

SPHERE PACKING BOUNDS VIA SPHERICAL CODES

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ABSTRACT. The sphere packing problem asks for the greatest density of a packing of congruent balls in Euclidean space. The current best upper bound in all sufficiently high dimensions is due to Kabatiansky and Levenshtein in 1978. We revisit their argument and improve their bound by a constant factor using a simple geometric argument, and we extend the argument to packings in hyperbolic space, for which it gives an exponential improvement over the previously known bounds. Additionally, we show that the Cohn-Elkies linear programming bound is always at least as strong as the Kabatiansky-Levenshtein bound; this result is analogous to Rodemich's theorem in coding theory. Finally, we develop hyperbolic linear programming bounds and prove the analogue of Rodemich's theorem there as well.

1. INTRODUCTION

What is the densest arrangement of non-overlapping, congruent balls in \mathbb{R}^n ? This problem has a long history and has been extensively studied [CS99], and it has strong connections with physics and information theory [C10]. With the proof of Kepler's conjecture by Hales [H05], the sphere packing problem has been solved in up to three dimensions, but no proof of optimality is known in any higher dimension, and there are only a few dozen cases in which there are even plausible conjectures for the densest packing. In \mathbb{R}^8 and \mathbb{R}^{24} there are upper bounds that are remarkably close to the densities of the E_8 and Leech lattices, respectively; for example, Cohn and Kumar [CK04, CK09] came within a factor of $1 + 10^{-14}$ of the density of E_8 and a factor of $1 + 1.65 \cdot 10^{-30}$ of the density of the Leech lattice. However, in most dimensions we must be content with much cruder bounds. In this paper, we will slightly improve the best upper bounds known in high dimensions, show how to obtain them via linear programming bounds, and extend them to hyperbolic space.

The *density* of a sphere packing in \mathbb{R}^n is the fraction of space covered by the balls in the packing. More precisely, let $B_R^n(x)$ denote the ball of radius R centered at x ; then the density of a packing is the limit as $R \rightarrow \infty$ of the fraction of $B_R^n(x)$ covered by the packing (the limit is independent of x if it exists). Of course this limit need not exist, but one can replace it with the *upper density* defined with a limit superior, and one can show that the least upper bound of the upper densities of all sphere packings in \mathbb{R}^n is actually achieved as the density of a packing (see [G63]). Let $\Delta_{\mathbb{R}^n}$ denote this maximal packing density.

A *spherical code* in dimension n with minimum angle θ is a set of points on the unit sphere in \mathbb{R}^n with the property that no two points subtend an angle less than θ at the origin. In other words, $\langle x, y \rangle \leq \cos \theta$ for all pairs of distinct points x, y in the spherical code. Let $A(n, \theta)$ denote the greatest size of such a spherical code.

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In this paper, we consider the problem of finding upper bounds for packing density. Linear programming bounds have proven to be a powerful tool. This technique was first developed by Delsarte [D72] in the setting of error-correcting codes, and his method can be extended to many other settings. In particular, Delsarte, Goethals, and Seidel [DGS77] and Kabatiansky and Levenshtein [KL78] independently formulated a linear program for proving upper bounds on $A(n, \theta)$. Using this approach, Kabatiansky and Levenshtein found excellent upper bounds on $A(n, \theta)$ for large n , and they then applied a geometric argument to deduce a bound on $\Delta_{\mathbb{R}^n}$. Their upper bound is currently the best bound known for $n \geq 115$ (see Appendix A). It has the asymptotic form

$$(1.1) \quad \Delta_{\mathbb{R}^n} \leq 2^{-(0.5990\dots+o(1))n},$$

while the best lower bound known remains $2^{-(1+o(1))n}$ despite recent improvements [V11, V13].

Cohn and Elkies [CE03] found a more direct approach to bounding sphere packing densities, with no need to consider spherical codes. Their technique set new records in every case with $n \geq 4$ for which the calculations were carried out; see Appendix A for more details, and see Theorem 1.4 in [LOV12] for subsequent improvements when $n = 4, 5, 6, 7$, and 9 . However, despite the evidence from low dimensions, the asymptotic behavior of the Cohn-Elkies bound is far from obvious and it has been unclear whether it improves on, or even matches, the Kabatiansky-Levenshtein bound asymptotically. Until this paper, it was only known how to use the Cohn-Elkies linear program to match the “second-best bound” by Levenshtein [L79] (see Section 6 of [CE03]).

