Supplementary Material for: Dionysian Hard Sphere Packings are Mechanically Stable at Vanishingly Low Densities

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I. CONSTRUCTING A DIONYSIAN PACKING IN TWO DIMENSIONS

To construct a Dionysian packing in two dimensions, we do the following:

1. Create a chain of n kissing circles labeled $a_1 - a_n$ which have unit radius and centers that lie on a convex function $f(x)$ given by equation 6 such that the coordinates of each circle are $(x, f(x))$. The values used in this manuscript can be found in table I. If we give the bridges $h_\infty = 1 + \sqrt{3}$, we end up with nice monodisperse crystalline structures at infinity. However, because the radii of b circles oscillate between two values, these values of h_∞ will eventually cause overlapping to occur. To prevent this, we perturb these values by 0.05
2. Place a circle b_1 of radius 1 that kisses a_1 and a_2
3. Place circle b_m, where $m \in [2, n-1]$, such that it kisses a_m, a_{m+1}, and b_{m-1}
4. Place circle b_n such that it kisses a_{n-1} and a_n and so that its center lies at $a_{nx}+1$ where a_{nx} is the x coordinate of circle a_n
5. Place circle c_m, where $m \in [1, n-1]$, such that it lies on $y = 0$ and kisses circles b_m and b_{m+1}
6. Reflect the ensemble of circles about the x axis
7. Reflect the ensemble of circles about the line normal to the x axis that passes through the center of b_n
8. Generate three of these bridges and connect them such that they share a_1 circles and lie along the contact vectors of the triangular packing
9. Contain the circle ensemble in a rhombus with periodic boundary conditions
10. Place seven identical circles inside the cavity between bridges such that they form a honeycomb pattern and each of the six outer circles touch two copies of b_1
11. Place six identical circles in the cavity each of which touches an a circle and two of the circles in the honeycomb arrangement

II. CONSTRUCTING A DIONYSIAN PACKING IN THREE DIMENSIONS

The construction process is very similar in three dimensions, but with the following changes

1. The values for the curve are different and can be found in table I
2. The coordinates of a spheres have the form $\left(a_x, a_y, 0\right)$, the coordinates of b spheres have the form $\left(b_x, b_y, b_y\right)$, and the coordinates of c spheres have the form $\left(c_x, 0, 0\right)$
3. The a and b spheres each have three copies that are rotated 45 degrees about the x axis
4. The sphere ensemble is reflected about the plane perpendicular to the x axis that passes through the center of b_n
5. Six of these bridges are created and connected such that they share sphere a_1 and lie along the contact vectors of the primitive cell for the FCC packing

6. The spheres in the empty cavity formed by the bridges are different. Generate thirteen equal sized spheres, f, in the shape of an fcc crystal such that one sphere is in the very middle of the cavity and the other twelve touch four b spheres associated with the ends of the bridges. Connecting these bridges will naturally create two differently sized holes. In the six larger holes, create a dimer of equally sized circles, m, such that they touch: each other, a b sphere, two a spheres, and an f sphere. Also in these larger holes, place a sphere, p, that touches eight of these m sphere and an f sphere. In the eight smaller holes, place a triangle of equally sized spheres, q, that touch each other, three a spheres and an f sphere

d	f_0	h_∞	δ
2	$2\sqrt{3}$	$\left(1+\sqrt{3}\right)+0.05$	0.01
3	$\sqrt{6}$	$\left(1+\sqrt{2}\right)+0.025$	0.01

Table I. The values we used to parameterize curve $\mathcal{C}$ for various dimensions d according to equation 9

For a visual representation of the construction in two dimensions, see FIG. 1.

III. TRIVIAL EXTENSION TO HIGHER DIMENSIONS

We can prove that extending this construction to higher dimensions will not work. The generalized construction is given by parameterizing the positions of the a spheres as

$$\vec{a}_m = \left(a_{mx}, a_{my}, 0, 0, \ldots\right) \text{ and } \vec{b}_m = \left(b_{mx}, b_{my}, b_{my}, b_{my}, \ldots\right)$$

for $m \in [1, n]$. The a spheres will each have $2(d-1)$ copies given by

$$\left(a_{mx}, -a_{my}, 0, 0, \ldots\right), \left(a_{mx}, 0, a_{my}, 0, \ldots\right), \left(a_{mx}, 0, -a_{my}, 0, \ldots\right), \left(a_{mx}, 0, 0, a_{my}, 0, \ldots\right), \ldots$$

and the b spheres will each have 2^{d-1} copies given by

$$\left(b_{mx}, -b_{my}, b_{my}, b_{my}, \ldots\right), \left(b_{mx}, b_{my}, -b_{my}, b_{my}, \ldots\right), \left(b_{mx}, -b_{my}, -b_{my}, b_{my}, \ldots\right), \ldots$$

