New Lower Bound for the Optimal Ball Packing Density of Hyperbolic 4-space *

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Abstract

In this paper we consider ball packings of 4-dimensional hyperbolic space, and show that it is possible to exceed the conjectured 4-dimensional realizable packing density upper bound due to L. Fejes-Tóth (Regular Figures, 1964). We give seven examples of horoball packing configurations that yield higher densities of $\approx 0.71644896$ where horoballs are centered at ideal vertices of Coxeter simplices that make up fundamental domains of certain Coxeter simplex reflection groups.

1 Introduction

2 Introduction

Let $X$ denote a space of constant curvature, either the $n$-dimensional sphere $S^n$, Euclidean space $E^n$, or hyperbolic space $H^n$ with $n \geq 2$. In discrete mathematics, a common question to ask is to find the highest possible packing density of $X$ by congruent balls of a given radius $\ddot{i}$, $\dddot{i}$. Most is known for Euclidean cases. The densest

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possible lattice packings are known for dimensions $\mathbb{E}^2$ through $\mathbb{E}^8$, however mostly only bounds are known in higher dimensional cases. Furthermore, not much is known about irregular packings of $\mathbb{E}^n$ when $n > 3$. One major recent development has been the settling of the long standing Kepler conjecture, part of Hilbert’s 18th problem, by Thomas Hales at the turn of the 21st century. Hales’ computer assisted proof was largely based on a program set forward by L. Fejes-Toth in the 1950’s [5].

It is well known that the definition of density is critical in hyperbolic space, by convention we shall consider the local densities of balls with respect to their Dirichlet-Voronoi cells [14]. In the case of Coxeter simplex tilings these coincide with the Coxeter simplices. A Coxeter simplex is an $n$-dimensional simplex in $X$ such that each of its dihedral angles is a submultiple of $\pi$ or zero. The group generated by reflections to the sides of a Coxeter simplex is called a Coxeter simplex reflection group. Such reflections give a discrete group of isometries of $X$ with the original Coxeter simplex as its fundamental domain, hence the groups give regular tessellations of $X$. The Coxeter group is finite for $S^n$, and infinite for $\mathbb{E}^n$, $H^n$.

In $H^n$ we allow unbounded simplices with ideal vertices at infinity $\partial H^n$. Coxeter Simplexes exist only for dimensions $n = 2, 3, \ldots, 9$, furthermore only a finite number of them exist in dimensions $n \geq 3$. Johnson et al. computed the volumes of all Coxeter simplices in hyperbolic $n$-space [10], [13]. Such simplices are the most elementary building blocks of hyperbolic manifolds of which volume is an important topological invariant.

In an $n$-dimensional space $X$ of constant curvature ($n \geq 2$) define the simplicial density function $d_n(r)$ to be the density of $n + 1$ spheres of radius $r$ mutually touching one another with respect to the simplex spanned by the centers of the spheres. L. Fejes Tóth and H. S. M. Coxeter conjectured that the packing density of balls of radius $r$ in $X$ cannot exceed $d_n(r)$. This conjecture has been proved by C. A. Rogers for Euclidean space $\mathbb{E}^n$ [20]. The 2-dimensional spherical case was settled by L. Fejes Tóth in [8], and in [3] K. Böröczky proved the following generalization:

**Theorem 2.1 (K. Böröczky).** In an $n$-dimensional space of constant curvature consider a packing of spheres of radius $r$. In spherical space suppose that $r < \frac{\pi}{4}$. Then the density of each sphere in its Dirichlet-Voronoi cell cannot exceed the density of $n + 1$ spheres of radius $r$ mutually touching one another with respect to the simplex spanned by their centers.

The monotonicity of the $d_n(r)$ is proven for dimension three [4]. for high enough dimensions the results of Marshall show that $d_n(r)$ is a strictly increasing function of $r$ [16].

The above density upper bound in hyperbolic space $\mathbb{H}^3$ is $\approx 0.85327613$ which is not realized by packing regular balls. However, it is attained by a horoball packing of $\mathbb{H}^3$ where the ideal centers of horoballs lie on the absolute figure of $\mathbb{H}^3$, for example the ideal regular simplex tiling with Coxeter-Schlaffi symbol $(3, 3, 6)$. Bowen and Radin give results on the uniqueness and irregularity of packings in [19], [2].

In the previous paper [15] we proved that the above known optimal ball packing arrangement in $\mathbb{H}^3$ is not unique. We gave several new examples of horoball packing arrangements based on totally asymptotic Coxeter tilings that yield the Böröczky–Florian
packing density upper bound \[4\]. Furthermore, by admitting horoballs of different types at each vertex of a totally asymptotic simplex and generalizing the simplicial density function to \(\mathbb{H}^n\) for \((n \geq 2)\), we find the Böröczky type density upper bound is no longer valid for the fully asymptotic simplices in cases \(n \geq 3\) \[25\], \[26\]. For example, the density of such optimal, locally densest packing is \(\approx 0.77038\) which is larger than the analogous Böröczky type density upper bound of \(\approx 0.73046\) for \(\mathbb{H}^4\). However these ball packing configurations are only locally optimal and cannot be extended to the entirety of the hyperbolic spaces \(\mathbb{H}^n\). Further open problems and conjectures on 4-dimensional hyperbolic space packings are discussed in \[7\]. A universal formula is known for the inradius of a hyperbolic truncated n-simplex that uses its gram matrix \[9\].

