OPTIMAL HOROBALL PACKING DENSITIES FOR KOSZUL-TYPE TILINGS
IN HYPERBOLIC 3-SPACE

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ABSTRACT. We determine the optimal horoball packing densities for the Koszul-type
Coxeter simplex tilings in $\mathbb{H}^3$. We give a family of horoball packings parameterized by
the Busemann function and symmetry group that achieve the simplicial packing density
upper bound $d_3(\infty) = \left(2\sqrt{3}\Lambda\left(\frac{\pi}{3}\right)\right)^{-1} \approx 0.853276$ where $\Lambda$ is the Lobachevsky
function.

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1. INTRODUCTION

This is the fifth paper in a series on optimal horoball packing densities of all Koszul-type
noncompact Coxeter simplex tilings in $\mathbb{H}^n$. In [14], we showed that the classical example
of the horoball packing in $\mathbb{H}^3$ that achieves the Böröczky-type simplicial packing density
upper bound $d_3(\infty)$ (cf. Theorem 2) is not unique, and showed several new examples using
horoballs of different types. In [15–17] we considered the dimensions $4 \leq n \leq 9$ where
Koszul-type tilings exist. In [15], we found seven horoball packings of Coxeter simplex
tilings in $\mathbb{H}^4$ that yield densities of $5\sqrt{2}/\pi^2 \approx 0.71645$, counterexamples to L. Fejes Tóth’s
conjecture for the maximal packing density of $\frac{5-\sqrt{5}}{4} \approx 0.69098$ in his foundational book
Regular Figures [8, p. 323]. In [16, 17] we constructed the densest known ball packing in
$\mathbb{H}^6$ with $6 \leq n \leq 9$, for example in $\mathbb{H}^5$ the optimal packing density is $\frac{5}{\pi\zeta(3)}$ where $\zeta(\cdot)$ is
the Riemann Zeta function.
In the present paper we extend [14] to the Koszul simplex groups of dimension \( n = 3 \). We summarize the results in this paper in Theorems 3-6 as follows, where \( \Lambda(\theta) = -\frac{1}{2} \int_0^\theta \ln \left( 2 \sin \left( \frac{t}{2} \right) \right) \, dt \) is the Lobachevsky function.

**Theorem 1.** The optimal horoball packing density for noncompact Coxeter simplex tilings in \( \mathbb{H}^3 \) of \( d_3(\infty) = \left( 2 \sqrt{3} \Lambda \left( \frac{\pi}{2} \right) \right)^{-1} = 0.85328 \ldots \) is realized in tilings by eight simplex groups in the \([3,3,6]\) commensurability class.

Upper bounds for the packing density were published by Kellerhals [11] using the simplicial density function \( d_n(\infty) \). This bound is strict for \( n = 3 \).

Relative to [14], in this paper the notion of ‘horoball type’ with respect to a fundamental domain is strengthened using isometry invariant Busemann functions. We use Busemann functions to parameterize horoballs centered at \( \xi \in \partial \mathbb{H}^n \) with respect to a marked reference point \( o \in \mathbb{H}^n \) (alternatively a reference horoball through \( \xi \) and \( o \)) in the model of \( \mathbb{H}^n \), see Section 3.3. This new point of view shows that the optimal packings cannot be made equivalent by repartitioning, a nontrivial hyperbolic isometry, or some paradoxical construction, and clarifies our earlier results prior to [13,17].

2. BACKGROUND

Let \( X \) denote a space of constant curvature, either the 3-dimensional sphere \( S^3 \), Euclidean space \( \mathbb{E}^3 \), or hyperbolic space \( \mathbb{H}^3 \). An important question of discrete geometry is to find the highest possible packing density in \( X \) by congruent non-overlapping balls of a given radius \([6,7]\). The definition of packing density is critical in hyperbolic space as shown by B"or"oczky [4], for the standard paradoxical construction see \([7,23]\). The most widely accepted notion of packing density considers the local densities of balls with respect to their Dirichlet–Voronoi cells (cf. \([4,11]\)). In order to study horoball packings in \( \mathbb{H}^3 \), we use an extended notion of such local density.

Let \( B \) be a horoball of packing \( \mathcal{B} \), and \( P \in \mathbb{H}^3 \) an arbitrary point. Define \( d(P, B) \) to be the shortest distance from point \( P \) to the horosphere \( S = \partial B \), where \( d(P, B) \leq 0 \) if \( P \in B \). The Dirichlet–Voronoi cell \( D(B, B) \) of horoball \( B \) is the convex body

\[
D(B, B) = \{ P \in \mathbb{H}^3 \mid d(P, B) \leq d(P, B'), \ \forall B' \in \mathcal{B} \}.
\]

Both \( B \) and \( D \) have infinite volume, so the standard notion of local density is modified. Let \( Q \in \partial \mathbb{H}^3 \) denote the ideal center of \( B \), and take its boundary \( S \) to be the one-point compactification of Euclidean plane. Let \( B_C(r) \subset S \) be the Euclidean ball with center \( C \in S \setminus \{ Q \} \). Then \( Q \) and \( B_C(r) \) determine a convex cone \( C(r) = \text{cone}_Q \{ B_C(r) \} \subset \mathbb{H}^3 \) with apex \( Q \) consisting of all hyperbolic geodesics passing through \( B_C(r) \) with limit point \( Q \). The local density \( \delta_3(B, B) \) of \( B \) to \( D \) is defined as

\[
\delta_3(B, B) = \lim_{r \to \infty} \frac{\text{vol}(B \cap C(r))}{\text{vol}(D \cap C(r))}.
\]

This limit is independent of the choice of center \( C \) for \( B_C(r) \).

In the case of periodic ball or horoball packings, this local density defined above extends to the entire hyperbolic space via its symmetry group, and is related to the simplicial density function (defined below) that we generalized in \([26,27]\). In this paper we shall use such definition of packing density (cf. Section 3).

A Coxeter simplex is a top dimensional simplex in \( X \) with dihedral angles either integral submultiples of \( \pi \) or zero. The group generated by reflections on the sides of a Coxeter simplex is a Coxeter simplex reflection group. Such reflections generate a discrete group
of isometries of $X$ with the Coxeter simplex as the fundamental domain. Hence the groups give regular tessellations of $X$ if the fundamental simplex is characteristic. The Coxeter groups are finite for $S^3$, and infinite for $\mathbb{E}^3$ or $\mathbb{H}^3$.

There are non-compact Coxeter simplices in $\mathbb{H}^n$ with ideal vertices on $\partial \mathbb{H}^n$, however only for dimensions $2 \leq n \leq 9$; furthermore, only a finite number exist in dimensions $n \geq 3$. Johnson et al. [9] found the volumes of all Coxeter simplices in hyperbolic $n$-space. Such simplices are the most elementary building blocks of hyperbolic manifolds, the volume of which is an important topological invariant.

In $n$-dimensional space $X$ of constant curvature ($n \geq 2$), define the simplicial density function $d_n(r)$ to be the density of $n + 1$ mutually tangent balls of radius $r$ in the simplex spanned by their centers. L. Fejes Tóth and H. S. M. Coxeter conjectured that the packing density of balls of radius $r$ in $X$ cannot exceed $d_n(r)$. Rogers [24] proved this conjecture in Euclidean space $\mathbb{E}^n$. The 2-dimensional spherical case was settled by L. Fejes Tóth [8], and Böröczky [4] gave a proof for the extension:

**Theorem 2** (K. Böröczky), In an $n$-dimensional space of constant curvature, consider a packing of spheres of radius $r$. In the case of spherical space, assume that $r < \frac{n+1}{n}$. 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.

In hyperbolic 3-space, the monotonicity of $d_3(r)$ was proved by Böröczky and Florian in [5]. In [13] Marshall showed that for sufficiently large $n$, function $d_n(r)$ is strictly increasing in variable $r$. Kellerhals [11] showed $d_n(r) < d_{n-1}(r)$, and that in cases considered by Marshall the local density of each ball in its Dirichlet–Voronoi cell is bounded above by the simplicial horoball density $d_n(\infty)$. Theorem 2 is extended to the horoball case in [4] §6 as a remark.