The purpose of this paper is fourfold. In Section 2 we improve the Kabatiansky-Levenshtein bound by a constant factor by giving a simple modification of their geometric argument relating spherical codes to sphere packings. (This does not change the exponential decay rate in bound (1.1)). In Section 3 we show that in every dimension n , the Cohn-Elkies linear program can always match the Kabatiansky-Levenshtein approach. This further demonstrates the power of the linear programming bound for sphere packing. In Section 4 we prove an analogue of the Kabatiansky-Levenshtein bound in hyperbolic space. The resulting bound behaves the same as (1.1) asymptotically, and it is exponentially better than the best bound previously known in hyperbolic space. Finally, in Section 5, we develop the theory of hyperbolic linear programming bounds (based partly on unpublished work of Cohn, Lurie, and Sarnak) and prove that they too subsume the Kabatiansky-Levenshtein approach.

2. GEOMETRIC ARGUMENT

In all sufficiently high dimensions, the best upper bound currently known for sphere packing density is given by Kabatiansky and Levenshtein [KL78] (see also Chapter 9 of [CS99] and Chapter 8 of [Z99]). They first obtain an upper bound on $A(n, \theta)$ using linear programming and then use the inequality

$$(2.1) \quad \Delta_{\mathbb{R}^n} \leq \sin^n(\theta/2)A(n+1, \theta).$$

The inequality was derived using a simple geometric argument. Here we improve it using an equally simple argument.

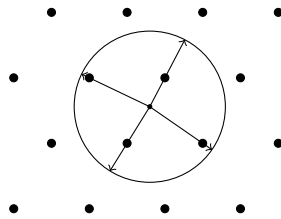


FIGURE 1. Proof of Proposition 2.1.

Proposition 2.1. *For all $n \geq 1$ and $\pi/3 \leq \theta \leq \pi$,*

$$(2.2) \quad \Delta_{\mathbb{R}^n} \leq \sin^n(\theta/2)A(n, \theta).$$

Since the unit sphere in \mathbb{R}^n can be embedded in the unit sphere in \mathbb{R}^{n+1} via a hyperplane through the origin, we always have $A(n, \theta) \leq A(n + 1, \theta)$, with strict inequality when $\theta \leq \pi/2$. The applications of (2.1) have $\pi/3 \leq \theta \leq \pi/2$, so Proposition 2.1 will be a strict (though small) improvement. Neither inequality is useful in low dimensions; for example, when $n = 2$ and $\theta = \pi/3$, Proposition 2.1 says that $\Delta_{\mathbb{R}^2} \leq 3/2$. However, these inequalities are valuable in high dimensions.

For the sake of comparison, let us first recall the proof of (2.1).

Proof of (2.1). Suppose we have a sphere packing in \mathbb{R}^n of density Δ using unit spheres. Consider a sphere S_R^n in \mathbb{R}^{n+1} of radius R (to be chosen later), and place the sphere packing in \mathbb{R}^n onto a hyperplane through the center of S_R^n , with the packing translated so that at least ΔR^n of the sphere centers are contained in S_R^n . This is always possible by an averaging argument: a randomly chosen translation will lead to an average of ΔR^n sphere centers in S_R^n . Project the sphere centers onto the upper hemisphere of S_R^n , orthogonally to the hyperplane. The projections of the sphere centers are still at least distance two apart, and thus separated by angles of at least θ , where $\sin(\theta/2) = 1/R$. Therefore, $\Delta R^n \leq A(n + 1, \theta)$, which is the bound that we wanted to prove, and we can achieve any angle by choosing R accordingly. \square

Our motivation for revisiting this argument is that it feels somewhat unnatural to lift to a higher dimension in the process. Our proposition shows that a stronger inequality can be obtained without going to a higher dimension. The proof is similar to the techniques of [HST10] and [BM07], but this application appears to be new.