The second author has an extensive program in finding globally and locally optimal ball packings in \(\mathbb{H}^n, S^n\), and the eight Thurston geometries arising from Thurston’s geometrization conjecture \[21\], \[22\], \[23\], \[24\], \[25\], \[26\], \[27\] and \[28\]. Packing density is defined to be the ratio of the volume of a fundamental domain of the symmetry group of a tiling to the volume of the ball pieces contained in the interior of the fundamental domain. Packing densities can be global or local depending on whether the density obtained in the fundamental domain can be generalized to the entire space.

In this paper we continue our investigation of ball packings in hyperbolic 4-space. Using horoball packings, allowing horoballs of different types, we find seven counterexamples (which are realized by allowing one-, two-, or three horoball types) to one of L. Fejes-Tóth’s conjectures found in the concluding section of the book Regular Figures \[8\]:

Finally we draw attention to the tessalations \\(\{5, 3, 3, 3\}\) of 4-dimensional hyperbolic space, the cell-inspheres and cell circumspheres of which are also expected to form a closest packing and loosest covering. The corresponding densities are \((5 - \sqrt{5})/4 = 0.690\.\.\.)\) and \((4 + 6\sqrt{5})/\sqrt{125} = 1.557\.\.\.) .

3 Higher Dimensional Hyperbolic Geometry

We use the Cayley–Klein ball model, and the projective interpretation of hyperbolic geometry. This has the advantage of greatly simplifying our calculations in higher dimensions as compared to other models such as the Poincaré model. In this section we give a brief review of notions used in this paper. For a general discussion and background of hyperbolic geometry and projective models of the Thurston geometries see \[17\] and \[18\].

3.1 The Projective Model

We use the projective model in Lorentzian \((n + 1)\)-space \(\mathbb{E}^{1,n}\) of signature \((1,n)\), i.e. \(\mathbb{E}^{1,n}\) is the real vector space \(\mathbb{V}^{n+1}\) equipped with the bilinear form of signature \((1,n)\)

\[
\langle \mathbf{x}, \mathbf{y} \rangle = -x^0 y^0 + x^1 y^1 + \cdots + x^n y^n
\] (1)
where the non-zero real vectors $\mathbf{x} = (x^0, x^1, \ldots, x^n) \in V^{n+1}$ and $\mathbf{y} = (y^0, y^1, \ldots, y^n) \in V^{n+1}$ represent points in projective space $P^n(\mathbb{R})$. $\mathbb{H}^n$ is represented as the interior of the absolute quadratic form

$$Q = \{ [x] \in P^n | \langle x, x \rangle = 0 \} = \partial \mathbb{H}^n$$

in real projective space $P^n(V^{n+1}, V_{n+1})$. All proper interior points $x \in \mathbb{H}^n$ are characterized by $\langle x, x \rangle < 0$.

The boundary points $\partial \mathbb{H}^n$ in $P^n$ represent the absolute points at infinity of $\mathbb{H}^n$. Points $y$ with $\langle y, y \rangle > 0$ lie outside $\partial \mathbb{H}^n$ and are called the outer points of $\mathbb{H}^n$. Take $P([x]) \in P^n$, a point $[y] \in P^n$ is said to be conjugate to $[x]$ relative to $Q$ when $\langle x, y \rangle = 0$. The set of all points conjugate to $P([x])$ form a projective (polar) hyperplane

$$pol(P) := \{ [y] \in P^n | \langle x, y \rangle = 0 \}.$$

Hence the bilinear form $Q$ in (1) induces a bijection or linear polarity $V^{n+1} \rightarrow V_{n+1}$ between the points of $P^n$ and its hyperplanes. A point $X[x]$ and a hyperplane $\alpha[a]$ are called incident if the value of the linear form $\alpha$ evaluated on vector $x$ is equal to zero (i.e., $\alpha x = 0$ where $x \in V^{n+1} \setminus \{0\}$, and $a \in V_{n+1} \setminus \{0\}$). Similarly, straight lines in $P^n$ are characterized by the 2-subspaces of $V^{n+1}$ or $(n-1)$-spaces of $V_{n+1}$ [17].