The simplicial packing density upper bound classically given in series form $d_3(\infty) = (1 + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{7}} + \ldots)^{-1} = 0.85327\ldots$ cannot be achieved by packing regular balls, instead it is realized by horoball packings of $\mathbb{H}^3$, the regular ideal simplex tiling $\mathbb{H}^3$. More precisely, the centers of horoballs in $\partial \mathbb{H}^3$ lie at the vertices of the ideal regular Coxeter simplex tiling with Schl"afli symbol $[3,3,6]$.

In three dimensions the Böröczky-type bound for horoball packings are used for volume estimates of cusped hyperbolic manifolds [1,20], more recently [2,19]. Lifts of horoball neighborhoods of cusps give horoball packings in the universal cover $\mathbb{H}^n$, and for some discrete torsion free subgroup of isometries $\mathbb{H}^n/\Gamma$ is a cusped hyperbolic manifold where the cusps lift to ideal vertices of the fundamental domain. In this setting a manifold with a single cusp has a well defined maximal cusp neighborhood, while manifolds with multiple cusps have a range of non-overlapping cusp neighborhoods with boundaries with nonempty tangential intersection, these lift to different horoball types in the universal cover. An important application is Adams’ proof that the Geiseking manifold is the noncompact hyperbolic 3-manifold of minimal volume [11]. Kellerhals then used the Böröczky-type bounds to estimate volumes of higher dimensional hyperbolic manifolds [12].

In [14] we proved that the classical horoball packing configuration in $\mathbb{H}^3$ realizing the Böröczky-type upper bound is not unique. We gave several examples of different regular horoball packings using horoballs of different types, that is horoballs that have different relative densities with respect to the fundamental domain, that yield the Böröczky–Florian-type simplicial upper bound [5].
We remark that the second-named author studied the case of simply truncated Coxeter orthoschemes in $\mathbb{H}^3$ where the density upper bound is not achieved [28].

3. Preliminaries

We use the projective Cayley–Klein model of hyperbolic geometry to preserves lines and convexity for the packing of simplex tilings with convex fundamental domains. Hyperbolic symmetries are modeled as Euclidean projective transformations using the projective linear group $\text{PGL}(4, \mathbb{R})$. In this section we review some key concepts, for a general discussion of the projective models of Thurston geometries see [21][22].

3.1. The Projective Model of $\mathbb{H}^3$. Let $\mathbb{E}^{1,3}$ denote $\mathbb{R}^4$ with the Lorentzian inner product $\langle x, y \rangle = -x_0y_0 + x_1y_1 + x_2y_2 + x_3y_3$ where non-zero real vectors $x, y \in \mathbb{R}^4$ represent points in projective space $\mathbb{P}^3 = \mathbb{P}(\mathbb{E}^4)$, equipped with the quotient topology of the natural projection $\Pi : \mathbb{E}^4 \setminus \{0\} \rightarrow \mathbb{P}^3$. Partitioning $\mathbb{E}^{1,3}$ into $\mathbb{Q}_+ = \{ v \in \mathbb{R}^4 | \langle v, v \rangle > 0 \}$, $\mathbb{Q}_0 = \{ v | \langle v, v \rangle = 0 \}$, and $\mathbb{Q}_- = \{ v | \langle v, v \rangle < 0 \}$, the proper points of hyperbolic 3-space $\mathbb{H}^3 = \Pi(\mathbb{Q}_+)$, $\partial\mathbb{H}^3 = \Pi(\mathbb{Q}_0)$ are the boundary or ideal points, we will refer to points in $\Pi(\mathbb{Q}_+)$ as outer points, and $\mathbb{H}^3 = \mathbb{H}^3 \cup \partial\mathbb{H}^3$ as extended hyperbolic space.

Points $[x], [y] \in \mathbb{P}^3$ are conjugate when $\langle x, y \rangle = 0$. The set of all points conjugate to $[x]$ form a projective (polar) hyperplane $\text{pol}([x]) = \{ [y] \in \mathbb{P}^3 | \langle x, y \rangle = 0 \}$. Hence $\mathbb{Q}_0$ induces a duality $\mathbb{R}^4 \leftrightarrow \mathbb{R}_4$ between the points and hyperplanes of $\mathbb{P}^3$. Point $[x]$ and hyperplane $[a]$ are incident if the value of the linear form $\alpha$ evaluated on vector $x$ is zero, i.e. $\alpha x = 0$ where $x \in \mathbb{R}^4 \setminus \{0\}$, and $\alpha \in \mathbb{R}_4 \setminus \{0\}$. Similarly, the lines in $\mathbb{P}^3$ are given by 2-subspaces of $\mathbb{R}_4$ or dual 2-subspaces of $\mathbb{R}_4$ [21].

Let $P \subset \mathbb{H}^3$ be a polyhedron bounded by a finite set of hyperplanes $H^i$ with unit normals $b^i \in \mathbb{R}_4$ directed towards the interior of $P$:

$$H^i = \{ x \in \mathbb{H}^3 | \langle b^i, x \rangle = 0 \} \quad \text{with} \quad \langle b^i, b^j \rangle = 1.$$  

In this paper $P$ is assumed to be an acute-angled polyhedron with proper or ideal vertices. The Gram matrix of $P$ is $G(P) = \{ \langle b^i, b^j \rangle \}_{i,j}, i, j \in \{0, 1, 2, 3\}$ is symmetric with signature $(1, 3)$, its entries satisfy $\langle b^i, b^j \rangle = 1$ and $\langle b^i, b^j \rangle \leq 0$ for $i \neq j$ where

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

This is summarized in the Coxeter graph of the polytope $\Sigma(P)$. The graph nodes correspond to the hyperplanes $H^i$ and are connected if $H^i$ and $H^j$ are not perpendicular ($i \neq j$). If connected the positive weight $k$ where $\alpha_{ij} = \pi/k$ is indicated on the edge, unlabeled edges denote an angle of $\pi/3$. Coxeter diagrams appear in Table [1].

In this paper we set the sectional curvature of $\mathbb{H}^3$, $K = -k^2$, to be $k = 1$. The distance $d$ between two proper points $[x]$ and $[y]$ is given by

$$\cosh d = \frac{-\langle x, y \rangle}{\sqrt{\langle x, x \rangle \langle y, y \rangle}}.$$
The projection \([y]\) of point \([x]\) on plane \([u]\) is given by
\[
(3) \quad y = x - \frac{(x, u)}{(u, u)} u,
\]
where \([u]\) is the pole of the plane \([u]\).

3.2. Horospheres and Horoballs in \(\mathbb{H}^3\). A horosphere in \(\mathbb{H}^3\) is as hyperbolic 3-sphere with infinite radius centered at an ideal point \(\xi \in \partial \mathbb{H}^3\) obtained as a limit of spheres through \(x \in \mathbb{H}^3\) as its center \(c \rightarrow \xi\). Equivalently, a horosphere is a 2-surface orthogonal to the set of parallel straight lines passing through \(\xi \in \partial \mathbb{H}^3\). A horoball is a horosphere together with its interior.

To derive the equation of a horosphere, fix a projective coordinate system for \(\mathbb{H}^3\) with standard basis \(a_i, 0 \leq i \leq 3\) so that the Cayley–Klein ball model of \(\mathbb{H}^3\) is centered at \(O = (1, 0, 0, 0)\), and orient it by setting point \(\xi \in \partial \mathbb{H}^3\) to lie at \(A_0 = (1, 0, 0, 1)\). The equation of a horosphere with center \(\xi = A_0\) passing through interior point \(S = (1, 0, 0, s)\) is derived from the equation of the the boundary sphere \(-x^0x^0 + x^1x^1 + x^2x^2 + x^3x^3 = 0\), and the plane \(x^0 - x^3 = 0\) tangent to the boundary sphere at \(\xi = A_0\). The general equation of the horosphere is
\[
(4) \quad 0 = \lambda(-x^0x^0 + x^1x^1 + x^2x^2 + x^3x^3) + \mu(x^0 - x^3)^2.\]
Evaluating at \(S\) obtain
\[
\lambda(-1 + s^2) + \mu(-1 + s)^2 = 0 \quad \text{and} \quad \frac{\lambda}{\mu} = \frac{1 - s}{1 + s}.
\]
For \(s \neq \pm 1\), the equation of a horosphere in projective coordinates is
\[
(5) \quad (s - 1) \left(-x^0x^0 + \sum_{i=1}^{3} (x^i)^2\right) - (1 + s)(x^0 - x^3)^2 = 0.
\]

In \(\mathbb{H}^3\) there exists an isometry \(g \in \text{Isom}(\mathbb{H}^3)\) for any two horoballs \(B\) and \(B'\) such that \(gB = B'\). However, it is often useful to distinguish between certain horoballs of a packing: we shall use the notion of horoball type with respect to the fundamental domain of a tiling (lattice) as introduced in [27]. In Section 3.3 we show that this coincides with the Busemann function up to scaling, hence is isometry invariant.