We consider $\vec{a}_1 = \left(0, a_y, 0, \ldots\right)$ with unit radius and $\vec{b}_1 = \left(1, b_y, b_y, \ldots\right)$ with radius b_r. If we enforce that these two spheres kiss, we can solve for a_y. We can then find that b_y has a maximum value of

$$b_y^* = \sqrt{\frac{b_r(b_r+2)}{(d-2)(d-1)}}.$$

Because b_1 cannot overlap with one of it's copies, $b_y \geq b_r$. This along with the above equation means that

$$b_r \leq \sqrt{\frac{b_r(b_r+2)}{(d-2)(d-1)}}$$

or for $d > 2$,

$$b_r \leq \frac{2}{d^2-3d+1}.$$

We also know that in steady state, the sum of the radii for b_m and b_{m+1} will be 2. This means that setting b_m to have a radius less than 1 gives b_{m+1} a radius greater than 1. Therefore, if we substitute $b_r = 1$, we arrive at an upper bound for d :

$$d \leq \frac{3+\sqrt{13}}{2} \approx 3.30278$$

which means that this construction does not extend to dimensions higher than three. We do conjecture that a different construction procedure exists to generate Dionysian packings in higher dimensions.

IV. MINIMAL CURVATURE FOR THREE DIMENSIONAL DIONYSIAN PACKINGS

We remarked in the text that the curves $\mathcal{C}$ have a very subtle amount of curvature in three dimensions. Given a and b spheres of radius 1, the tightest Dionysian bridge configuration one can achieve has an a sphere with $a_y = (1+\sqrt{2})$. Any tighter and the b spheres will overlap. The loosest configuration has $a_y = \sqrt{6}$. Any looser and the b spheres will no longer be contained. (See table I). If our packing begins with the loosest configuration and ends with the tightest, the curve will decrease in height by $\sqrt{6}/(1+\sqrt{2}) - 1 = 1.46\%$ which is subtle.

V. AMORPHOUS SHEAR STABILIZED SYSTEMS

We generate amorphous shear stabilized systems by finding the traceless forces on strain degrees of freedom as given in equation 4 of the manuscript. We then use the FIRE algorithm on these strain degrees of freedom to adjust the lattice vectors and apply an affine strain. Because $\mathrm{Tr}(\varepsilon) = 0$ is just the linear approximation for volume conservation, we also rescale the lattice vectors after each minimization step. Once a shear stabilized packing is found, we alternate between minimizing the system and uniformly decreasing the radius of each particle in order to maintain the polydispersity. After rattlers are removed and the system is at one state of self stress, we find the mechanical properties.

VI. COMPUTING THE STIFFNESS MATRIX

We first consider our extended rigidity matrix for which

$$R_{x\langle ij\rangle(k\gamma)} = (\delta_{jk} - \delta_{ik})\, n_{ij}^{\gamma} \tag{1}$$

$$R_{\varepsilon\langle ij\rangle(\alpha\beta)} = n_{ij}^{\alpha} n_{ij}^{\beta} \sigma_{ij} \tag{2}$$

for contact $\langle ij\rangle$, particle k, and dimension γ. Here, also note that n_{ij}^{γ} is the normalized contact vector between particle j and particle i and σ_{ij} is the sum of the radii of particles i and j.

In order to find the stiffness matrix, we define the extended hessian, which is

$$H = \begin{pmatrix} H_{xx} & H_{x\varepsilon} \\ H_{x\varepsilon}^T & H_{\varepsilon\varepsilon} \end{pmatrix} \tag{3}$$

where H_{xx} is the second derivative of the energy function with respect to positional degrees of freedom, $H_{\varepsilon\varepsilon}$ is the second derivative with respect to strain degrees of freedom, and $H_{x\varepsilon}$ are mixed derivatives.

From Hooke's law, we know that

$$H \begin{pmatrix} \Delta\vec{x} \\ \vec{\varepsilon} \end{pmatrix} = \begin{pmatrix} -\vec{F} \\ \vec{\sigma} \end{pmatrix} \tag{4}$$

where $\Delta\vec{x}$ is a perturbation vector of the particles and $\vec{\sigma}$ is the stress. To find the stiffness matrix, we solve for the non-affine perturbation $\Delta\vec{x}_{\mathrm{na}}$ that leave the spatial forces unchanged but imposes a stress:

$$H \begin{pmatrix} \Delta\vec{x}_{\mathrm{na}} \\ \vec{\varepsilon} \end{pmatrix} = \begin{pmatrix} \vec{0} \\ \vec{\sigma} \end{pmatrix}. \tag{5}$$

If we solve this system of equations for $\vec{\sigma}$, we find that $C\vec{\varepsilon} = \vec{\sigma}$ where the stiffness matrix is

$$C = \left[H_{\varepsilon\varepsilon} - H_{x\varepsilon}^T \left(H_{xx}\right)^{-1} H_{x\varepsilon} \right]. \tag{6}$$

The term, $\left(H_{xx}\right)^{-1}$ is the Moore-Penrose pseudoinverse [1] of the singular matrix H_{xx}. While the algebra is simple, care must be taken to prove that it is valid to use the pseudoinverse for hyperstatic jammed packings.