Let $P \subset \mathbb{H}^n$ denote a polyhedron bounded by a finite set of hyperplanes $H^i$ with unit normal vectors $b^i \in V_{n+1}$ directed towards the interior of $P$:

$$H^i := \{ x \in \mathbb{H}^d | \langle x, b^i \rangle = 0 \} \quad \text{with} \quad \langle b^i, b^i \rangle = 1.$$

In this paper $P$ is assumed to be an acute-angled polyhedron with either proper or ideal vertices. The Grammian matrix $G(P) := (\langle b^i, b^j \rangle)_{i, j \in \{0, 1, 2 \ldots n\}}$ of normal vectors $b^i$ to the hyperplanes of $P$ is an indecomposable symmetric matrix of signature $(1, n)$ with entries $\langle b^i, b^i \rangle = 1$ and $\langle b^i, b^j \rangle \leq 0$ for $i \neq j$ with the following geometric meaning

$$\langle b^i, b^j \rangle = \begin{cases} 0 & \text{if } H^i \perp H^j, \\ -\cos \alpha_{ij} & \text{if } H^i, H^j \text{ intersect along an edge of } P \text{ at angle } \alpha_{ij}, \\ -1 & \text{if } H^i, H^j \text{ are parallel in the hyperbolic sense,} \\ -\cosh l_{ij} & \text{if } H^i, H^j \text{ admit a common perpendicular of length } l_{ij}. \end{cases}$$

This is visualized using the weighted graph or scheme of the polytope $\sum(P)$. The graph nodes correspond to the hyperplanes $H^i$ and are connected if $H^i$ and $H^j$ not perpendicular ($i \neq j$). If they are connected we write the positive weight $k$ where $\alpha_{ij} = \pi/k$ on the edge, and unlabeled edges denote an angle of $\pi/3$. For examples see the Coxeter diagrams in Table[1].

In this paper we set the sectional curvature of $\mathbb{H}^n$, $K = -k^2$, to be $k = 1$. The distance $d$ of two proper points $[x]$ and $[y]$ is calculated by the formula

$$\cosh d = \frac{-\langle x, y \rangle}{\sqrt{\langle x, x \rangle \langle y, y \rangle}}.$$
The perpendicular foot $Y[y]$ of point $X[x]$ dropped onto plane $[u]$ is computed as

$$y = x - \frac{(x, u)}{(u, u)}u,$$

where $u$ is the pole of the plane $[u]$.

### 3.2 Horospheres and Horoballs in $\mathbb{H}^n$

A horosphere in $\mathbb{H}^n$ ($n \geq 2$) is a hyperbolic $n$-sphere with infinite radius centered at an ideal point on $\partial\mathbb{H}^n$. Equivalently, a horosphere is an $(n-1)$-surface orthogonal to the set of parallel straight lines passing through a point of the absolute quadratic surface. A horoball is a horosphere together with its interior.

In order to derive the equation of a horosphere, we introduce a projective coordinate system for $\mathbb{P}^n$ with a vector basis $a_i$ ($i = 0, 1, 2, \ldots, n$) so that the Cayley-Klein ball model of $\mathbb{H}^n$ is centered at $(1, 0, 0, \ldots, 0)$, and select an arbitrary point at infinity to lie at $A_0 = (1, 0, \ldots, 0, 1)$. The equation of a horosphere with center $A_0 = (1, 0, \ldots, 1)$ passing through point $S = (1, 0, \ldots, 0, s)$ is derived from the equation of the absolute sphere

$$-x_0^2 + x_1^2 + x_2^2 + \cdots + x_n^2 = 0,$$

and the plane $x_0 - x_n = 0$ tangent to the absolute sphere at $A_0$. The general equation of the horosphere is

$$0 = \lambda(-x_0^2 + x_1^2 + x_2^2 + \cdots + x_n^2) + \mu(x_0 - x_n)^2.$$

The horosphere passes through point $S = (1, 0, \ldots, 0, s)$ for some $s$, so

$$\lambda(-1 + s^2) + \mu(-1 + s)^2 = 0 \quad \text{and} \quad \frac{\lambda}{\mu} = \frac{1 - s}{1 + s}.$$

If $s \neq \pm 1$, then the equation for a horosphere in projective coordinates is

$$(s - 1) \left(-x_0^2 + \sum_{i=1}^{n} (x_i)^2\right) - (1 + s)(x_0 - x_n)^2 = 0,$$

and in cartesian coordinates where $h_i = \frac{x_i}{x_0}$ it becomes

$$\frac{2}{1 - s} \left(\sum_{i=1}^{n} h_i^2\right) + 4 \left(\frac{h_d - \frac{a_{d+1}}{a_{d+1}}}{1 - s}\right)^2 = 1.$$

In a $n$-dimensional hyperbolic space any two horoballs are congruent in the classical sense, each having an infinite radius. However, it is often useful to distinguish between certain horoballs of a packing. We use the notion of horoball type with respect to the packing as introduced in [26].

Two horoballs of a horoball packing are said to be of the same type or equipacked if and only if their local packing densities with respect to a given cell (in our case a Coxeter simplex) are equal. If this is not the case, then we say the two horoballs are of different type. For example in the above discussion horoballs centered at $A_0$ passing through $S$ with different values for the final coordinate $s$ are of different type relative to an appropriate cell.

