Appendix to "Geometrical Frustration and Static Correlations in a Simple Glass Former"

GEOMETRICAL TILINGS OF SIMPLICES

We review the regular polytopes and hyperbolic coverings that correspond to defectless tilings of simplices on spaces of constant curvature. In particular, we aim to show the following.

1. A regular tiling of tetrahedra is found on the sphere that inscribes the remarkably large 4D platonic polytope $\{3,3,5\}$. The inscribing sphere's curvature, $\pi^2/25$, is notably much smaller than that of the generalized octahedron $\{3,3,4\}$, $\pi^2/4$.

2. By contrast, on the d-dimensional sphere with $d > 3$, $\{3^{d-1},4\}$ is the only way to obtain a regular tiling of simplices resulting in large geometrical frustration of the corresponding Euclidean space, which hints at a possible limit role of simplex ordering in 3D.

3. The regular simplicial tiling $\{3,3,3,6\}$ is found on a hyperbolic space of curvature larger (in absolute value) than the curvature of the sphere that inscribes the tiling $\{3,3,3,4\}$, while the hyperbolic tiling $\{3,3,6\}$'s infinite edge length disqualifies it as a possible reference.

4. The homogeneous statistical honeycomb $\{3,3,\bar{q}\}$ gives is an upper limit for the density of simplex tiling in $d=3$, and a lower limit to $\bar{q}$.

Notations

We first establish some notation. The Euclidean space of dimension d is denoted $\mathbb{R}^d$ and the hyperbolic space of dimension d is denoted H^d. The sphere (or hypersphere) of (surface) dimension d is the set of all vectors of length 1 in $\mathbb{R}^{d+1}$ and is denoted S^d. Hence S^2 is the standard radius one sphere in $\mathbb{R}^3$ we all know and love.

Following Schläfli's notation (see [1, Chapter 7]), the polytope $\{a_1,\ldots,a_d\}$ is composed of polytopes $\{a_1,\ldots,a_{d-1}\}$ with vertex figure $\{a_2,\ldots,a_d\}$. The *vertex figure* of a d-dimensional polytope is a $(d-1)$-dimensional polytope whose vertices are obtained by taking the middle of each edge emanating from a vertex. This inductive definition deserves an illustration. The basic example is $\{p\}$, the regular polygon of p sides in $\mathbb{R}^2$. Next we have the regular polytopes in $\mathbb{R}^3$. Those are represented by the symbols $\{p,q\}$ for a polytope having faces made of $\{p\}$s and vertex figures made of $\{q\}$s. Note that because the polytope is regular, one can inscribe all the vertices on a sphere and thus $\{p,q\}$ gives a tiling of the sphere S^2. For instance, the cube $\{4,3\}$ is composed of squares (the regular polygon $\{4\}$) and the vertex figure is $\{3\}$, a triangle. The cubic tiling $\{4,4\}$ in $\mathbb{R}^2$ is composed of 4 squares surrounding each vertex.

Throughout the text, we use a measure q of the number of tetrahedra sharing a particular edge between nearest-neighbor pairs and $\bar{q}$ for the average amongst all pairs of nearest-neighbor. This quantity generalizes to higher-dimensional setting in the following manner: in a d-dimensional space (be it $\mathbb{R}^d, S^d$ or H^d), a set of $(i+1)$ points all nearest-neighbors to each other form a i-simplex (generalized tetrahedron). A 1-simplex is a line segment, a 2-simplex is a tetrahedron, etc. As in three-dimensional system, the dimension $(d-2)$-simplices play an important role. We call them *spindles*. Given a particular $(d-2)$-simplex, we let q measure the number of d-simplexes that contain it. Obviously, $\bar{q}$ is the average of q over all spindles.