Proof of Proposition 2.1. See Figure 1. Suppose we have a packing of unit spheres in \mathbb{R}^n with density Δ . Let S_R^{n-1} be a sphere in \mathbb{R}^n of radius $R \leq 2$ (to be chosen later), located so that it contains at least ΔR^n of the centers of the spheres in the packing but its center is not one of them. Such a location always exists, by the same averaging argument as above (a randomly chosen location will contain an average of ΔR^n sphere centers). Now, project the sphere centers from the packing onto the surface of S_R^{n-1} using rays starting from the center of S_R^{n-1} . It follows from the lemma below that the projections are separated by angles of at least θ , where $\sin(\theta/2) = 1/R$. Therefore, $\Delta R^n \leq A(n, \theta)$, as desired, and we can achieve any angle of $\pi/3$ or more using $R \leq 2$. \square

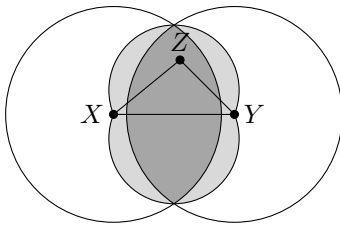


FIGURE 2. Pictorial proof of Lemma 2.2. The bounds $|XZ| \leq R$ and $|YZ| \leq R$ place Z in the dark gray region, which is the intersection of the two disks centered at X and Y with radius $R \leq 2$. The light gray region contains all points P with $\angle XPY \geq \theta$. Since the dark region is contained inside the light region, it follows that $\angle XZY \geq \theta$.

Note that the proof breaks down if $R > 2$, because two projected sphere centers can even coincide.

Lemma 2.2. *Suppose $R \leq 2$. If XYZ is a triangle with $|XY| \geq 2$, $|XZ| \leq R$, $|YZ| \leq R$, then $\angle XZY \geq \theta$, where $\sin(\theta/2) = 1/R$.*

Proof. See Figure 2 for a pictorial proof. For an algebraic proof, let $x = |XZ|$, $y = |YZ|$, $z = |XY|$, and $\gamma = \angle XZY$. By the law of cosines, $\cos \gamma = (x^2 + y^2 - z^2)/(2xy)$. By taking partial derivatives, we see that the expression $(x^2 + y^2 - z^2)/(2xy)$ is maximized in the domain $0 \leq x, y \leq R$ and $z \geq 2$ at $(x, y, z) = (R, R, 2)$. Therefore, $\cos \gamma \leq 1 - 2R^{-2} = 1 - 2\sin^2(\theta/2) = \cos \theta$. It follows that $\gamma \geq \theta$. \square

Inequalities (2.1) and (2.2) can be stated a little more naturally in terms of packing density on the sphere. A spherical code on S^{n-1} with minimal angle θ and size $A(n, \theta)$ corresponds to a packing with spherical caps of angular radius $\theta/2$ with density

$$(2.3) \quad A(n, \theta) \frac{\int_0^{\theta/2} \sin^{n-2} x \, dx}{\int_0^\pi \sin^{n-2} x \, dx}.$$

In other words, it covers this fraction of the sphere. Now if we let $\Delta_{S^{n-1}}(\theta)$ denote the optimal packing density, then (2.2) implies

$$(2.4) \quad \frac{1}{n} \log \Delta_{\mathbb{R}^n} \lesssim \frac{1}{n} \log \Delta_{S^{n-1}}(\theta),$$

where $f(n) \lesssim g(n)$ means $f(n) \leq h(n)$ for some function h with $h(n) \sim g(n)$ (i.e., $\lim_{n \rightarrow \infty} h(n)/g(n) = 1$). This simply amounts to verifying that

$$\frac{1}{n} \log \frac{\int_0^{\theta/2} \sin^{n-2} x \, dx}{\int_0^\pi \sin^{n-2} x \, dx} \sim \log \sin \frac{\theta}{2}$$

for fixed θ satisfying $0 < \theta \leq \pi$. Furthermore, it is known that

$$(2.5) \quad \frac{1}{n} \log \Delta_{S^{n-1}}(\theta) \lesssim \frac{1}{n+1} \log \Delta_{S^n}(\phi)$$

for $0 < \theta < \phi \leq \pi/2$ (see (17) in [L75]). Thus, the exponential rate of the packing density for spherical caps is weakly increasing as a function of angle, and Euclidean space naturally occurs as the zero angle limit.