In order to compute the volumes of horoball pieces, we use the classical formulas of János Bolyai from the mid 19-th century:

\[5\]
1. The hyperbolic length $L(x)$ of a horospheric arc belonging to chord segment $x$ is determined by
   \[ L(x) = 2 \sinh \left( \frac{x}{2} \right). \]  
   (10)

2. The intrinsic geometry of a horosphere is Euclidean, so the $(n-1)$-dimensional volume $\mathcal{A}$ of a polyhedron $\mathcal{A}$ on the surface of the horosphere can be calculated as in $\mathbb{E}^{n-1}$. The volume of the horoball piece $\mathcal{H}(\mathcal{A})$ determined by $\mathcal{A}$ and the aggregate of axes drawn from $\mathcal{A}$ to the center of the horoball is
   \[ \text{Vol}(\mathcal{H}(\mathcal{A})) = \frac{1}{n-1} \mathcal{A}. \]  
   (11)

4 Horoball packings of Coxeter Simplices with Ideal Vertices

An approach to describing Coxeter tilings involves analysis of their symmetry groups. If $\mathcal{T}$ is a Coxeter tiling, then any rigid motion moving one cell into another maps the entire tiling onto itself. The Coxeter group of a Coxeter tiling $\mathcal{T}$ is denoted by $\Gamma_{\mathcal{T}}$. Any simplex cell of $\mathcal{T}$ can act as the fundamental domain $\mathcal{F}_{\mathcal{T}}$ of $\Gamma_{\mathcal{T}}$ generated by reflections on its $(n-1)$-dimensional hyperface facets. A complete discussion of hyperbolic Coxter simplex volumes for dimensions $n \geq 3$ is given in [10]. In Table 1 we list all the nine cocompact or asymptotic Coxter simplices in hyperbolic 4-space that have at least one ideal vertex, and their volumes.

We define the density of a horoball packing $\mathcal{B}_{\mathcal{T}}$ of a Coxeter simplex tiling $\mathcal{T}$ as
   \[ \delta(\mathcal{B}_{\mathcal{T}}) = \frac{\sum_{i=1}^{n} \text{Vol}(B_i \cap \mathcal{F}_{\mathcal{T}})}{\text{Vol}(\mathcal{F}_{\mathcal{T}})} \]  
   (12)

where $\mathcal{F}_{\mathcal{T}}$ denotes the fundamental domain simplex of the tiling $\mathcal{T}$, $n$ is the number of ideal vertices of $\mathcal{F}_{\mathcal{T}}$, and $B_i$ are the horoballs centered at the ideal vertices. We allow horoballs of different types at the asymptotic vertices of the tiling. A horoball type is allowed if it gives a packing, i.e. no two horoballs have an interior point in common. In addition we require that no horoball may extend beyond the facet opposite the vertex where it is centered in order that the packing preserve the Coxeter symmetry group of the tiling. If these conditions are satisfied we can use the Coxeter group $\mathcal{T}$ associated to a tiling to extend the packing density from the fundamental domain simplex $\mathcal{F}_{\mathcal{T}}$ to all of $\mathbb{H}^4$. We denote the optimal horoball packing density
   \[ \delta_{\text{opt}}(\mathcal{T}) = \sup_{\mathcal{B}_{\mathcal{T}} \text{ packing}} \delta(\mathcal{B}_{\mathcal{T}}). \]  
   (13)

The Coxeter simplex tilings are related through the subgroup structure of their Coxeter symmetry groups pictured in Figure [11][11][12]. Let $\Gamma_1$ and $\Gamma_2$ be two Coxeter symmetry groups of the Coxeter tilings $\mathcal{T}_1$ and $\mathcal{T}_2$. If the index of Coxeter group $\Gamma_1$ in $\Gamma_2$ is two, i.e. $|\Gamma_1 : \Gamma_2| = 2$, then the Coxeter two groups differ by one reflection, and the fundamental domain of $\Gamma_2$ is obtained from that of $\Gamma_1$ by domain doubling, that is by taking certain pairs of neighboring domains and merging by removing a facet. In
| Coxeter Diagram | Notation | Witt Symbol | Simplex Volume | Packing Density |
|-----------------|----------|-------------|----------------|-----------------|
| Simply Asymptotic | 
| ![Diagram](image) | [4, 3^2,1] | $\mathcal{S}_4$ | $\pi^2/1440$ | 0.71644896 |
| | ![Diagram](image) | [3, 3[^4]] | $\mathcal{P}_4$ | $\pi^2/720$ | 0.71644896 |
| | ![Diagram](image) | [3, 4, 3, 4] | $\mathcal{R}_4$ | $\pi^2/864$ | 0.60792710 |
| | ![Diagram](image) | [3, 4, 3^{1,1}] | $\mathcal{O}_4$ | $\pi^2/432$ | 0.60792710 |
| | ![Diagram](image) | [(3^2, 4, 3, 4)] | $\widehat{FR}_4$ | $\pi^2/108$ | 0.71644896 |
| Doubly Asymptotic | 
| ![Diagram](image) | [4, 3, \_4] | $\mathcal{N}_4$ | $\pi^2/288$ | 0.71644896 |
| | ![Diagram](image) | [4, 3[^4]] | $\mathcal{BP}_4$ | $\pi^2/144$ | 0.71644896 |
| Triply Asymptotic | 
| ![Diagram](image) | [4, 3^{1,1,1}] | $\mathcal{M}_4$ | $\pi^2/144$ | 0.71644896 |
| | ![Diagram](image) | [3[^3]×\_] | $\mathcal{DP}_4$ | $\pi^2/72$ | 0.71644896 |

Table 1: Notation and volumes for asymptotic Coxeter Simplices in $\mathbb{H}^4$.