Schläfli's notation and spindles

Of primary importance for this paper is the relation between Schläfli's notation and the number q. Let $\{a_1,\ldots,a_d\}$ be a regular tiling in $\mathbb{R}^d$ or S^d. One can show that $q = a_d$. Instead of exhibiting the proof of this result, we give an example. Consider the simple cubic tiling of $\mathbb{R}^d$, given by $\{4,3^{d-2},4\}$. Here, a $(d-2)$-dimensional hypercube is given, for example, by $x_1 = x_2 = 0$ and $0 \leq x_i \leq 1$ for $3 \leq i \leq d$. The various d-dimensional hypercubes containing this $(d-2)$-dimensional hypercube are given by $\pm x_1, \pm x_2 \in [0,1]$, where the signs are chosen independently. Hence $q = 4$.

Note that any polytope $\{a_1,\ldots,a_d\}$ in $\mathbb{R}^{d+1}$ can be seen as inscribed in a sphere S^d whose center is the center of mass of the polytope. By inflating the polytope to make it round, we see that it produces a regular tiling of S^d. For

Tetrahedral honeycomb	in	curvature
$\{3,6\}$	$\mathbb{R}^2$	0
$\{3,q\}$ with $q \geq 7$	H^2	$-4\text{arccosh}^2(2^{-1}\csc\frac{\pi}{q})$
600-cell $\{3,3,5\}$	S^3	$\pi^2/25 \simeq 0.39$
octahedron $\{3^{n-1},4\}$	S^n	$\pi^2/4 \simeq 2.47$
$\{3,3,3,6\}$	H^4	$-4\text{arccosh}^2\tau \simeq -4.505$

TABLE I: Summary of tiling results with the curvature reported setting $\sigma = 1$.

instance, the hypercube $\{4,3^{d-2}\}$ in $\mathbb{R}^d$ is also a tiling of S^{d-1}. By looking at the usual case $\{4,3\}$, one sees that it gives $q = 3$ on S^2. The same argument illustrates that for the tiling $\{4,3^{d-1}\}$ of S^d, one also has $q = 3$.

Various tilings in various spaces

Consider the case of the generalized octahedron, $\{3^{d-1},4\}$, in $\mathbb{R}^{d+1}$. It gives a regular tiling of S^d with $q = 4$. This tiling is dual in $\mathbb{R}^{d+1}$ to $\{4,3^{d-1}\}$ which can be thought as the cube $[-1,1]^{d+1}$. So the vertices of the dual generalized octahedron are $\pm\vec{e}_i$ for the standard basis $\{\vec{e}_1,\ldots,\vec{e}_{d+1}\}$ of $\mathbb{R}^{d+1}$. Obviously, the distance between two vertices is $\sqrt{2}$ via straight line, or $\frac{\pi}{2}$ in S^d. To obtain a unit distance in S^d, one has to rescale the sphere to be of radius $\frac{2}{\pi}$, hence the sphere has a curvature $\frac{\pi^2}{4} \simeq 2.47$.

As pointed by [2, p.20], the 120 vertices of the 600-cell $\{3,3,5\}$ all belong to the hypersphere S^3 with radius equal to the golden ratio ($\tau = \frac{1+\sqrt{5}}{2}$) if the edges are of unit length. The alternative expression $\tau = \frac{1}{2}\csc(\frac{\pi}{10})$ is useful for our computation. Indeed, imagine a isosceles triangle whose equal sides measure τ and opposite side measure 1. The angle opposite to the side of measure 1 is

$$\theta = 2\arcsin\left(\frac{1}{2\tau}\right) = 2\arcsin\left(\sin(\frac{\pi}{10})\right) = \frac{\pi}{5}.$$

So, if one desires the spherical distance between vertices in the $\{3,3,5\}$ regular tiling of S^3 to be 1, the radius must be $\frac{\tau}{\tau\pi/5} = \frac{5}{\pi}$. The curvature of this sphere is thus $\frac{\pi^2}{25} \simeq 0.39$.

The tiling $\{3,3,6\}$ in hyperbolic 3-space H^3 is somewhat of a degenerate case. Despite the cells being of finite volume, all of its vertices are at infinity hence the edge length is infinite, which makes the curvature impossible to rescale; see [3, p.202]. In H^4 however, the tiling $\{3,3,3,5\}$ is perfectly well-defined, with finite distance between vertices. According to [3, p.204 and table p.213], the edge-length is 2φ and $\cosh\varphi = \tau$, hence the edge-length is $2\text{arccosh}\tau \simeq 2.12$. The expressions obtained by Coxeter are consistent with the results in standard hyperbolic space of curvature -1. Rescaling the space to make the edge-length 1 changes the curvature to $-\left(2\text{arccosh}\tau\right)^2 \simeq -4.505$.