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 particular cell (in our case a Coxeter simplex) are equal, otherwise the two horoballs are of different type. For example, the horoballs centered at \(A_0\) passing through \(S\) with different values for the final coordinate \(s \in (-1, 1)\) are of different type relative to a given cell, and the set of all horoballs centered at vertex \(A_0\) is a one-parameter family.

Volumes of horoball pieces are given by János Bolyai’s classical formulas from the mid 19-th century. The hyperbolic length \(L(x)\) of a horospherical arc contained in a chord segment of length \(x\) is
\[
(6) \quad L(x) = 2 \sinh \left(\frac{x}{2}\right).
\]
The intrinsic geometry of a horosphere is Euclidean, so the area \(A\) of a polygon \(A\) on the surface of the horosphere can be calculated as in \(\mathbb{E}^2\). The volume of the horoball piece \(\mathcal{H}(A)\) bounded by \(A\), the set consisting of the union of geodesic segments joining \(A\) to the center of the horoball, is
\[
(7) \quad \text{vol}(\mathcal{H}(A)) = \frac{1}{2} A.
\]
3.3. The Busemann function in $\mathbb{H}^3$. Define the Busemann function on $\mathbb{H}^3$ as the map $\beta : \mathbb{H}^3 \times \mathbb{H}^3 \times \partial \mathbb{H}^3 \to \mathbb{R}$ with $\beta(x, y, \xi) = \lim_{z \to \xi} (d(x, z) - d(y, z))$, where the limit $z \to \xi$ is taken along any geodesic in $\mathbb{H}^3$ ending at boundary point $\xi$. The Busemann function satisfies $\beta(x, x, \xi) = 0$, antisymmetry $\beta(x, y, \xi) = -\beta(y, x, \xi)$, the cocycle property $\beta(x, y, \xi) + \beta(y, z, \xi) = \beta(x, z, \xi)$ for all $x, y, z \in \mathbb{H}^3$, and is invariant under actions of $\text{Isom}(\mathbb{H}^3)$. A horosphere centered at $\xi$ through $o$ is the level set of the Busemann function $\text{Hor}_\xi(o) = \{x \in \mathbb{H}^3 | \beta(x, o, \xi) = 0\}$, while a horoball is the sublevel set $\text{Hor}_\xi(o) = \{x \in \mathbb{H}^3 | \beta(x, o, \xi) \leq 0\}$. The space of all horospheres $\text{Hor}(\mathbb{H}^3)$ gives an $\mathbb{R}$-fibration $h : \text{Hor}(\mathbb{H}^3) \to \partial \mathbb{H}^3$ where $\text{Hor}_\xi(o) \to \xi$. The Busemann function then is an oriented distance between two concentric horospheres $\text{Hor}_\xi(o_1)$ and $\text{Hor}_\xi(o_2)$. For Busemann functions in Hadamard spaces defined by various authors cf. [3, 13].

Set reference point $o \in \mathbb{H}^3$ for the model at $o = (1, 0, 0, 0)$ and reference horosphere $\text{Hor}_\xi(o)$ at $\xi = (1, 0, 0, 1)$. The $s$-parameter of horosphere $\text{Hor}_\xi(x)$ is $s = \text{th}(\beta(o, x, \xi))$ where $\text{th}(\cdot)$ is the hyperbolic tangent function. A choice of reference point $o \in \mathbb{H}^3$ gives a trivialization of the fibration according to diagram

$\text{Hor}(\mathbb{H}^3) \xrightarrow{\varphi_o} \partial \mathbb{H}^3 \times \mathbb{R}$

where $\text{Hor}_\xi(x) \mapsto (\xi, \beta(o, x, \xi))$. An element $g \in \text{Isom}(\mathbb{H}^3)$ acts on a horosphere as an additive cocycle

$g.\text{Hor}_\xi(x) = \text{Hor}_{g.\xi}(gx) \mapsto (g\xi, \beta(o, gx, g\xi)) = (g\xi, \beta(g^{-1}o, x, \xi))$

$= (g\xi, \beta(o, x, \xi) + \beta(g^{-1}o, o, \xi))$.

Let $\hat{s} = \text{arcth}(s)$ then $g$ acts on the trivialization by

$g(\xi, \hat{s}) = (g\xi, \hat{s} + \beta(g^{-1}o, o, \xi))$.

In summary Busemann functions are related to the $s$-parameters by scaling and describe packing configurations relative to a marked point $o$ in an isometry invariantly.

4. Packing Density in the Projective Model

In this section we define packing density and collect three Lemmas used in Section 5 to find the optimal packing densities for the Koszul simplex tilings.

Let $\mathcal{T}$ be a Coxeter tiling of $\mathbb{H}^3$ [10]. The symmetry group of a Coxeter tiling $\Gamma_\mathcal{T}$ contains its Coxeter group, and isometric mapping between two cells in $\mathcal{T}$ preserves the tiling. Any simplex cell of $\mathcal{T}$ acts as a fundamental domain $\mathcal{F}_\mathcal{T}$ of $\Gamma_\mathcal{T}$, and the Coxeter group is generated by reflections on the 2-dimensional faces of $\mathcal{F}_\mathcal{T}$. In this paper we consider only noncompact or Koszul-type Coxeter simplices, that is simplices with one or more ideal vertex, then the orbifold $\mathbb{H}^3/\Gamma_\mathcal{T}$ has at least one cusp. In Table 1 we list the 23 Koszul-type Coxeter simplices in $\mathbb{H}^3$ and their volumes. For a detailed discussion of the volume formulae for the other hyperbolic Coxeter simplices of dimensions $n \geq 3$, see Johnson et al. [9].

Define the density of a regular horoball packing $\mathcal{B}_\mathcal{T}$ of Coxeter simplex tiling $\mathcal{T}$ as

$$\delta(\mathcal{B}_\mathcal{T}) = \frac{\sum_{i=1}^{m} \text{vol}(B_i \cap \mathcal{F}_\mathcal{T})}{\text{vol}(\mathcal{F}_\mathcal{T})}.$$
\( \mathcal{F}_T \) denotes the simplex fundamental domain of tiling \( T \), \( m \) the number of ideal vertices of \( \mathcal{F}_T \), and \( B_i \) the horoball centered at the \( i \)-th ideal vertex. We allow horoballs of different types at each asymptotic vertex of the tiling. A particular set of horoballs \( \{ B_i \}_{i=1}^m \) with different horoball types is allowed if it gives a packing: no two horoballs may have an interior point in common, and we require that no horoball extend beyond the face opposite the vertex where it is centered. The second condition ensures that the packing remains invariant under the actions of \( \Gamma_T \) with \( \mathcal{F}_T \). With these conditions satisfied, the packing density in \( \mathcal{F}_T \) extends to the entire \( \mathbb{H}^3 \) by actions of \( \Gamma_T \). In the case of Coxeter simplex tilings, Dirichlet–Voronoi cells coincide with the Coxeter simplices. We denote the optimal horoball packing density as

\[
\delta_{\text{opt}}(T) = \sup_{B_T \text{ packing}} \delta(B_T).
\]

Let \( \mathcal{F}_T \) denote the simplicial fundamental domain of Coxeter tiling \( T \) with vertex set \( \{ A_i \}_{i=0}^3 \in \mathbb{P}(E^{1,3}) \), where \( A_0 = (1, 0, 0, 1) \) is ideal and \( A_1 = (1, 0, 0, 0) \) is the center of the model \( O \). Vertex coordinates \( A_2, A_3 \) then are set according to the dihedral angles of \( \mathcal{F}_T \) indicated in the Coxeter diagrams in Table 1 see Tables 2, 8 for a choice of vertices, here \( u_i \) denote the hyperplane opposite to vertex \( A_i \).

