finding the jamming threshold of sphere packings [10,11]. The jamming threshold is the lowest density that can be achieved for strictly jammed configurations. However, while this threshold has mostly been explored for monodisperse configurations, we show that lower density packings can be found by expanding the search space to include polydispersity.

The method we employ is inspired by the construction of the Böröczky bridge packing [12,13] for which locally stable bridges of circles can be constructed with arbitrary length. These bridges lead to packings with asymptotically zero density, but only satisfy the very weakest definition of stability; they are only *locally* stable or locally jammed [7–13]. Following the spirit of the Böröczky bridge packing and allowing for the radii of the spheres to be additional degrees of freedom, we achieve Dionysian packings subject to periodic boundary conditions at arbitrarily low densities. This demonstrates that the lower density bound for mechanically stable, repulsive circle, and sphere packings is precisely zero.

To determine if a packing is strictly jammed, we model it as a spring network in which spheres interact through a harmonic contact potential in their overlaps. We examine whether or not the spring network represents a minimum with respect to position degrees of freedom x as well as symmetric affine, volume-preserving strain degrees of freedom ε [9,14], where the potential is

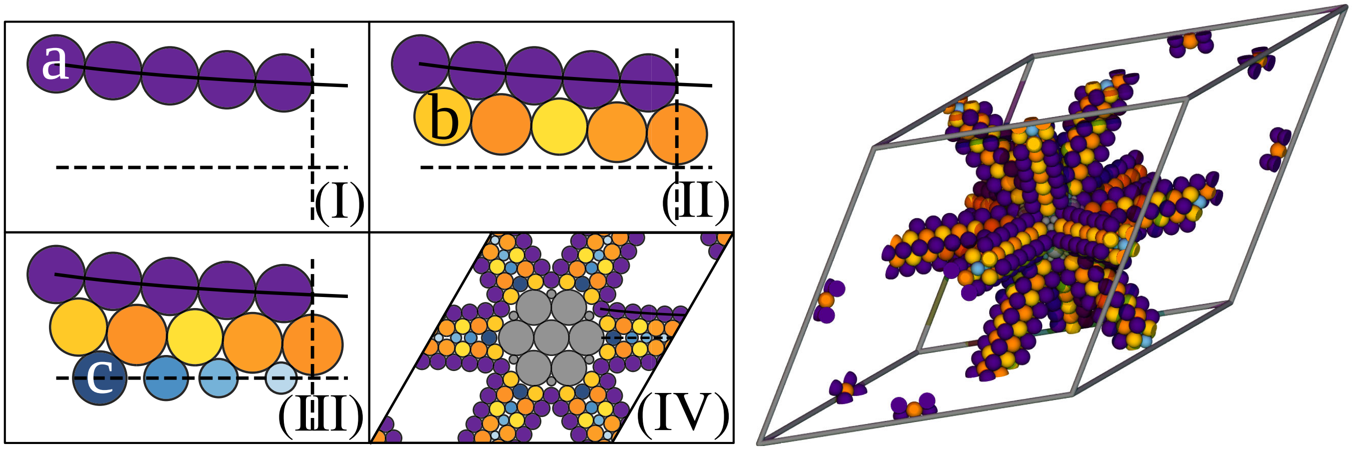

FIG. 1. The construction of a Dionysian packing in two and three dimensions. Left: (I) A row of $n = 5$ circles a (purple) lie on a strictly convex curve $\mathcal{C}$ such that each circle kissing its neighbors. (II) A row of $n = 5$ circles b (orange and yellow) are placed such that they kiss two circles a from below and a circle b on either side. The rightmost b circle is constrained such that its center lies on the vertical line tangent to the rightmost a circle. (III) A row of $n - 1 = 4$ circles c (blue) lie on a horizontal line and kiss two b circles above. (IV) A bridge is formed by reflecting the circles about the dotted lines of symmetry. Three bridges are combined and their centers are filled as shown (gray). Because of the periodic boundary conditions, each of the bridges wraps around the unit cell to contact the central gray spheres twice such that each unit cell contains six half-bridges or three full bridges. The resulting packing, which is jammed and shear stable, has a very low density and is a Dionysian packing in the limit as $n \to \infty$. Right: A three dimensional mechanically stable packing at arbitrarily low densities. Such a construction contains the same three types of spheres as in the two dimensional analog but with additional symmetries and an entirely unrelated set of spheres filling the void region (gray). The three dimensional Dionysian packing has a much narrower set of convex curves $\mathcal{C}$ for which overlaps do not occur (as detailed in the Supplemental Material [16]). This requires a much more subtle curvature of $\mathcal{C}$ which is not apparent to the naked eye in this figure.