Figure 1: Lattice of Subgroups of cocompact Coxeter groups in $\mathbb{H}^4$. Number of stars in the superscript ** and *** indicate that the fundamental simplex of the group has two or three ideal vertices.
the case of asymptotic Coxeter simplices if $|\Gamma_1 : \Gamma_2| = 2$ and the number of asymptotic vertices of the domains of $\Gamma_1$ and $\Gamma_2$ are equal, then the new fundamental domain is obtained by removing a facet adjacent to the asymptotic vertices. If the number of asymptotic vertices increase by one, then the cells of $\Gamma_2$ are obtained by removing a facet opposite to the asymptotic vertices of $\Gamma_1$ and merging the cells. The relationship between the volumes of the cells of $\Gamma_1$ and $\Gamma_2$ when $|\Gamma_1 : \Gamma_2| = m$ are given by $Vol(F_{\Gamma_1}) = m \, Vol(F_{\Gamma_2})$. If the index of the groups is two, then the packing density $\delta(B_{\Gamma_1})$ of the bigger group can be realized in the smaller group $\Gamma_2$.

4.1 Simply Asymptotic Cases

We compute of optimal horoball packing density for the Coxeter simplex tiling in case $\mathcal{S}_4$. The other simply asymptotic cases are obtained using the same method. Case $\mathcal{T}_4$ was previously computed in [21] by the second author.

**Proposition 4.1.** The optimal horoball packing density for simply asymptotic Coxeter simplex tiling $\mathcal{T}_{S_4}$ is $\delta_{opt}(\mathcal{S}_4) \approx 0.71644896$.

**Proof.** For the fundamental simplex $F_{\mathcal{T}_{S_4}}$ of the Coxeter tiling $\mathcal{T}_{S_4}$, we fix coordinates for the vertices $A_0, A_1, \ldots, A_4$ to satisfy the angle requirements. Our choices for vertices and forms corresponding to the hyperplane $[u_i]$ opposite vertex $A_i$ are given in Table [2]. To maximize the packing density we determine the maximal horoball type $B_0(s)$ centered at ideal vertex $A_0$ that fits into the fundamental domain $F_{\mathcal{T}_{S_4}}$. We find the horoball type parameter $s$ corresponding to the “radius” of the horoball when the horoball $B_0(s)$ is tangent to the hyperface plane $[u_0]$ bounding the fundamental simplex opposite of $A_0$. The perpendicular foot $F_0[f_0]$ of vertex $A_0$ on plane $[u_0]$, 

$$f_0 = a_0 - \frac{\langle a_0, u_0 \rangle}{\langle u_0, u_0 \rangle} u_0 = \left(1, 0, -\frac{2}{5}, -\frac{1}{5}, 0\right),$$ 

is the point of tangency of the horoball and hyperface $u_0$ of the the simplex cell.

Plugging in $F_0$ and solving equation (9) we find that the horoball with type parameter $s = \frac{-1}{9}$ is the optimal horoball type. The equation of horosphere $B_0 = B_0(-\frac{1}{9})$ centered at $A_0$ passing through $F_0$ is

$$\frac{9}{5} \left(h_1^2 + h_2^2 + h_3^2\right) + \frac{81}{25} \left(h_4 - \frac{4}{9}\right)^2 = 1. \quad (15)$$

The intersections $H_i[h_i]$ of the horosphere $B_0$ and the simplex edges are found by parameterizing the simplex edges as $h_i(\lambda) = \lambda a_0 + a_i$ ($i = 1, 2, 3, 4$), and computing their intersections with the horosphere. See Figure [2], and Table [2] for the intersection points. The volume of the horospherical tetrahedron determines the volume of the horoball piece by equation (11). In order to determine the data of the horospherical tetrahedron we compute the hyperbolic distances $l_{ij}$ by the formula (5) $l_{ij} = d(H_i, H_j)$ where $d(h_i, h_j) = \text{arccos} \left(\frac{-\langle h_i, h_j \rangle}{\sqrt{\langle h_i, h_i \rangle \langle h_j, h_j \rangle}}\right)$. Moreover, the horospherical distances $L_{ij}$ can be calculated by the formula (10). The intrinsic geometry of the horosphere...
is Euclidean so we use the Cayley-Menger determinant to find the volume $A$ of the horospherical tetrahedron $A$,

$$A = \frac{1}{288} \begin{vmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & L_{12}^2 & L_{13}^2 & L_{14}^2 \\ 1 & L_{12}^2 & 0 & L_{23}^2 & L_{24}^2 \\ 1 & L_{13}^2 & L_{23}^2 & 0 & L_{34}^2 \\ 1 & L_{14}^2 & L_{24}^2 & L_{34}^2 & 0 \end{vmatrix} \approx 0.0147314.$$ (16)