The proof of the Kabatiansky-Levenshtein bound (1.1) on $\Delta_{\mathbb{R}^n}$ uses the following bound on $A(n, \theta)$ for $0 < \theta < \pi/2$, which is derived using the linear programming bound for spherical codes (see Theorem 4 in [KL78]):

$$(2.6) \quad \frac{1}{n} \log A(n, \theta) \lesssim \frac{1 + \sin \theta}{2 \sin \theta} \log \frac{1 + \sin \theta}{2 \sin \theta} - \frac{1 - \sin \theta}{2 \sin \theta} \log \frac{1 - \sin \theta}{2 \sin \theta}.$$

The bound (1.1) is then deduced by setting (2.6) into (2.1) and choosing θ to minimize the resulting bound,¹ which turns out to happen at $\theta = 1.0995\dots \approx 0.35\pi$. If we now apply our new inequality (2.2) in place of (2.1), then we obtain an improvement in the bound by a factor of $\mathcal{A}_{n+1}/\mathcal{A}_n$, where $\mathcal{A}_n = (1.2635\dots + o(1))^n$ is the Kabatiansky-Levenshtein bound on $A(n, 1.0995\dots)$. Thus, we obtain an improved sphere packing bound by a factor of 1.2635\dots on average, in the sense that the geometric mean of the improvement factors over all dimensions from 1 to N tends to 1.2635\dots as $N \rightarrow \infty$.

3. LINEAR PROGRAMMING BOUNDS

In [KL78] the upper bound on the maximum sphere packing density $\Delta_{\mathbb{R}^n}$ was derived by first giving an upper bound for the maximum size $A(n, \theta)$ of a spherical code using linear programming, and then using (2.1) to compare the two quantities. We refer to this method as the Kabatiansky-Levenshtein approach. Cohn and Elkies [CE03] took a more direct approach to bounding $\Delta_{\mathbb{R}^n}$, by setting up a different linear program. In this section, we show that the Cohn-Elkies linear program can always prove at least as strong a bound on $\Delta_{\mathbb{R}^n}$ as the Kabatiansky-Levenshtein approach.

This theorem is the continuous analogue of a theorem of Rodemich [R80] in coding theory (see Theorem 3.5 of [D94] for a proof of Rodemich's theorem, since Rodemich published only an abstract). Let $A(n, d)$ denote the maximum size of a binary error-correcting code of block length n and minimal Hamming distance d (i.e., a subset of $\{0, 1\}^n$ with every two elements differing in at least d positions), and let $A(n, d, w)$ denote the maximum size of such a code with constant weight w (i.e., every element of the subset has exactly w ones). The current best bounds on $A(n, d)$ and $A(n, d, w)$ for large n are by McEliece, Rodemich, Rumsey, and Welch [MRRW77], using linear programming bounds. As in the Kabatiansky-Levenshtein approach, some of the best bounds on $A(n, d)$ were obtained using bounds on $A(n, d, w)$ along with an analogue of Proposition 2.1 known as the Bassalygo-Elias inequality [B65]:

$$(3.1) \quad A(n, d) \leq \frac{2^n}{\binom{n}{w}} A(n, d, w).$$

¹Let us clarify a potentially confusing point. The fact that $\theta = 1.0995\dots$ minimizes the bound may, at first, seem to be at odds with (2.4) and (2.5), where we said that the exponential rate of the packing density $\Delta_{S^{n-1}}(\theta)$ is weakly increasing in θ . Both statements are correct. The bound in (2.6) is a preliminary bound on $A(n, \theta)$, which can be improved for θ less than the critical value 1.0995\dots by incorporating (2.5). This improvement yields the same bound on $\Delta_{\mathbb{R}^n}$ for all $\theta \leq 1.0995\dots$

The proof of (3.1) is by an easy averaging argument. In analogy with sphere packing, error-correcting codes play the role of sphere packings while constant weight codes play the role of spherical codes. Rodemich proved that any upper bound on $A(n, d)$ obtained using the linear programming bound for $A(n, d, w)$ combined with (3.1) can be obtained directly via the linear programming bound for $A(n, d)$. Theorem 3.4 below is the continuous analogue of Rodemich's theorem.