$$U = \frac{1}{4}\sum_{i}\sum_{j\neq i}\xi_{ij}^{2} \tag{1}$$

and ξ_{ij} is the normalized overlap between spheres i and j.

We require force balance on all degrees of freedom. The forces on the position degrees of freedom are

$$F_i^\alpha = -\frac{\partial U}{\partial x_i^\alpha} = \sum_{k\in\partial i}\left(\frac{\xi_{ik}n_{ik}^\alpha}{r_i + r_k}\right) = 0, \tag{2}$$

where n_{ik}^α is the α component of the normalized contact vector pointing from particle k to particle i and r_i is the radius of sphere i. Forces on the strain degrees of freedom are

$$-\frac{\partial U}{\partial \varepsilon^{\alpha\beta}} = \frac{1}{4}\sum_{i}\sum_{j\in\partial i}\frac{\xi_{ij}}{r_i + r_j}\left(n_{ij}^\alpha x_{ij}^\beta + n_{ij}^\beta x_{ij}^\alpha\right) \tag{3}$$

for spheres i and j in Cartesian directions α and β, where $\varepsilon^{\alpha\beta}$ is the strain degree of freedom and x_{ij}^α is the contact vector which is not normalized.

These forces are subject to the volume-preserving constraint $\mathrm{Tr}(\varepsilon) = 0$ [9] so that force balance is achieved when

$$-\frac{\partial U}{\partial \varepsilon^{\alpha\beta}}\bigg|_{\mathrm{Tr}(\varepsilon)=0} = -\frac{\partial U}{\partial \varepsilon^{\alpha\beta}} + \frac{\delta^{\alpha\beta}}{d}\sum_{\gamma=1}^{d}\frac{\partial U}{\partial \varepsilon^{\gamma\gamma}} = 0. \tag{4}$$

Because this derivative is proportional to overlap, it is trivially zero for any packing where overlaps do not occur. To ensure that these packings are at a critical point due to a balancing of strain degrees of freedom, we evaluate the derivative with infinitesimal overlap.

The rigidity matrix [15] in conjunction with a linear programming algorithm [8–10] is used to determine if packings are strictly jammed. The rigidity matrix R_x relates a perturbation of the particles $\vec{x}$ with the stresses on the bonds $\vec{b}$ such that $\vec{b} = R_x\vec{x}$. However, perturbing the particles is not our only degree of freedom to explore when considering whether or not a packing is strictly jammed as we must also consider bulk deformations of the system as encoded in strain degrees of freedom. We define the extended rigidity matrix as $R = (R_x R_\varepsilon)$, where R_x is the ordinary rigidity matrix and R_ε relates the bond stresses to the strain degrees of freedom. (See Supplemental Material [16] for more information.) However, applying a strain that increases the volume of the periodic cell will allow all of the bonds to break, unjamming the packing. As such, we apply a constraint preventing the strain matrix ε from having volume changing deformations [9].