The volume of the optimal horoball piece in the fundamental simplex is

$$Vol(B_0 \cap F_{S_4}) = \frac{1}{n-1} A \approx \frac{1}{3} \cdot 0.0147314 \approx 0.00491046.$$ (17)

Hence by the Coxeter group $\Gamma_{S_4}$ the optimal horoball packing density of the Coxeter Simplex tiling $T_{S_4}$ becomes

$$\delta_{opt}(S_4) = \frac{Vol(B_0 \cap F_{S_4})}{Vol(F_{S_4})} \approx \frac{0.00491046}{\pi^2/1440} \approx 0.71644896.$$ (18)

The same method carries over to all other simply asymptotic Coxeter simplex tilings. Similar computations summarized in Table 2 show that

**Corollary 4.2.** The optimal horoball packing density for simply asymptotic Coxeter simplex tiling $T_\Gamma$, $\Gamma \in \{S_4, T_4, F_4\}$ is $\delta_{opt}(\Gamma) \approx 0.71644896$. 

Figure 2: Simply asymptotic case (a) Horosphere $B_0$ intersecting the sides of the simplex at $H_1, H_2,$ and $H_3$. (b) Horospheric tetrahedron on hyperface opposite $A_0$. 

$\Box$
### Coxeter Simplex Tilings

| Witt Symb. | $\mathcal{S}_4$ | $\mathcal{T}_4$ | $\mathcal{P}_4$ | $\mathcal{O}_4$ | $FR_4$ |
|------------|-----------------|-----------------|-----------------|-----------------|--------|
| $A_0$      | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$ |
| $A_1$      | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$ |
| $A_2$      | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$ |
| $A_3$      | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$ |
| $A_4$      | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$ |

### Vertices of Simplex

| $u_0$      | $(0,0,0,1)$     | $(0,0,0,1)$     | $(0,0,0,1)$     | $(0,0,0,1)$     | $(0,0,0,1)$     |
| $u_1$      | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   |
| $u_2$      | $(0,0,0,1)$     | $(0,0,0,1)$     | $(0,0,0,1)$     | $(0,0,0,1)$     | $(0,0,0,1)$     |
| $u_3$      | $(0,0,0,1)$     | $(0,0,0,1)$     | $(0,0,0,1)$     | $(0,0,0,1)$     | $(0,0,0,1)$     |
| $u_4$      | $(0,0,0,1)$     | $(0,0,0,1)$     | $(0,0,0,1)$     | $(0,0,0,1)$     | $(0,0,0,1)$     |

### Maximal horball parameter $s$

| $s$        | $-1/9$          | $-3/19$         | $0$             | $5/19$          | $7/17$ |

### Intersections $H_i = B(A_0, s) \cap A_0 A_i$ of horballs with simplex edges

| $H_1$      | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   |
| $H_2$      | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   |
| $H_3$      | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   |
| $H_4$      | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   | $(1,0,0,0,1)$   |

### Volume of horball pieces

| $Vol(B_0 \cap \mathcal{F})$ | $0.00491046$ | $0.00582093$ | $0.00699444$ | $0.01388898$ | $0.0555556$ |

### Optimal Packing Density

| $\delta_{opt}$ | $0.71644896$ | $0.71644896$ | $0.67072710$ | $0.67072710$ | $0.71644896$ |

Table 2: Data for simply asymptotic Tilings in Cayley-Kleinball model of radius 1 centered at $(1,0,0,0,0)$
4.2 Multiply asymptotic case

In cases where the Coxeter simplex has multiple asymptotic vertices we allow horoballs of different types at different vertices. The equations for horoballs centered at \((1, 0, 0, 0, -1)\) and \((1, 0, 1, 0, 0)\) with where \(h_i = \frac{1}{2^n}\) are

\[
\frac{2 \left( h_1^2 + h_2^2 + h_3^2 \right)}{s + 1} + \frac{4 (h_4 + \frac{1}{s})^2}{(s + 1)^2} = 1, \tag{19}
\]

and

\[
\frac{2 \left( h_1^2 + h_2^2 + h_3^2 \right)}{1 - s} + \frac{4 (h_4 - \frac{1}{s})^2}{(1 - s)^2} = 1. \tag{20}
\]

Analogously to the simply asymptotic case, first we find the bound for the largest possible horoball type at each asymptotic vertex. Such horoball is tangent to the face opposite its center. We pick one horoball to be of the largest type, and increase the size of the other horoballs until they become tangent. We then vary the types horoballs within the allowable bounds to find the optimal packing density. The following lemma proved in \([25]\) gives the relationship between the volumes of two tangent horoball pieces centered at certain vertices of a tiling as we continuously vary their types.