Lemma 1 describes a procedure for finding the optimal horoball packing density in the fundamental domain \( \mathcal{F}_T \) with a single ideal vertex \( A_0 \). Packing density is maximized by the largest horoball type admissible in cell \( \mathcal{F}_T \) centered at \( A_0 \). Let \( B_0(s) \) denote the 1-parameter family of horoballs centered at \( A_0 \) where \( s \)-parameter related to the Busemann function measures the “radius” of the horoball, the minimal Euclidean signed distance between the horoball and the center of the model \( O \), taken negative if the horoball contains the model center.

**Lemma 1** (Local horoball density). The local optimal horoball packing density of simply asymptotic Coxeter simplex \( \mathcal{F}_T \) is \( \delta_{\text{opt}}(\Gamma) = \frac{\text{vol}(B_0(\mathcal{F}_T))}{\text{vol}(\mathcal{F}_T)} \).

**Proof.** The maximal horoball \( B_0(s) \) opposite \( A_0 \) with fundamental domain \( \mathcal{F}_T \) is tangent to the face of the simplex given by \( u_0 \). This tangent point of \( B_0(s) \) and hyperface \( u_0 \) is \( f_0 \) the projection of vertex \( A_0 \) on plane \( u_0 \) given by,

\[
f_0 = a_0 - \frac{(a_0, u_0)}{(u_0, u_0)} u_0.
\]

The value of the \( s \)-parameter for the maximal horoball can be read from the equation of the horosphere through \( A_0 \) and \( f_0 \). The intersections \( [h_i] \) of horosphere \( \partial B_0 \) and the edges of the simplex \( \mathcal{F}_T \) are found by parameterizing the edges \( h_i(\lambda) = \lambda a_0 + a_i \) \( 1 \leq i \leq 3 \) then finding their intersections with \( \partial B_0 \). The volume of the horospherical triangle determines the volume of the horoball piece by equation (7). The data for the horospherical triangle is obtained by finding hyperbolic distances \( l_{ij} \) via equation (2), \( l_{ij} = d(H_i, H_j) \) where \( d(h_i, h_j) = \arccos \left( \frac{-\langle h_i, h_j \rangle}{\sqrt{\langle h_i, h_i \rangle \langle h_j, h_j \rangle}} \right) \). Moreover, the horospherical distances \( L_{ij} \) are found by formula (6). The intrinsic geometry of a horosphere is Euclidean, so the Cayley-Menger determinant gives the volume \( \mathcal{A} \) of the horospheric 2-simplex \( \mathcal{A} \),

\[
\mathcal{A} = \frac{1}{16} \begin{vmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & L_{1,2}^2 & L_{1,3}^2 \\ 1 & L_{1,2}^2 & 0 & L_{2,3}^2 \\ 1 & L_{1,3}^2 & L_{2,3}^2 & 0 \end{vmatrix}.
\]
The volume of the horoball piece contained in the fundamental simplex is

\[ \text{vol}(B_0 \cap F_{\Gamma}) = \frac{1}{2} A. \]

The locally optimal horoball packing density of Coxeter Simplex \( F_{\Gamma} \) is

\[ \delta_{\text{opt}}(F_{\Gamma}) = \frac{\text{vol}(B_0 \cap F_{\Gamma})}{\text{vol}(F_{\Gamma})}. \]

**Lemma 2.** The optimal horoball packing density \( \delta_{\text{opt}}(\Gamma) \) of tiling \( T_{\Gamma} \) and the local horoball packings density \( \delta_{\text{opt}}(F_{\Gamma}) \) are equal.

**Proof.** The local construction the the proof of Lemma 1 is preserved by the isometric actions of \( g \in \Gamma \). The Coxeter group \( \Gamma \) extends the optimal local horoball packing density from the fundamental domain \( F_{\Gamma} \) to the entire tiling \( T_{\Gamma} \) of \( \mathbb{H}^3 \), that is \( \delta_{\text{opt}}(\Gamma) = \delta_{\text{opt}}(F_{\Gamma}) = \frac{\text{vol}(B_0 \cap F_{\Gamma})}{\text{vol}(F_{\Gamma})}. \)

The volumes of two tangent horoball pieces centered at two distinct ideal vertices of the fundamental domain as the horoball type is continuously varied are related in the Lemma 3.

In \( \mathbb{H}^3 \) let \( \tau_1 \) and \( \tau_2 \) be two congruent convex cones with vertices at \( C_1, C_2 \in \partial \mathbb{H}^3 \) that share a common geodesic edge \( C_1C_2 \). Let \( B_1(x) \) and \( B_2(x) \) denote two horoballs centered at \( C_1 \) and \( C_2 \) respectively, mutually tangent at \( I(x) \in C_1C_2 \). Define \( I(0) \) as the point with \( V(0) = 2\text{vol}(B_1(0) \cap \tau_1) = 2\text{vol}(B_2(0) \cap \tau_2) \) for the volumes of the horoball sectors.

**Lemma 3 ([26]).** Let \( x \) be the hyperbolic distance between \( I(0) \) and \( I(x) \), then

\[ V(x) = \text{vol}(B_1(x) \cap \tau_1) + \text{vol}(B_2(x) \cap \tau_2) \]
\[ = V(0) e^{2x} + e^{-2x} = V(0) \cosh(2x) \]

is strictly convex and strictly increasing as \( x \to \pm \infty \).

**Proof.** See our paper [26] for a proof.

5. The Optimal Packing Densities of the Koszul Simplex Tilings

In this section we determine the optimal horoball packing densities of the Koszul-type Coxeter simplex tilings in \( \mathbb{H}^3 \). Table 1 summarizes the tilings and their optimal packing densities. Fig. 1 shows the lattice of subgroups for the different commensurability classes of groups. The Witt symbols will denote the various \( \Gamma \) groups.
### Table 1