We quantify the degree of stability by calculating the resistance of the packing to compressive deformations and shear deformations via the bulk and shear moduli, respectively. These quantities can be calculated simultaneously by computing the stiffness matrix C [17] for the packing. This matrix has the property $\vec{\sigma} = C\vec{\epsilon}$, where $\vec{\sigma}$ is the stress experienced by the packing when a particular strain $\vec{\epsilon}$ is applied. The stiffness matrix can be computed in terms of the rigidity matrix as well as the states of self-stress for R_x. The matrix of states of self-stress S is an orthonormal basis for the zero modes of R_x^T such that $R_x^T S = \vec{0}$. The states of self-stress represent the basis of stresses that can be placed on the bonds without causing particle perturbations. Using these terms, the stiffness matrix can be computed as

$$C = R_\epsilon^T S S^T R_\epsilon. \tag{5}$$

(See Supplemental Material [16] for a derivation and an explanation of this equation.)

To explicitly satisfy the constraints for shear stability and jamming, we focus on creating a packing which is locally stable and has a high number of contacts per particle z, and then test for stability. As illustrated in Fig. 1 and described in more detail in the Supplemental Material [16], this is achieved by placing n circles labeled a, where n is an odd integer greater than 2, on a strictly convex curve $\mathcal{C}$ such that they kiss their neighbors. A new row of circles b is then placed below so that each b circle kissing two a neighbors from below and a b neighbor on each side. Finally, the centers of circles c are placed on a line of zero slope and constrained to touch two b circles from below. Applying the appropriate symmetries, a stable bridge is formed. This construction can be replicated and the bridges can be joined such that a circle packing is formed without overlapping regions. This packing, with the addition of thirteen circles filling the largest void, is a Dionysian packing for particular construction parameters. Our bridge placement for the two dimensional Dionysian packing is based on the contact network of the triangular lattice.

In the limit of an infinitely large bridge, we find that every a circle has four contacts, every b has six, and every c has four. The asymptotic number ratio of this packing is $a:b:c = 2:2:1$. This means that there are $z = (2\times 4 + 2\times 6 + 4)/5 = 4\frac{4}{5}$ contacts per particle in two dimensions, which is larger than is required by the Maxwell rule for shear stable and jammed systems [18].

For the Böröczky locally jammed packing [12,13], the two dimensional version can be used to create a locally jammed packing in any dimension by elevating the circles to spheres of the desired dimension and stacking the result. Such a trivial procedure will not work to extend the Dionysian construction because it results in structures which are not convex and so are subject to zero energy modes. To create a three dimensional Dionysian packing, we instead construct a set of six bridges in three dimensions and combine them as shown in Fig. 1. A three dimensional bridge is constructed very similarly to the two dimensional bridge and exploits the symmetries of three dimensional space.

In the limit of an infinitely large bridge, we find that every a sphere has six contacts, every b has eight, and every c has eight. The asymptotic number ratio for these spheres is $a:b:c = 4:4:1$. This means that there are $z = (4\times 6 + 4\times 8 + 8)/9 = 7\frac{1}{9}$ contacts per particle in three dimensions, which is larger than is required by the Maxwell rule for shear stable and jammed systems [18].

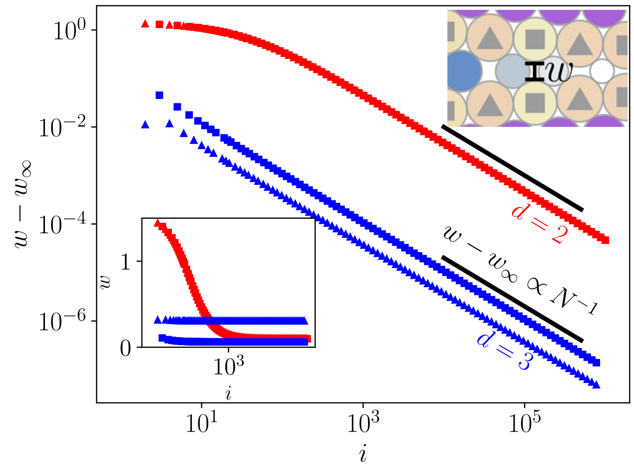

FIG. 2. Top right inset: demonstration of the definition of a gap for a circle. The b circles, indexed by i, oscillate in size and are separated into two categories labeled by squares and triangles. Bottom left inset: The gap value for both square and triangular marked spheres asymptotes in two and three dimensions. When the asymptotic gap value is subtracted, the gap sizes follow a power law of N^{-1} as they reach their respective asymptotic values.