Still following [3, Chapter 10], one sees that the regular tilings in H^5 are not tetrahedral and that there are no regular tilings in hyperbolic space of six or more dimensions. In H^2, any $\{3,q\}$ with $q > 6$ is possible, with edge-length 2φ where $\cosh\varphi = \frac{\cos\frac{\pi}{3}}{\sin\frac{\pi}{q}} = \frac{\csc\frac{\pi}{q}}{2}$; [3, p.201]. Rescaling to get edge-length 1, one gets a curvature $-4\text{arccosh}^2(2^{-1}\csc\frac{\pi}{q})$.

The results for $d \geq 3$ are summarized in Table I. Note that in the H^2 case, the packing of an increasing number of hyperbolic triangles around a vertex, keeping the edge-length 1, makes the curvature go down from approximately -1.19 (for $\{3,7\}$), to -2.34 (for $\{3,8\}$), to -3.44 (for $\{3,9\}$), with limit $-\infty$ as $q \to \infty$.

Statistical honeycomb

Coxeter suggested that nature tries to approximate regular tilings $\{p,3,3\}$ for p between 5 and 6 in soap froth [4, Chap. 22]. Obviously, the soap froth itself produces an irregular tiling, but one could look at the average structure, the *statistical honeycomb*. Taking its dual, as suggested by [5], we consider the corresponding statistical honeycomb $\{3,3,\bar{q}\}$ produced by wrapping as many tetrahedra as possible around a given spindle, even if that means wrapping a fraction of a tetrahedron. Because the angle formed by two adjacent edges in a perfectly regular tetrahedron is $\arccos(1/3)$, the ideal number is thus $\bar{q} = \frac{2\pi}{\arccos(1/3)} \simeq 5.1043$.

As proposed in Ref. [5], we can consider an ideal configuration where every bond belongs to $\bar{q}$ tetrahedra. In the Voronoi decomposition corresponding to this configuration, the cells have Z identical faces corresponding to the Z nearest neighbors of a particle, each of them being a polygon with $\bar{q}$ faces. This Voronoi cell can be seen as living on the surface of a sphere. If it has V vertices and E edges, we must thus have $V - E + Z = 2$, using Euler's relation. Counting the pairs (*edge*,*face*), with *edge* adjacent to *face*, in two different ways, we get $2E = Z\bar{q}$, and counting the pairs (*edge*,*vertex*) in two different ways, we get $3V = Z\bar{q}$. Overall, we obtain that in this ideal structure, each particle has a number of neighbors

$$Z = \frac{12}{6 - \bar{q}} \simeq 13.4.$$

Note that in this construction, all quantities are also by definition their own average.

Now one can compute the volume occupied by that fictitious Voronoi cell, and obtain, as did Ref. [5], a volume of

$$\begin{aligned} V_{\text{cell}} &= \frac{Z}{3}\frac{\sigma}{2}\text{area}(\bar{q}\text{-sided regular polygon}) \\ &= \frac{Z\sigma^3\bar{q}\cot(\frac{\pi}{\bar{q}})}{144}. \end{aligned}$$

The packing fraction is then given by

$$\varphi = \frac{V_{\text{sphere}}}{V_{\text{cell}}} = \frac{\frac{4}{3}\pi(\frac{\sigma}{2})^3}{V_{\text{cell}}} \simeq 0.7796.$$

It should be noted that this result is also Roger's bound on the maximal packing fraction for any sphere packing in 3D, not only simplex tilings. In all cases, it gives an upper bound on the density of simplex tilings in 3D systems.

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[4] H. S. M. Coxeter. *Introduction to geometry*. John Wiley & Sons Inc., New York, second edition, 1969.
[5] D. R. Nelson and F. Spaepen. Polytetrahedral order in condensed matter. *Solid State Physics*, 42:1–90, 1989.