3.1. LP bounds for spherical codes. We begin by reviewing the linear programming bounds for spherical codes. We follow the approach of Kabatiansky and Levenshtein [KL78], based on their inequality on the mean.

Let S^{n-1} denote the unit sphere in \mathbb{R}^n . A function $f: [-1, 1] \rightarrow \mathbb{R}$ is *positive definite* if for all N and all $x_1, \dots, x_N \in S^{n-1}$, the matrix $(f(\langle x_i, x_j \rangle))_{1 \leq i, j \leq N}$ is positive semidefinite. (Note that this property depends on the choice of n ; when necessary for clarity, we will say such a function is *positive definite on S^{n-1}* .) Equivalently, for all $x_1, \dots, x_N \in S^{n-1}$ and $t_1, \dots, t_N \in \mathbb{R}$,

$$\sum_{1 \leq i, j \leq N} t_i t_j f(\langle x_i, x_j \rangle) \geq 0.$$

A result of Schoenberg [S42] characterizes continuous positive-definite functions as the nonnegative linear combinations of the Gegenbauer polynomials $C_k^{n/2-1}$ for $k = 0, 1, 2, \dots$. Recall that the polynomials C_k^α are orthogonal with respect to the measure $(1-t^2)^{\alpha-1/2} dt$ on $[-1, 1]$. When $\alpha = n/2 - 1$, this measure arises naturally (up to scaling) as the orthogonal projection of the surface measure from S^{n-1} onto a coordinate axis.

Given a positive-definite function g , define \bar{g} to be its average

$$\bar{g} = \frac{\int_{-1}^1 g(t) (1-t^2)^{(n-3)/2} dt}{\int_{-1}^1 (1-t^2)^{(n-3)/2} dt}$$

with respect to this measure. Equivalently, \bar{g} is the expectation of $g(\langle x, y \rangle)$ with x and y chosen independently and uniformly at random from S^{n-1} . If

$$g(t) = \sum_{k \geq 0} c_k C_k^{n/2-1}(t),$$

then $\bar{g} = c_0$.

Theorem 3.1 (Delsarte-Goethals-Seidel [DGS77], Kabatiansky-Levenshtein [KL78]). *If $g: [-1, 1] \rightarrow \mathbb{R}$ is continuous and positive definite on S^{n-1} , $g(t) \leq 0$ for all $t \in [-1, \cos \theta]$, and $\bar{g} > 0$, then*

$$A(n, \theta) \leq \frac{g(1)}{\bar{g}}.$$

Let $A^{\text{LP}}(n, \theta)$ denote the best upper bound on $A(n, \theta)$ that could be derived using Theorem 3.1. In other words, it is the infimum of $g(1)/\bar{g}$ over all valid auxiliary functions g .

We will give a proof of this theorem following the approach of [KL78], as preparation for giving a new proof of Theorem 3.3 below.

Proof. Let \mathcal{C} be any spherical code in S^{n-1} with minimal angle at least θ , let μ be the surface measure on S^{n-1} , normalized to have total measure 1, let δ_x be a delta

function at the point x , and let

$$\nu = \sum_{x \in \mathcal{C}} \delta_x + \lambda \mu,$$

where λ is a constant to be determined. We have

$$\iint g(\langle x, y \rangle) d\nu(x) d\nu(y) \geq 0,$$

because we can approximate the integral with a sum and use the positive definiteness of g . This inequality amounts to

$$\lambda^2 \bar{g} + 2\lambda |\mathcal{C}| \bar{g} + \sum_{x, y \in \mathcal{C}} g(\langle x, y \rangle) \geq 0.$$

Because $\langle x, y \rangle \leq \cos \theta$ for distinct points $x, y \in \mathcal{C}$ and $g(t) \leq 0$ for $t \in [-1, \cos \theta]$, we have

$$\sum_{x, y \in \mathcal{C}} g(\langle x, y \rangle) \leq \sum_{x \in \mathcal{C}} g(\langle x, x \rangle) = |\mathcal{C}| g(1).$$