Not all convex curves $\mathcal{C}$ result in viable packings; some choices of $\mathcal{C}$ result in overlapping of spheres in the limit as n approaches infinity. While infinitely many viable choices of $\mathcal{C}$ are possible, for simplicity we choose curves that fit the form

$$f(x) = \frac{(f_0 - h_\infty)^2}{(f_0 - h_\infty) - x\delta} + h_\infty, \tag{6}$$

where f_0 is the height of the curve at $x = 0$, δ is the slope of the curve at $x = 0$, and $h_\infty = \lim_{x\to\infty} f(x)$. The values used in this manuscript are different between the two and three dimensional versions. (See Supplemental Material [16]).

For these parameters, we can track the smallest distance w between the b spheres and their reflected counterparts as seen in Fig. 2. From this figure, we see a very clear power law and conclude that in the limit of infinitely large bridges, no unwanted additional contacts are created. This means that regardless of the value of n we choose, there are no overlaps for our Dionysian packing subject to the chosen curves $\mathcal{C}$. Because the length of our bridges increases with n but the other spatial dimensions do not, this construction results in packings with a density that falls like n^{1-d}.

Using the aforementioned linear programming algorithm on our Dionysian packings, we find that they are both jammed and shear stable for every n studied up to $n = 105$

($N = 3145$) with packing fraction 0.0558 in two dimensions and $n = 25$ ($N = 2731$) with packing fraction 0.0128 in three dimensions.

In addition to demonstrating jamming and shear stability, we quantify the level of stability by calculating the shear, G, and bulk, K, moduli [19,20] shown in Fig. 3. The two dimensional dionysian packing is isotropic and has a single shear modulus, G. However, the three dimensional Dionysian packing, like the FCC crystal upon which it was based, has two independent shear moduli, G_{100} and G_{110} [21]. These moduli in two dimensions can be calculated from the stiffness matrix as $K = (C_{11} + C_{12})/2$ and $G = C_{33}$. In three dimensions, these are calculated as $K = (C_{11} + 2C_{12})/2$, $G_{100} = C_{44}$, and $G_{110} = (C_{11} - C_{12})/2$.