We can take this result further by considering that for systems without prestresses, such as ours, the extended hessian can also be written as

$$H = R^T R \tag{7}$$

$$= \begin{pmatrix} R_x^T R_x & R_x^T R_\varepsilon \\ R_\varepsilon^T R_x & R_\varepsilon^T R_\varepsilon \end{pmatrix} \tag{8}$$

so that

$$C = \left[R_\varepsilon^T R_\varepsilon - R_\varepsilon^T R_x \left(R_x^T R_x\right)^{-1} R_x^T R_\varepsilon\right]. \tag{9}$$

This can be further simplified by applying the singular value decomposition [2] for R_x. We can define the left singular vectors as U which correspond to the linearly independent basis of bond stresses, the right singular vectors, V, which correspond to normal modes, and Σ which is the rectangular diagonal matrix of singular values. Given this,

$$R_x = U\Sigma V^T. \tag{10}$$

If we make this substitution in equation 9, we find that

$$C = \left[R_\varepsilon^T R_\varepsilon - R_\varepsilon^T U\Sigma \left(\Sigma^T\Sigma\right)^{-1} \Sigma^T U^T R_\varepsilon\right] \tag{11}$$

$$= R_\varepsilon^T \left(\mathbf{1} - U\Sigma \left(\Sigma^T\Sigma\right)^{-1} \Sigma^T U^T\right) R_\varepsilon \tag{12}$$

$$= R_\varepsilon^T \left(UU^T - U\Sigma \left(\Sigma^T\Sigma\right)^{-1} \Sigma^T U^T\right) R_\varepsilon \tag{13}$$

$$= R_\varepsilon^T U \left(\mathbf{1} - \Sigma \left(\Sigma^T\Sigma\right)^{-1} \Sigma^T\right) U^T R_\varepsilon. \tag{14}$$

The pseudoinverse of a diagonal matrix such as $\Sigma^T\Sigma$ is a diagonal matrix where the nonzero entries are inverted and the zero entries remain zero. To simplify this, we can rewrite Σ. If we let there be f floppy modes, s states of self stress, and z nonzero singular values, then we can choose to express Σ as

$$\Sigma = \begin{pmatrix} Q_{z\times z} & \mathbf{0}_{z\times f} \\ \mathbf{0}_{s\times z} & \mathbf{0}_{s\times f} \end{pmatrix} \tag{15}$$

where Q is the diagonal matrix of non-zero singular values and where we have explicitly assumed that $s > f$. This assumption will always hold for shear stabilized packings where $f = d$ corresponds to trivial floppy modes. Also note that this form of Σ assumes that the left and right singular vectors are arranged in a corresponding way. Substituting this equation into equation 14, we find that

$$C = R_\varepsilon^T U \left(\mathbf{1} - \begin{pmatrix} Q_{z\times z} & \mathbf{0}_{z\times f} \\ \mathbf{0}_{s\times z} & \mathbf{0}_{s\times f} \end{pmatrix} \begin{pmatrix} \left(Q_{z\times z}^2\right)^{-1} & \mathbf{0}_{z\times f} \\ \mathbf{0}_{f\times z} & \mathbf{0}_{f\times f} \end{pmatrix} \begin{pmatrix} Q_{z\times z} & \mathbf{0}_{z\times s} \\ \mathbf{0}_{f\times z} & \mathbf{0}_{f\times s} \end{pmatrix}\right) U^T R_\varepsilon \tag{16}$$

$$= R_\varepsilon^T U \left(\mathbf{1} - \begin{pmatrix} \mathbf{1}_{z\times z} & \mathbf{0}_{z\times s} \\ \mathbf{0}_{s\times z} & \mathbf{0}_{s\times s} \end{pmatrix}\right) U^T R_\varepsilon \tag{17}$$

$$= R_\varepsilon^T U \begin{pmatrix} \mathbf{0}_{z\times z} & \mathbf{0}_{z\times s} \\ \mathbf{0}_{s\times z} & \mathbf{1}_{s\times s} \end{pmatrix} U^T R_\varepsilon. \tag{18}$$

In this equation, the $\mathbf{1}_{s\times s}$ term corresponds to the entries associated with states of self stress. As such,

$$C = R_\varepsilon^T S S^T R_\varepsilon \tag{19}$$

where S is the matrix of states of self stress for R_x. Again, this expression is valid under the assumption that the packing has no prestress and is strictly jammed.

We can understand this result by considering how each term interacts with an arbitrary strain, $\vec{\varepsilon}$. This arbitrary strain results in bond stresses, $\vec{b} = R_\varepsilon\vec{\varepsilon}$. However, these bond stresses will very likely result in perturbations of the particles which will bring the packing out of force balance. The SS^T term removes any components of the bond stresses that are inconsistent with the states of self stress and therefore would cause particle movements. This new set of bond stresses is then passed through R_ε^T and gives the stress vector, $\vec{\sigma}$.

[1] in *Generalized Inverses: Theory and Applications*, CMS Books in Mathematics, edited by A. Ben-Israel and T. N. E. Greville (Springer) pp. 40–51.
[2] V. Klema and A. Laub, 10.1109/TAC.1980.1102314.