| Coxeter Diagram | Notation | Witt Symbol | Simplex Volume | Packing Density |
|-----------------|----------|-------------|----------------|-----------------|
| Commensurable to $[3, 3, 6]$ | | | | |
| ![Diagram](attachment:diagram1.png) | $[3, 3, 6]$ | $V_3$ | $\frac{1}{6} \Lambda \left( \frac{\pi}{3} \right)$ | $\Theta = \frac{1}{2\sqrt{3}} \Lambda \left( \frac{\pi}{3} \right)$ |
| ![Diagram](attachment:diagram2.png) | $[3, 6, 3]$ | $Y_3$ | $\frac{1}{2} \Lambda \left( \frac{\pi}{3} \right)$ | $\Theta \approx 0.853276$ |
| ![Diagram](attachment:diagram3.png) | $[6, 3^{[3]}]$ | $VP_3$ | $\frac{3}{2} \Lambda \left( \frac{\pi}{3} \right)$ | $\Theta$ |
| ![Diagram](attachment:diagram4.png) | $[3^{[3], [3]}]$ | $PP_3$ | $3 \Lambda \left( \frac{\pi}{3} \right)$ | $\Theta$ |
| ![Diagram](attachment:diagram5.png) | $[3, 3^{[3]}]$ | $P_3$ | $\frac{1}{2} \Lambda \left( \frac{\pi}{3} \right)$ | $\Theta$ |
| ![Diagram](attachment:diagram6.png) | $[6, 3, 6]$ | $Z_3$ | $\frac{3}{4} \Lambda \left( \frac{\pi}{3} \right)$ | $\Theta$ |
| ![Diagram](attachment:diagram7.png) | $[4, 3, 6]$ | $BV_3$ | $\frac{1}{10} \Lambda \left( \frac{\pi}{3} \right)$ | $\rho = \frac{2}{5 \sqrt{3}} \Lambda \left( \frac{\pi}{3} \right)$ |
| ![Diagram](attachment:diagram8.png) | $[4, 3^{[3]}]$ | $BP_3$ | $\frac{5}{10} \Lambda \left( \frac{\pi}{3} \right)$ | $\rho \approx 0.682620$ |
| ![Diagram](attachment:diagram9.png) | $[4, 3^{[3], [1], [1]}]$ | $DV_3$ | $\frac{5}{20} \Lambda \left( \frac{\pi}{3} \right)$ | $\Theta$ |
| ![Diagram](attachment:diagram10.png) | $[3^{[3]}] \times [1]$ | $DP_3$ | $\frac{5}{20} \Lambda \left( \frac{\pi}{3} \right)$ | $\Theta$ |
| ![Diagram](attachment:diagram11.png) | $[3^{[3], [3]}]$ | $\hat{V}_3$ | $\frac{5}{20} \Lambda \left( \frac{\pi}{3} \right)$ | $\rho$ |
| Commensurable to $[3, 4, 4]$ | | | | |
| ![Diagram](attachment:diagram12.png) | $[3, 4, 4]$ | $\overline{R}_3$ | $\frac{1}{4} \Lambda \left( \frac{\pi}{3} \right)$ | $\sigma = \frac{3}{4G}$ |
| ![Diagram](attachment:diagram13.png) | $[3, 4^{[1], [1]}]$ | $\overline{O}_3$ | $\frac{1}{4} \Lambda \left( \frac{\pi}{3} \right)$ | $\sigma \approx 0.818808$ |
| ![Diagram](attachment:diagram14.png) | $[3^{[2], [4]}]$ | $\overline{BR}_3$ | $\frac{3}{8} \Lambda \left( \frac{\pi}{3} \right)$ | $\sigma$ |
| ![Diagram](attachment:diagram15.png) | $[4, 4, 4]$ | $N_3$ | $\frac{1}{2} \Lambda \left( \frac{\pi}{3} \right)$ | $\sigma$ |
| ![Diagram](attachment:diagram16.png) | $[4^{[1], [1], [1]}]$ | $\overline{M}_3$ | $\Lambda \left( \frac{\pi}{3} \right)$ | $\sigma$ |
| ![Diagram](attachment:diagram17.png) | $[4^{[4]}]$ | $\overline{RR}_3$ | $2 \Lambda \left( \frac{\pi}{3} \right)$ | $\sigma$ |
| Nonarithmetic | | | | |
| Commensurable to $[5, 3, 6]$ | | | | |
| ![Diagram](attachment:diagram18.png) | $[5, 3, 6]$ | $HV_3$ | $0.17150 \ldots$ | $0.550841 \ldots$ |
| ![Diagram](attachment:diagram19.png) | $[5, 3^{[3]}]$ | $HP_3$ | $0.34300 \ldots$ | $0.550841 \ldots$ |
| Other Nonarithmetic | | | | |
| ![Diagram](attachment:diagram20.png) | $[(3^{[3], [6]}]$ | $\overline{AV}_3$ | $0.364107 \ldots$ | $0.838825 \ldots$ |
| ![Diagram](attachment:diagram21.png) | $[(3, 4, 3, 6)]$ | $\overline{BV}_3$ | $0.525840 \ldots$ | $0.747914 \ldots$ |
| ![Diagram](attachment:diagram22.png) | $[(3, 5, 3, 6)]$ | $\overline{HV}_3$ | $0.672985 \ldots$ | $0.655381 \ldots$ |
| ![Diagram](attachment:diagram23.png) | $[(3, 4^{[3]}]$ | $\overline{CR}_3$ | $0.556282 \ldots$ | $0.767195 \ldots$ |

The 23 asymptotic Coxeter Simplices in $\mathbb{H}^3$ with optimal packing densities, $\Lambda$ is the Lobachevsky function and $G$ is Catalan’s constant.
5.1. **Commensurability Class of** [3, 3, 6]. The eleven groups in the commensurability class include the symmetries of the totally asymptotic hyperbolic tetrahedron and cube. We express the optimal packing densities in terms of the Lobachevsky function.

**Theorem 3.** The optimal horoball packing density of Coxeter simplex tilings $\mathcal{T}_\Gamma$, $\Gamma \in \{V_3, P_3, BV_3, BP_3, VV_3, PP_3, PV_3, DV_3, DP_3\}$ is $\delta_{opt}(\Gamma) = \frac{1}{2\sqrt{3}\Lambda(\frac{\pi}{3})} \approx 0.853276$.

The optimal horoball packing density of Coxeter simplex tilings $\mathcal{T}_\Gamma$, $\Gamma \in \{BV_3, BP_3, VV_3\}$ is $\delta_{opt}(\Gamma) = \frac{2}{5\sqrt{3}\Lambda(\frac{\pi}{3})} \approx 0.682620$.

**Proof.** Consider four cases based on the number of ideal vertices. The data is summarized in Tables 2-4.

(1) Coxeter simplices $\mathcal{F}_\Gamma$ with $\Gamma \in \{V_3, P_3, BV_3, BP_3\}$ have a single ideal vertex (see Fig. 1). The local optimal packing densities follow from Lemma 1 and extend to $H^3$ by Lemma 2. Coordinates for $\{A_i\}$, forms of hyperplanes $\{u_i\}$ opposite each $A_i$, horoball parameter $s$ for optimal horoballs, and intersection point coordinates are given in Tables 2-3.
(2) Coxeter simplices $\mathcal{F}_\Gamma$ with $\Gamma \in \{ T_3, Z_4, D_{7,3}, D_{5,3}, \hat{V}V_3 \}$ have two ideal vertices. We defer the details of this case to Theorem 6 that considers the nonarithmetic cases, the data for the computations is given in Table 2. See [14], §3.2.4 or [15, §3.2.4] for early versions of the argument for cases $\hat{V}V_3$ (denoted $\mathcal{O}_{(3,6,3)}$) and $D_{7,3}$.

(3) Case $\Gamma = \hat{V}P_3$ has three ideal vertices. Follow the method of [16, §3.2.2–3.2.3], the data for the computation is given in Table 2.

(4) Case $\Gamma = \hat{P}P_3$ is the ideal regular simplex and is a main result of [14, §4.2].

□

In addition cf. [15, §3.2.4] or [15, §3.2.5] describing techniques for domain doubling cases of fundamental domains. Fig. 2 describes the optimal packing structures with respect to the ratio of the volume of each horoball in a fundamental simplex cell.

| Witt Symb. | $V_3$ | $\hat{V}V_3$ | $\hat{V}P_3$ |
|------------|-------|-------------|-------------|
| Vertices of Simplex |
| $A_0$ | $(1, 0, 0, 1)^*$ | $(1, 0, 0, 1)^*$ | $(1, 0, 0, 1)^*$ |
| $A_1$ | $(1, 0, 0, 0)$ | $(1, 0, 0, 0)$ | $(1, 0, 0, 0)$ |
| $A_2$ | $(1, 1, 0, 0)$ | $(1, 1, 0, 0)$ | $(1, \sqrt{3}, -1/2, 0)^*$ |
| $A_3$ | $(1, 1, \sqrt{3}, 0)$ | $(1, 1, \sqrt{3}, 0)$ | $(1, \sqrt{3}, 1, 0)^*$ |
| The form $u_i$ of sides opposite $A_i$ |
| $u_0$ | $(0, 0, 0, 1)$ | $(0, 0, 0, 1)$ | $(0, 0, 0, 1)$ |
| $u_1$ | $(1, -2, 0, -1)$ | $(1, -2, 0, -1)$ | $(1, -2\sqrt{3}, 0, -1)$ |
| $u_2$ | $(0, -\sqrt{3}, 1, 0)$ | $(0, -\sqrt{3}, 1, 0)$ | $(0, -\sqrt{3}, 1, 0)$ |
| $u_3$ | $(0, 0, 1, 0)$ | $(0, 0, 1, 0)$ | $(0, \sqrt{3}, 1, 0)$ |
| Maximal horoball-type parameter $s_i$ for horoball $B_i$ at $A_i$ |
| $s_0$ | 0 | 0 | 0 |
| $s_1$ | $1/2$ | $1/2$ | $1/2$ |
| $s_2$ | $1/2$ | $1/2$ | $1/2$ |
| Horoball Parameters |
| $B_0 \rightarrow$ | $(0, 0, 1)$ | $(0, 0, 1)$ | $(0, 0, 1)$ |
| $B_1 \rightarrow$ | $(1, 1, 1, 1)$ | $(1, 1, 1, 1)$ | $(1, 1, 1, 1)$ |
| $B_2 \rightarrow$ | $(1, 1, 1, 1)$ | $(1, 1, 1, 1)$ | $(1, 1, 1, 1)$ |
| Packing Ratios w.r.t. $\delta_{opt}$ |
| $B_0 \rightarrow$ | $\hat{O}$ | $(1/2, 1/2)\hat{O}$ | $(1/2, 1/2)\hat{O}$ |
| $B_1 \rightarrow$ | $\hat{O}$ | $(1/2, 1/2)\hat{O}$ | $(1/2, 1/2)\hat{O}$ |
| $B_2 \rightarrow$ | $\hat{O}$ | $(1/2, 1/2)\hat{O}$ | $(1/2, 1/2)\hat{O}$ |
| Optimal Horoball Packing Density |
| $\delta_{opt}$ | $\Theta$ | $\Theta$ | $\Theta$ |