Thus,

$$\lambda^2 \bar{g} + 2\lambda |\mathcal{C}| \bar{g} + |\mathcal{C}| g(1) \geq 0.$$

To derive the best bound on $|\mathcal{C}|$, we take $\lambda = -|\mathcal{C}|$. Then

$$0 \leq -|\mathcal{C}|^2 \bar{g} + |\mathcal{C}| g(1)$$

and hence

$$|\mathcal{C}| \leq \frac{g(1)}{\bar{g}},$$

as desired. \square

3.2. LP bounds in Euclidean space. The Kabatiansky-Levenshtein approach gives the following bound on $\Delta_{\mathbb{R}^n}$. The original version uses (2.1), but here we state the improved version using Proposition 2.1.

Corollary 3.2. *Suppose g satisfies the hypotheses of Theorem 3.1 with $\pi/3 \leq \theta \leq \pi$. Then*

$$\Delta_{\mathbb{R}^n} \leq \sin^n(\theta/2) \frac{g(1)}{\bar{g}}.$$

Let us recall the Cohn-Elkies linear programming bound. Given an integrable function $f: \mathbb{R}^n \rightarrow \mathbb{R}$, let \hat{f} denote its Fourier transform, normalized by

$$\hat{f}(t) = \int_{\mathbb{R}^n} f(x) e^{2\pi i \langle x, t \rangle} dt.$$

Let B_R^n denote the n -dimensional ball with radius R . The volume of the n -dimensional unit ball is $\text{vol}(B_1^n) = \pi^{n/2}/(n/2)!$, where $(n/2)! = \Gamma(n/2 + 1)$ for n odd.

Much like the case of spheres, a function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is *positive definite* if for all N and all $x_1, \dots, x_N \in \mathbb{R}^n$, the matrix $(f(x_i - x_j))_{1 \leq i, j \leq N}$ is positive semidefinite. A result of Bochner [B33] characterizes continuous positive-definite functions as the Fourier transforms of finite Borel measures. If f and \hat{f} are both integrable, then f is positive definite if and only if \hat{f} is nonnegative everywhere, by Fourier inversion and Bochner's theorem.

Theorem 3.3 (Cohn-Elkies [CE03]). *Suppose $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is continuous, positive definite, and integrable, $f(x) \leq 0$ for all $|x| \geq 2$, and $\widehat{f}(0) > 0$. Then*

$$\Delta_{\mathbb{R}^n} \leq \text{vol}(B_1^n) \frac{f(0)}{\widehat{f}(0)}.$$

The original version in [CE03] required suitable decay of f and \widehat{f} at infinity, and it was based on Poisson summation. These more restrictive hypotheses were removed in Section 9 of [CK07]. Here we give a more direct proof, although it has the disadvantage of not telling as much about what happens when equality holds as the Poisson summation proof does.

Proof. Without loss of generality, we can symmetrize to assume f is an even function (indeed, radially symmetric). This is not necessary for the proof, but it will simplify some of the expressions below.

Let \mathcal{P} be a packing with balls of radius 1, such that \mathcal{P} has density $\Delta_{\mathbb{R}^n}$. Given a radius $r > 0$, let S_r be the set of sphere centers from \mathcal{P} that lie within the ball of radius r about the origin, let V_r be the volume of that ball, and let $N_r = |S_r|$. Then

$$\lim_{r \rightarrow \infty} \text{vol}(B_1^n) \frac{N_r}{V_r} = \Delta_{\mathbb{R}^n}.$$

Let $R = r + \sqrt{r}$ (in fact, \sqrt{r} could be replaced with any function that tends to infinity but is $o(r)$). Consider the signed measure

$$\nu = \sum_{x \in S_r} \delta_x + \lambda \mu_R,$$

where δ_x is the delta function at x , μ_R is Lebesgue measure on the ball of radius R centered at the origin, and λ is a constant to be determined. As in the proof of Theorem 3.1,

$$\iint f(x-y) d\nu(x) d\nu(y) \geq 0,$$

because f is positive definite. Equivalently,

$$\lambda^2 \iint_{|x|, |y| \leq R} f(x-y) dx dy + 2\lambda \sum_{x \in S_r} \int_{|y| \leq R} f(x-y) dy + \sum_{x, y \in S_r} f(x-y) \geq 0.$$