Let \(\tau_1\) and \(\tau_2\) be two congruent \(n\)-dimensional convex pyramid-like regions with vertices at \(C_1\) and \(C_2\) sharing a common edge \(C_1C_2\). Let \(B_1(x)\) and \(B_2(x)\) denote two horoballs centered at \(C_1\) and \(C_2\) tangent at point \(I(x) \in C_1C_2\). Define the point of tangency \(I(0)\) (the “midpoint”) such that the equality \(V(0) = 2Vol(B_1(0) \cap \tau_1) = 2Vol(B_2(0) \cap \tau_2)\) holds for the volumes of the horoball sectors. See Figure \(3(a)\).

**Lemma 4.3 \([25]\).** Let \(x\) be the hyperbolic distance between \(I(0)\) and \(I(x)\), then

\[
V(x) = Vol(B_1(x) \cap \tau_1) + Vol(B_2(x) \cap \tau_2) = \frac{V(0)}{2} \left( e^{(n-1)x} + e^{-(n-1)x} \right)
\]

strictly increases as \(x \to \pm \infty\).

4.2.1 Doubly Asymptotic Case

**Proposition 4.4.** The optimal horoball packing density for Coxeter simplex tiling \(\mathcal{T}_{4,N}\) is \(\delta_{opt}(N_4) \approx 0.71644896\).

**Proof.** We parameterize the fundamental domain \(\mathcal{F}_{N_4}\) according to Table \(3\) so that the two asymptotic vertices are at two opposite poles of the ball model. Let the corner of the simplex at \(A_0\) be \(\tau_0\) and at \(A_3\) be \(\tau_3\). We place two horoballs \(B_0(0)\) and \(B_0(1/3)\) that pass through \((1, 0, 0, 0, s_0)\) and \((1, 0, 0, 0, s_3)\) respectively at \(A_0\) and \(A_3\). Let \(x_i = \tanh^{-1}(s_i)\) denote the hyperbolic distance of the center of the model \((1, 0, 0, 0, 0)\) and the point \(S = (1, 0, 0, 0, s_i)\). If the two horoballs \(B_0(0)\) and \(B_0(1/3)\) are tangent to their respective hyperfaces \([u_0]\) and \([u_3]\) then their interiors intersect, so the packing density is optimal when the horoballs are tangent at one point. Set \(s = s_0 = s_3\), see Figure \(3(b)\). Let \(B_i(s) = B_i(x)\), and define \(V_0(x) = Vol(B_0(x) \cap \tau_0)\) and \(V_3(x) = Vol(B_3(x) \cap \tau_3)\). With the techniques of Proposition \(5.1\) and horosphere equations \(9\).
and (20) we compute that $V_0(0) \approx 0.0138889$ and $V_3(0) \approx 0.00694444$. The corner of the simplex at $\tau_1$ is half the size of that at $\tau_3$ so we have that $2V_0(0) = V_3(0)$ when $x = s = 0$. By Lemma 4.3 we obtain

$$V(x) = V_0(0)e^{3x} + V_2(0)e^{-3x}$$

which is maximal when $x$ is the largest possible value allowed, when $s = 1/3$.

$$\delta_{opt}(N_4) = \frac{Vol(B_0(1/3) \cap F_{N_4}) + Vol(B_3(1/3) \cap F_{N_4})}{Vol(F_{N_4})} \approx 0.71644896.$$  

The data for the optimal horoball packing is summarized in Table 3. The symmetry group $\Gamma_{N_4}$ carries the density from the fundamental domain to the entire tiling.

Similarly to the above proof we obtain

**Corollary 4.5.** The optimal horoball packing density for Coxeter simplex tiling $\Gamma_{BP_4}$ is $\delta_{opt}(BP_4) \approx 0.71644896$.

Note that $|\Gamma_{N_4} : \Gamma_{BP_4}| = 2$ so the tilings are related by fundamental domain doubling. The optimal horoball configurations of $N_4$ and $BP_4$ are essentially the same.

### 4.2.2 Triply Asymptotic Case

We generalize the above results to the two triply asymptotic tilings using the subgroup relations of the multiply asymptotic tilings given in Figure 1. The indeces of the subgroups are

$$|\Gamma_{N_4} : \Gamma_{M_4}| = |\Gamma_{M_4} : \Gamma_{DP_4}| = |\Gamma_{BP_4} : \Gamma_{DP_4}| = 2,$$

so the fundamental domains are related by domain doubling, hence the optimal packing density is at least $\delta \approx 0.71644896$ for all multiply asymptotic cases. By repeated use of
Coxeter Simplex Tilings