**Table 2.** Data for multiply asymptotic Coxeter simplex tilings in the Cayley-Klein ball model of radius 1 centered at $(1, 0, 0, 0)$. Vertices marked with * are ideal.
Coxeter Simplex Tilings

| Witt Symb. | $P_3$ | $BV_3$ | $BP_3$ |
|------------|-------|--------|--------|
| $A_0$      | $(1, 0, 0, 1)^*$ | $(1, 0, 0, 1)^*$ | $(1, 0, 0, 1)^*$ |
| $A_1$      | $(1, 0, 0, 0)$  | $(1, 0, 0, 0)$  | $(1, 0, 0, 0)$  |
| $A_2$      | $(1, \frac{1}{2}, -\frac{\sqrt{3}}{2}, 0)$ | $(1, \frac{\sqrt{3}}{2}, 0, 0)$ | $(1, \frac{\sqrt{3}}{2}, -\frac{\sqrt{3}}{2}, 0)$ |
| $A_3$      | $(1, \frac{1}{2}, \frac{\sqrt{3}}{2}, 0)$  | $(1, \frac{\sqrt{3}}{2}, \frac{\sqrt{3}}{2}, 0)$  | $(1, \frac{\sqrt{3}}{2}, -\frac{\sqrt{3}}{2}, 0)$  |

The form $u_i$ of sides opposite to $A_i$

| $u_0$      | $(0, 0, 0, -1)$  | $(0, 0, 0, 1)$  | $(0, 0, 0, 1)$  |
| $u_1$      | $(1, -2, 0, -1)$  | $(1, -\sqrt{2}, 0, -1)$  | $(1, -\sqrt{2}, 0, -1)$  |
| $u_2$      | $(0, -\frac{\sqrt{3}}{2}, 1, 0)$  | $(0, -\frac{\sqrt{3}}{2}, 1, 0)$  | $(0, -\frac{\sqrt{3}}{2}, 1, 0)$  |
| $u_3$      | $(0, \frac{\sqrt{3}}{2}, 1, 0)$  | $(0, 0, 1, 0)$  | $(0, 0, 1, 0)$  |

Maximal horoball parameter $s_0$

| $s_0$ | 0 | 0 | 0 |

Intersections $H_i = B(A_0, s_0) \cap A_i A_i$ of horoballs with simplex edges

| $H_1$  | $(1, 0, 0, 0)$  | $(1, 0, 0, 0)$  | $(1, 0, 0, 0)$  |
| $H_2$  | $(1, \frac{1}{2}, -\frac{\sqrt{3}}{2}, \frac{1}{2})$ | $(1, \frac{\sqrt{3}}{2}, 0, \frac{1}{2})$ | $(1, \frac{\sqrt{3}}{2}, -\frac{1}{2} \sqrt{2}, \frac{1}{2})$ |
| $H_3$  | $(1, \frac{1}{2}, \frac{\sqrt{3}}{2}, \frac{1}{2})$ | $1, \frac{3}{4} \sqrt{2}, \frac{3}{4} \sqrt{2}, \frac{1}{4}$ | $(1, \frac{3}{4} \sqrt{2}, \frac{3}{4} \sqrt{2}, \frac{1}{4})$ |

Volume of maximal horoball piece

| $\text{vol}(B_0 \cap F)$ | $\frac{1}{8 \sqrt{3}}$ | $\frac{1}{3 \sqrt{3}}$ | $\frac{1}{4 \sqrt{3}}$ |

Optimal Packing Density

| $\delta_{\text{opt}}$ | $\Theta$ | $\rho$ | $\rho$ |

Table 3. Data for the simply asymptotic Coxeter simplex tilings in the projective Cayley–Klein ball model of radius 1 centered at (1,0,0,0), the * denotes an ideal vertex.
### Coxeter Simplex Tilings

#### Doubly Asymptotic Nonarithmetic

| Witt Symb. | $DV_3$ | $DP_3$ | $VV_3$ | $Z_3$ |
|------------|--------|--------|--------|-------|
| Vertices of Simplex |
| $A_0$ | $(1, 0, 0, 1)^*$ | $(1, 0, 0, 1)^*$ | $(1, 0, 0, 1)^*$ | $(1, 0, 0, 1)^*$ |
| $A_1$ | $(1, 0, 0, -1)^*$ | $(1, 0, 0, -1)^*$ | $(1, 0, 0, -1)^*$ | $(1, 0, 0, -1)^*$ |
| $A_2$ | $(1, \sqrt{3}/6, 0, 0)$ | $(1, \sqrt{3}/6, \sqrt{3}/6, 0)$ | $(1, \sqrt{4\sqrt{3} - 6}, 0, 2 - \sqrt{3})$ | $(1, \sqrt{3}/3, -1/3, 1/3)$ |
| $A_3$ | $(1, \sqrt{3}/6, \sqrt{3}/6, 0)$ | $(1, \sqrt{3}/6, -\sqrt{3}/6, 0)$ | $(1, 0, \sqrt{4\sqrt{3} - 6}, \sqrt{3} - 2)$ | $(1, \sqrt{3}/3; 1/3, -1/3)$ |

### The form $u_i$ of sides opposite $A_i$

| $u_0$ | $(1, -\sqrt{3}/2, -\sqrt{3}/2, 1)$ | $(1, -\sqrt{2}, 0, 1)$ | $(1, -\sqrt{4}/3, -1/\sqrt{3}, 1)$ | $(1, -\sqrt{3}, 1, 1)$ |
| $u_1$ | $(1, -\sqrt{3}/2, \sqrt{3}/2, -1)$ | $(1, -\sqrt{2}, 0, -1)$ | $(1, -\sqrt{4}/3, -1/\sqrt{3}, -1)$ | $(1, -\sqrt{3}, -1, -1)$ |
| $u_2$ | $(0, -\sqrt{3}/3, 1, 0)$ | $(0, \sqrt{12}/6, 1, 0)$ | $(0, \sqrt{4}/3, 1, 0)$ | $(0, -\sqrt{3}, 1, 0)$ |
| $u_3$ | $(0, 0, 1, 0)$ | $(0, -\sqrt{12}/6, 1, 0)$ | $(0, -\sqrt{4}/3, 1, 0)$ | $(0, \sqrt{3}, 1, 0)$ |

### Maximal horoball-type parameter $s_i$ for horoball $B_i$ at $A_i$

| Maximal horoball-type parameter $s_i$ for horoball $B_i$ at $A_i$ |
|----------------------|
| $s_0 \Rightarrow s_1$ | $-1 \Rightarrow -\frac{1}{3}$ | $-\frac{1}{3} \Rightarrow -\frac{2}{3}$ | $-2 + \sqrt{3} \Rightarrow 2 - \sqrt{3}$ | $0 \Rightarrow 0$ |
| $s_1 \Rightarrow s_0$ | $-\frac{1}{3} \Rightarrow -\frac{1}{3}$ | $-\frac{1}{3} \Rightarrow -\frac{2}{3}$ | $-2 + \sqrt{3} \Rightarrow 2 - \sqrt{3}$ | $0 \Rightarrow 0$ |