Because $f(x-y) \leq 0$ whenever x and y are distinct points in the packing,

$$\lambda^2 \iint_{|x|, |y| \leq R} f(x-y) dx dy + 2\lambda \sum_{x \in S_r} \int_{|y| \leq R} f(x-y) dy + N_r f(0) \geq 0.$$

Assuming r is large enough that $N_r > 0$, we set $\lambda = -N_r/V_r$ and divide by N_r to obtain

$$\frac{N_r}{V_r} \cdot \frac{1}{V_r} \iint_{|x|, |y| \leq R} f(x-y) dx dy - 2 \cdot \frac{N_r}{V_r} \cdot \frac{1}{N_r} \sum_{x \in S_r} \int_{|y| \leq R} f(x-y) dy + f(0) \geq 0.$$

It is not hard to compute the limits

$$\lim_{r \rightarrow \infty} \frac{1}{V_r} \iint_{|x|, |y| \leq R} f(x-y) dx dy = \widehat{f}(0)$$

and

$$\lim_{r \rightarrow \infty} \frac{1}{N_r} \sum_{x \in S_r} \int_{|y| \leq R} f(x-y) dy = \widehat{f}(0).$$

Specifically, when $|x| \leq r$, the y -integral covers all values of $x - y$ up to radius $R - r = \sqrt{r}$. As $r \rightarrow \infty$ these y -integrals converge to $\widehat{f}(0)$, and all but a negligible fraction of the values of x satisfying $|x| \leq R$ also satisfy $|x| \leq r$.

Thus, in the limit as $r \rightarrow \infty$ we find that

$$\frac{\Delta_{\mathbb{R}^n}}{\text{vol}(B_1^n)} \widehat{f}(0) - 2 \frac{\Delta_{\mathbb{R}^n}}{\text{vol}(B_1^n)} \widehat{f}(0) + f(0) \geq 0,$$

which is equivalent to the desired inequality. \square

Let $\Delta_{\mathbb{R}^n}^{\text{LP}}$ denote the optimal upper bound on $\Delta_{\mathbb{R}^n}$ using Theorem 3.3. Recall that $A^{\text{LP}}(n, \theta)$ denotes the optimal upper bound on $A(n, \theta)$ obtained using Theorem 3.1. Our next result compares the LP bound on the sphere packing density $\Delta_{\mathbb{R}^n}$ obtained from Corollary 3.2 with the one from Theorem 3.3.

Theorem 3.4. *For $\pi/3 \leq \theta \leq \pi$ and positive integers n ,*

$$\Delta_{\mathbb{R}^n}^{\text{LP}} \leq \sin^n(\theta/2) A^{\text{LP}}(n, \theta).$$

To prove Theorem 3.4, we will show that for any upper bound on $\Delta_{\mathbb{R}^n}$ obtained using a function g in Corollary 3.2, we can always find a function f that gives a matching bound using Theorem 3.3. In other words,

$$\sin^n(\theta/2) \frac{g(1)}{\overline{g}} = \text{vol}(B_1^n) \frac{f(0)}{\widehat{f}(0)}.$$

We have a similar conclusion for the original Kabatiansky-Levenshtein bound using (2.1) without the $\theta \geq \pi/3$ assumption. See the remarks following the proof.

Proof of Theorem 3.4. Let g be any function satisfying the hypotheses of Theorem 3.1. The idea is to construct a function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ based on g mimicking the geometric argument in the proof of Proposition 2.1. Let $R = 1/\sin(\theta/2)$, as in that proof.

Consider the integral

$$\int_{B_R^n(x) \cap B_R^n(y)} g \left(\left\langle \frac{x-z}{|x-z|}, \frac{y-z}{|y-z|} \right\rangle \right) dz,$$

where $B_R^n(x)$ is the ball of radius R centered at x . Note that

$$\left\langle \frac{x-z}{|x-z|}, \frac{y-z}{|y-z|} \right\rangle = \cos \angle xzy,$$

where $\angle xzy$ denotes the angle at z formed by x and y . This angle is not defined if $x = z$ or $y = z$, but these cases occur with measure zero.