| Witt Symb. | Doubly Asymptotic | Triply Asymptotic |
|------------|-------------------|------------------|
|            | \(N_4\)          | \(BP_4\)         | \(M_4\)          | \(DP_4\)         |
| Vertices of Simplex |
| \(A_0\)   | \((1, 0, 0, 0, 1)^*\) | \((1, 0, 0, 0, 1)^*\) | \((1, 0, 0, 0, 1)^*\) | \((1, 0, 0, 0, 1)^*\) |
| \(A_1\)   | \((1, 0, \frac{2}{3}, 0, \frac{1}{3})\) | \((1, 0, \frac{2}{3}, 0, \frac{1}{3})\) | \((1, 0, 1, 0, 0)^*\) | \((1, 0, 1, 0, 0)^*\) |
| \(A_2\)   | \((1, 0, \frac{2}{3}, \frac{1}{3}, 0)\) | \((1, -\frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0)\) | \((1, 0, \frac{1}{3}, \frac{1}{3}, 0)\) | \((1, -\frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0)\) |
| \(A_3\)   | \((1, 0, 0, 0, -1)^*\) | \((1, 0, 0, 0, -1)^*\) | \((1, 0, 0, 0, -1)^*\) | \((1, 0, 0, 0, -1)^*\) |
| \(A_4\)   | \((1, \frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0)\) | \((1, \frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0)\) | \((1, \frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0)\) | \((1, \frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0)\) |

The form \(u_i\) of sides opposite \(A_i\):

\[
\begin{align*}
  u_0 &= (1, 0, -2, 0, 1)^T, & (1, 0, -2, 0, 1)^T, & (1, 0, -1, -1, 1)^T, & (1, 0, -1, -1, 1)^T \\
  u_1 &= (0, 0, 1, -1, 0)^T, & (0, 0, 1, -1, 0)^T, & (0, 0, 1, -1, 0)^T, & (0, 0, 1, -1, 0)^T \\
  u_2 &= (0, -1, 0, 1, 0)^T, & (0, -1, 0, 1, 0)^T, & (0, -1, 0, 1, 0)^T, & (0, -1, 0, 1, 0)^T \\
  u_3 &= (-1, 0, 1, 1, 1)^T, & (-1, 0, 1, 1, 1)^T, & (-1, 0, 1, 1, 1)^T, & (-1, 0, 1, 1, 1)^T \\
  u_4 &= (0, 1, 0, 0, 0)^T, & (0, 1, 0, 0, 0)^T, & (0, 1, 0, 0, 0)^T, & (0, 1, 0, 0, 0)^T \\
\end{align*}
\]

Maximal horoball-type parameter \(s_i\) for horoball \(B_i\) at \(A_i\):

\[
\begin{align*}
  s_0 &= 0 & 0 & -1/3 & -1/3 \\
  s_1 &= - & - & 1/3 & 1/3 \\
  s_3 &= 1/3 & 1/3 & 1/3 & 1/3 \\
\end{align*}
\]

Volumes of optimal horoball pieces \(V_i = \text{Vol}(B_i \cap F_\Gamma)\):

\[
\begin{align*}
  V_0 &= 0.00461046 & 0.00982093 & 0.00461046 & 0.00982093 \\
  V_1 &= - & - & 0.00461046 & 0.00982093 \\
  V_2 &= 0.0196419 & 0.0392837 & 0.0392837 & 0.0785674 \\
\end{align*}
\]

Optimal Horoball Packing Density

\[
\delta_{opt} = 0.71644896, 0.71644896, 0.71644896, 0.71644896
\]

Table 3: Data for multiply asymptotic Coxeter simplex tilings in the Cayley-Klein ball model of radius 1 centered at \((1,0,0,0,0,0)\). Vertices marked with * are ideal.

Lemma 4.3 we can show that this value is the optimal packing density for all multiply asymptotic cases. We omit the technical details of the proof.

**Proposition 4.6.** The optimal horoball packing density for triply asymptotic Coxeter simplex tilings \(\Gamma \in \{M_4, DP_4\}\) is \(\delta_{opt}(\Gamma) \approx 0.71644896\).

The details of the results for multiply asymptotic tilings are given in Table 3.

## 5 Main Result: New Lower Bound for the Ball Packing Density of \(\mathbb{H}^4\)

The horoball packings described in this paper are the densest realizable packings of the entire space \(\mathbb{H}^4\) known to the authors at the time of writing. We summarize our results in the following theorem.
Theorem 5.1. In $\mathbb{H}^4$ the horoball packing density $\delta_{\text{opt}}(T_\Gamma) \approx 0.71644896$ is optimal in seven asymptotic Coxeter simplex tilings $\Gamma \in \{\overline{S}_4, \overline{P}_4, \overline{FR}_4, \overline{N}_4, \overline{M}_4, \overline{BP}_4, \overline{DP}_4\}$, if horoballs of different types are allowed at each asymptotic vertex of the tiling.

Remark 5.2. Consider two horoball packings to be in a same class, if their symmetry groups are isomorphic. In this sense we can distinguish between three different horoball packings of optimal density.

Our packing density is greater than the $(5 - \sqrt{5})/4 \approx 0.69098301$ value conjectured by L. Fejes-Tóth as the realizable packing density upper bound on pp. 323 of [8]. However it does not exceed the Böröczky–Florian upper bound for $\mathbb{H}^4$ of $\approx 0.73046$.

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