### Volumes of optimal horoball pieces $V_i = vol(B_i \cap F_\Gamma)$

| Volumes of optimal horoball pieces $V_i = vol(B_i \cap F_\Gamma)$ |
|----------------------|
| $V_{\max} B_0 \Rightarrow V_{B_1}$ | $\frac{1}{4\sqrt{3}} \Rightarrow \frac{1}{16\sqrt{3}}$ | $\frac{1}{2\sqrt{3}} \Rightarrow \frac{1}{8\sqrt{3}}$ | $\frac{\sqrt{3}}{4} \Rightarrow \frac{1}{4\sqrt{3}}$ | $\frac{\sqrt{3}}{16} \Rightarrow \frac{\sqrt{3}}{16}$ |
| $V_{B_0} \Leftarrow V_{\max} B_1$ | $\frac{1}{4\sqrt{3}} \Leftarrow \frac{1}{16\sqrt{3}}$ | $\frac{1}{2\sqrt{3}} \Leftarrow \frac{1}{8\sqrt{3}}$ | $\frac{\sqrt{3}}{4} \Leftarrow \frac{1}{4\sqrt{3}}$ | $\frac{\sqrt{3}}{16} \Leftarrow \frac{\sqrt{3}}{16}$ |

### Densities of horoball pieces $\delta_i = vol(B_i \cap F_\Gamma)$

| Densities of horoball pieces $\delta_i = vol(B_i \cap F_\Gamma)$ |
|----------------------|
| $(\delta_{\max} s_0, \delta s_1)$ | $(\frac{4}{3}, \frac{1}{3})\delta_{opt}$ | $(\frac{4}{3}, \frac{1}{3})\delta_{opt}$ | $(\frac{4}{3}, \frac{1}{3})\delta_{opt}$ | $(\frac{4}{3}, \frac{1}{3})\delta_{opt}$ |
| $(\delta_{s_0}, \delta_{\max} s_1)$ | $(\frac{4}{3}, \frac{1}{3})\delta_{opt}$ | $(\frac{4}{3}, \frac{1}{3})\delta_{opt}$ | $(\frac{4}{3}, \frac{1}{3})\delta_{opt}$ | $(\frac{4}{3}, \frac{1}{3})\delta_{opt}$ |

### Optimal Horoball Packing Density

| Optimal Horoball Packing Density |
|----------------------|
| $\delta_{opt}$ | $\Theta$ | $\Theta$ | $\rho$ | $\Theta$ |

---

Table 4. Data for doubly asymptotic Coxeter simplex tilings in the Cayley-Klein ball model of radius 1 centered at $(1, 0, 0, 0)$. Vertices marked with * are ideal.
5.2. Commensurability Class of $[3, 4, 4]$. This commensurability class contains the symmetries of the hyperbolic ideal regular octahedron, horoball packings of which we extensively studied in [14, §4.3]. In this paper, the optimal packing densities are expressed in terms of Catalan’s constant $G = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^2}$, equal to a quarter of the volume of the ideal hyperbolic octahedron.

**Theorem 4.** The optimal horoball packing density of Coxeter simplex tilings $T_\Gamma$, $\Gamma \in \{R_3, O_3, BR_3, N_3, M_3, RR_3\}$ is $\delta_{opt}(\Gamma) = \frac{3}{4}G \approx 0.818808$.

**Proof.** Follow methods as outlined in Theorem 3. The data is summarized in Tables 5 and 6. Note that $N_3, M_3$, and $RR_3$ which have more than a single ideal vertex form a domain doubling sequence [15].

In addition cf. [14, §4.3] for earlier partial results. Fig. 3 describes the optimal packing structures with respect to the ratio of the volume of each horoball in a fundamental simplex cell.
5.3. Nonarithmetic Cases. There are six nonarithmetic asymptotic Coxeter simplices in five commensurability classes, see Table I.
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Optimal horoball packing density

\( \frac{\phi}{\pi} \) at \( \hat{\Gamma} \).

Table 6. Data for multiply asymptotic Coxeter simplex tilings in the Cayley-Klein ball model of radius 1 centered at \((1, 0, 0, 0)\). Vertices marked with * are ideal.

5.3.1. The commensurability class of \([5, 3, 6]\). This commensurability class contains symmetries of the asymptotic hyperbolic dodecahedron, cf. [14 §5]. Both Coxeter simples in this commensurability class have a single ideal vertex, see Table 7. Their volumes are given in terms of the Lobachevsky function orthoscheme decompositions following [9]. We have \( \text{vol}(\hat{HV}_3) = \frac{1}{4} \Lambda(\frac{\pi}{4}) + \frac{1}{4} \Lambda(\frac{3\pi}{4}) \) and \( \text{vol}(\hat{HP}_3) = 2 \cdot \text{vol}(\hat{HV}_3) \).

Theorem 5. The optimal horoball packing density of Coxeter simplex tilings \( \hat{\Gamma}, \Gamma \in \{\hat{HV}_3, \hat{HP}_3\} \) is \( \delta_{\text{opt}}(\Gamma) \approx 0.550841 \).

Proof. Both Coxeter simples \( \hat{F}_\Gamma \) in \( \Gamma \in \{\hat{HV}_3, \hat{HP}_3\} \) have a single ideal vertex. The local optimal packing densities follow from Lemma 1 and extend to the entire space by Lemma 2. Coordinates for vertices \( \{A_i\} \), forms of hyperplanes \( \{u_i\} \) opposite each \( A_i \), optimal horoball parameters \( s \), and horoball intersection points, and a closed form of volume of the horoball intersection pieces with the \( \hat{F}_\Gamma \) are summarized in Table 7. \( \square \)

5.3.2. Commensurability classes of single simplices. The nonarithmetic coxeter simplices with cyclic diagrams can be dissected into orthoschemes, and their volume is then computed using volume formulas for orthoschemes [9]. The volume decompositions are given below, where \( \varphi = \frac{1 + \sqrt{5}}{2} \) is the golden ratio.

\[
\text{vol}(\hat{AV}_3) = \text{vol}([3, 3, 6]) + \text{vol}([3, 4, 4]) + \text{vol}([4, 4, 3]) + \text{vol}([3, 3, 3])
\]
The optimal horoball packing densities of Coxeter simplex tilings

| Coxeter Simplex Tilings | $HV_3$ | $HP_5$ |
|-------------------------|--------|--------|
| Vertices of Simplex     |        |        |
| $A_0$                   | $(1,0,0,1)^*$ | $(1,0,0,1)^*$ |
| $A_1$                   | $(1,0,0,0)$ | $(1,0,0,0)$ |
| $A_2$                   | $(1/2 (\sqrt{5} + 1), 0, 0)$ | $(1/2 (\sqrt{5} + 1), -\frac{1}{2}\sqrt{5 + 3}, 0)$ |
| $A_3$                   | $(1/2 (\sqrt{5} + 1), \frac{1}{2}\sqrt{5 + 3}, 0)$ | $(1/2 (\sqrt{5} + 1), \frac{1}{2}\sqrt{5 + 3}, 0)$ |
| Maximal horoball parameter $\delta_{opt}$ | $0.556841$ | $0.556841$ |

| Intersections $H_i = B(A_0, s_0) \cap A_0 A_i$ of horoballs with simplex edges |
|-------------------------|--------|
| $H_1$                   | $(1,0,0,0)$ |
| $H_2$                   | $(1/2 (9\sqrt{5} + 7), 0, 1/2 (4\sqrt{5} + 13))$ | $(1/2 (7\sqrt{5} + 5), -\frac{1}{2}\sqrt{5 + 10}, 1/2 (3\sqrt{5} + 10))$ |
| $H_3$                   | $(1/2 (7\sqrt{5} + 5), 1/2 (4\sqrt{5} + 3\sqrt{3} + 3), 1/2 (3\sqrt{5} + 10))$ | $(1/2 (7\sqrt{5} + 5), 1/2 (4\sqrt{5} + 3\sqrt{3} + 3), 1/2 (3\sqrt{5} + 10))$ |

| Volume of maximal horoball piece | $\frac{1}{12} (3\sqrt{5} + 7)$ | $\frac{1}{12} (3\sqrt{5} + 7)$ |