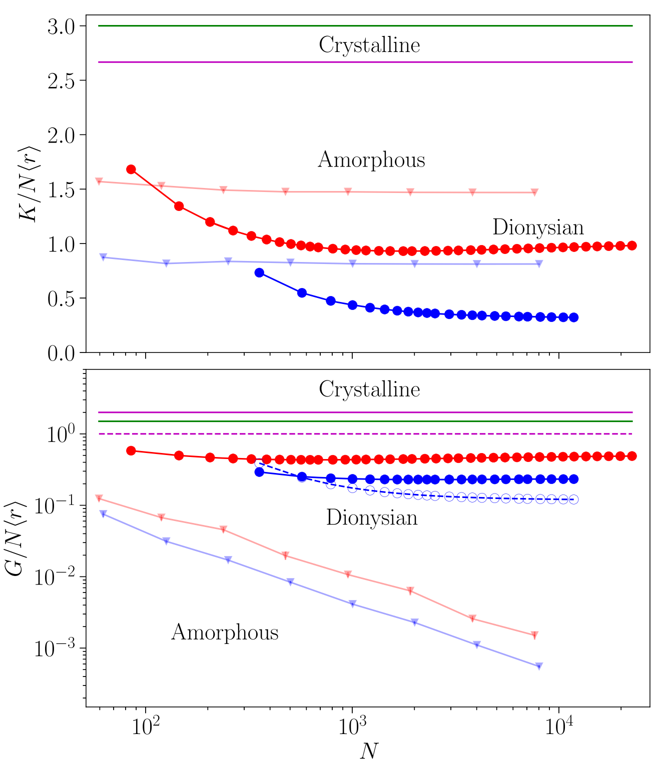

FIG. 3. The dimensionless bulk K and shear G moduli per sphere for Dionysian and amorphous packings in a unit cell as a function of the number of spheres N. The green line represents a two dimensional triangular packing, the magenta line represents a three dimensional FCC packing, and red and blue represent two dimensional and three dimensional packings, respectively. The dashed curves with open symbols represent G_{110}, the shear modulus in direction (1,1,0), whereas the solid curves with closed symbols represent G_{100}. The results are exact for the Dionysian packings and crystals. For the amorphous systems, sufficiently many systems were sampled to make the standard error bars smaller than the plot markers. In the limit of large N, the bulk modulus per sphere asymptotes to a positive value in two and three dimensions for all of the systems. The shear modulus for crystals and Dionysian packings plateaus for large N indicating that these remain very stiff. On the other hand, the amorphous packings have a shear modulus that decreases like $1/N$ [22].

To compare the mechanical properties of Dionysian packings with other purely compressive solids, we also studied the properties of crystals and shear-stabilized jammed packings. We generated shear-stabilized amorphous systems with monodisperse radii in three dimensions and 25% polydispersity in two dimensions drawn from a log-normal distribution. We then used a modified FIRE algorithm [23] that performs a constrained minimization with respect to both volume-preserving strains and positions as implemented in the pyCudaPacking software [24–26]. We created critically jammed and shear-stabilized packings by alternating between shear-stabilizing packings and uniformly decreasing the packing fraction and by extension the system pressure [27].

Figure 3 demonstrates that crystals, shear-stabilized jammed systems, and Dionysian packings all have a bulk modulus per particle that plateaus to a fixed value in the limit of large N. Similarly, the shear moduli per particle for crystals and Dionysian packings plateau for large N. In contrast, we confirm the claim by Dagois-Bohy *et al.* [22] that the shear modulus in shear-stabilized jammed systems decreases like $1/N$. These results indicate that Dionysian packings maintain their stability even as the density approaches zero, whereas amorphous systems are only marginally stable in the thermodynamic limit. Remarkably, Dionysian packings can be created without sacrificing stiffness.

Extension of our procedure to higher dimensions can be proven to not be viable due to unavoidable overlapping of spheres (see Supplemental Material [16]). We conjecture that higher dimensional Dionysian packings also have arbitrarily low densities, but to demonstrate this will require a novel construction.

Conclusions.—We find that the lower bound on density for mechanical stability of purely repulsive spheres is 0 (Dionysian) and the upper bound is 1 (Apollonian) in two and three dimensional sphere packings. In addition to this solution and the extension of our understanding of the limits associated with the jamming energy landscape, this discovery has implications for our fundamental understanding of mechanical stability. Where Apollonian packings can be used to create structures which fill space entirely, Dionysian packings can be used to create structures that utilize very little material and remain stiff. We prove that appreciably lighter weight materials can be constructed with no lower bounds. However, the experimental construction of such a system would necessarily be a major undertaking. Hard sphere systems do not exist in reality and must be replaced with high modulus soft-sphere particles. Real systems have shape and size imprecisions that make the physical construction process require additional theoretical investigation. Additionally, and perhaps most significantly, friction between physical particles adds a crucial layer of complication. While the structures offered here may not be the most well-suited for practical considerations, this work demonstrates that there must exist structures at every density which remain strictly jammed and can be tuned to one's particular needs.

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[16] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.128.018002 for additional information to construct Dionysian Packings, justification for the failure of trivial extensions to higher dimensions, analysis of curvature for bridges, and derivation of stiffness matrix.

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