Table 7. Data for the simply asymptotic Coxeter simplex tilings in the projective Cayley-Klein ball model of radius 1 centered at $(1,0,0,0)$, the $^*$ denotes an ideal vertex.

\[ (16) \quad \text{vol}(\hat{B}V_3) = \text{vol}([4, 3, 6]) + \text{vol} \left( [4, \arctan \sqrt{2}, \arccot \sqrt{2}] \right) + \text{vol} \left( [\arccot \frac{1}{\sqrt{2}}, \frac{\pi}{2} - \arctan \sqrt{2}, \frac{\pi}{3}] \right) + \text{vol}([3, 6, 3]) \]

\[ (17) \quad \text{vol}(\hat{H}V_3) = \text{vol}([5, 3, 6]) + \text{vol} \left( \left[ \frac{\pi}{5}, \arctan \varphi, \arccot \varphi \right] \right) \]

\[ + \text{vol} \left( [\arccot \varphi^{-1}, \frac{\pi}{2} - \arctan \varphi, \frac{\pi}{3}] \right) + \text{vol}([3, 6, 3]) \]

\[ (18) \quad \text{vol}(\hat{C}R_3) = \text{vol}([3, 4, 4]) + \text{vol}([4, 4, 4]) \]

\[ + \text{vol} \left( \left[ \frac{\pi}{3}, \arctan \frac{1}{\sqrt{2}}, \arccot \frac{1}{\sqrt{2}} \right] \right) \]

\[ + \text{vol} \left( [\arccot \sqrt{2}, \frac{\pi}{2} - \arctan \frac{1}{\sqrt{2}}, \frac{\pi}{4}] \right) \]

For the numerical values of the above volumes see Table 11

**Theorem 6.** The optimal horoball packing densities of Coxeter simplex tilings $\mathcal{T}_{A\hat{V}_3}$, $\mathcal{T}_{B\hat{V}_3}$, $\mathcal{T}_{H\hat{V}_3}$, and $\mathcal{T}_{C\hat{R}_3}$ are respectively $\delta_{opt}(\hat{A}V_3) = 0.838825$, $\delta_{opt}(\hat{B}V_3) = 0.747914$, $\delta_{opt}(\hat{H}V_3) = 0.655381$, and $\delta_{opt}(\hat{C}R_3) = 0.767195$. 
Proof. Each nonarithmetic simplex has two ideal vertices, see Table 8 for the data of the optimal packings. All cases follow as case $\Gamma = \hat{AV}_3$ given here. $\mathcal{F}_{\hat{AV}_3}$ has two ideal vertices $A_0$ and $A_1$, see Table 8. Let $B_0(\text{arctanh } s_0)$ and $B_1(\text{arctanh } s_1)$ denote horoballs with parameters $s_0$ and $s_1$ centered at $A_0$ and $A_1$. The equation for horosphere $\partial B_1$, is obtained by a rotation of $A_1$ to $A_0$ by $\text{Rot}_{A_1A_0} \in \text{PGL}(4, \mathbb{R})$, in coordinates

$$\text{Rot}_{A_1A_0} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}.$$  

Let $x_i = \text{arctanh } s_i = \beta(S_i, O, A_i)$ denote the hyperbolic distance of center of the model $A_1 = (1, 0, \ldots, 0)$ to $S_i = (1, 0, \ldots, 0, s_i)$ for $i \in \{0, 1\}$, rotated in the case of $A_1$. If horoball $B_0$ is maximal $s_0 = 0$. If horoball $B_1$ is maximal then $s_1 = \frac{1}{17} \left( 3 - 4\sqrt{3} \right)$. These two maximal horoballs $B_0(\text{arctanh } 0)$ and $B_1(\text{arctanh } \frac{1}{17} \left( 3 - 4\sqrt{3} \right))$ are tangent to hyperfaces $[u_0]$ and $[u_1]$ respectively, and to each other at $H_1$. By two invocations of Lemma 1 and then Lemma 2 the optimal backing packing density is

$$
\delta_{\text{opt}}(\Gamma) = \frac{1}{16\sqrt{3}} + \frac{1}{27} \left( 2\sqrt{3} + 3 \right) \approx 0.838825.
$$

Lemma 3 implies that this value is indeed optimal. 

$\square$
## Coxeter Simplex Tilings

### Doubly Asymptotic Nonarithmetic

| Win Symb. | Coxeter Simplex Tilings | | BV₁ | BV₂ |
|---|---|---|---|---|
| A₀ | (1.0, 0, 1)^* | (1.0, 1.0)^* | (1.0, 1.0)^* | (1.0, 1.0)^* |
| A₁ | (1.0, -1, 0)^* | (1.0, -1, 0)^* | (1.0, -1, 0)^* | (1.0, -1, 0)^* |
| A₂ | (1.0, √3, 0) | (1.0, √3, 0) | (1.0, √3, 0) | (1.0, √3, 0) |
| A₃ | (1.0, √3 + ½, √3 + ½, 0) | (1.0, (√7 + 1), (√7 - 1), 0) | (1.0, (2√7 + 1), (2√7 - 1), 0) | (1.0, (2√7 + 1), (2√7 - 1), 0) |

### Densities of horoball pieces

| δ | BV₁ | BV₂ |
|---|---|---|
| δ₀₀ | 0.951455 | 0.839825 | 0.747914 | 0.655384 |

### The form uₘ of sides opposite Aₘ

| u₀ | (0, 0, 1) | (0, 0, 1) | (0, 0, 1) | (0, 0, 1) |
| u₁ | (1, -1, -√2, -√2) | (1, -1, -√2, -√2) | (1, -1, -√2, -√2) | (1, -1, -√2, -√2) |
| u₂ | (1, -1, -1, -1) | (1, -1, -1, -1) | (1, -1, -1, -1) | (1, -1, -1, -1) |
| u₃ | (1, 0, 1, 0, 0) | (1, 0, 1, 0, 0) | (1, 0, 1, 0, 0) | (1, 0, 1, 0, 0) |

### Maximal horoball-type parameter sₘ for horoball Bₘ, at Aₘ

| max s₀ | s₀ = 0 =⇒ s₁ = 0.5 |
| max s₁ | s₁ = (15 - 6√5)/2 =⇒ s₀ = (15 - 6√5)/2 |
| max s₂ | s₂ = (15 - 6√5)/4 =⇒ s₁ = (15 - 6√5)/4 |
| max s₃ | s₃ = (15 - 6√5)/8 =⇒ s₂ = (15 - 6√5)/8 |

### Volumes of optimal horoball pieces V₁ = vol(B₁ ∩ F₁)

| V₁ | V₂ | V₃ |
|---|---|---|
| (2√3 + 3) | (2√3 + 3) | (2√3 + 3) |
| (2√3 + 3) | (2√3 + 3) | (2√3 + 3) |
| (2√3 + 3) | (2√3 + 3) | (2√3 + 3) |
| (2√3 + 3) | (2√3 + 3) | (2√3 + 3) |

### Densities of horoball pieces δ = vol(B₁ ∩ F₁)

| δ₁₂ | 0.853553, 0.146447 | 0.881854, 0.118146 | 0.908249, 0.091751 |
| δ₃₂ | 0.853553, 0.146447 | 0.881854, 0.118146 | 0.908249, 0.091751 |

### Optimal Horoball Packing Density

| δopt | 0.807195 | 0.839825 | 0.747914 | 0.655384 |

### Table 8

Data nonarithmetic Coxeter simplex tilings with two ideal vertices in the Cayley-Klein ball model of radius 1 centered at (1, 0, 0, 0). Vertices marked with * are ideal.
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