The integral depends only on $|x - y|$, so there is a radial function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ satisfying

$$f(x - y) = \int_{B_R^n(x) \cap B_R^n(y)} g \left(\left\langle \frac{x-z}{|x-z|}, \frac{y-z}{|y-z|} \right\rangle \right) dz.$$

We claim that f is positive definite. Indeed, let χ_R denote the characteristic function of $B_R^n(0)$. Then we can rewrite f as

$$f(x - y) = \int_{\mathbb{R}^n} \chi_R(x - z) \chi_R(y - z) g \left(\left\langle \frac{x-z}{|x-z|}, \frac{y-z}{|y-z|} \right\rangle \right) dz.$$

For any $x_1, \dots, x_N \in \mathbb{R}^n$ and $t_1, \dots, t_N \in \mathbb{R}$, we can expand

$$\sum_{1 \leq i, j \leq N} t_i t_j f(x_i - x_j)$$

as

$$\int_{\mathbb{R}^n} \sum_{1 \leq i, j \leq N} (t_i \chi_R(x_i - z))(t_j \chi_R(x_j - z)) g \left(\left\langle \frac{x_i - z}{|x_i - z|}, \frac{x_j - z}{|x_j - z|} \right\rangle \right) dz.$$

This expression is nonnegative, because g is positive definite on the unit sphere in \mathbb{R}^n and we can use $t_i \chi_R(x_i - z)$ as coefficients. This shows that f is positive definite on \mathbb{R}^n . It is also integrable, because it has compact support (it vanishes past radius $2R$).

If $|x - y| \geq 2$, then by Lemma 2.2,

$$\left\langle \frac{x - z}{|x - z|}, \frac{y - z}{|y - z|} \right\rangle \leq \cos \theta$$

for all $z \in B_R^n(x) \cap B_R^n(y) \setminus \{x, y\}$. Since $g(t) \leq 0$ for all $t \in [-1, \cos \theta]$ by hypothesis, it follows that $f(x - y) \leq 0$ whenever $|x - y| \geq 2$. Thus, we have verified that f satisfies all the hypotheses of Theorem 3.3 except $\widehat{f}(0) > 0$, which we will check shortly. We have $f(0) = \text{vol}(B_R^n)g(1)$ and

$$\begin{aligned} \widehat{f}(0) &= \int_{\mathbb{R}^n} f(x - 0) dx \\ &= \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \chi_R(x - z) \chi_R(-z) g \left(\left\langle \frac{x - z}{|x - z|}, \frac{-z}{|-z|} \right\rangle \right) dx dz \\ &= \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \chi_R(u) \chi_R(v) g \left(\left\langle \frac{u}{|u|}, \frac{v}{|v|} \right\rangle \right) du dv \\ &= \text{vol}(B_R^n)^2 \bar{g}. \end{aligned}$$

Therefore $\widehat{f}(0) > 0$ and

$$\text{vol}(B_1^n) \frac{f(0)}{\widehat{f}(0)} = \text{vol}(B_1^n) \frac{\text{vol}(B_R^n) g(1)}{\text{vol}(B_R^n)^2 \bar{g}} = \frac{1}{R^n} \frac{g(1)}{\bar{g}} = \sin^n(\theta/2) \frac{g(1)}{\bar{g}},$$

as desired. \square

When $\theta < \pi/3$ we can similarly match the Kabatiansky-Levenshtein bound obtained using (2.1) by adapting the above proof for the corresponding geometric argument. Let $\pi: B_1^n \rightarrow \{x \in S^n : x_{n+1} \geq 0\}$ denote the map that orthogonally projects the unit disk in the hyperplane $\mathbb{R}^n \times \{0\}$ in \mathbb{R}^{n+1} to the upper half of the unit sphere in \mathbb{R}^{n+1} . For any g in Theorem 3.1 that gives a bound for $A(n+1, \theta)$, let

$$f(x - y) = \int_{B_R^n(x) \cap B_R^n(y)} g \left(\left\langle \pi \left(\frac{x - z}{R} \right), \pi \left(\frac{y - z}{R} \right) \right\rangle \right) dz.$$

A similar argument shows that f is positive definite and $f(x) \leq 0$ whenever $|x| \geq 2$. We have $f(0) = \text{vol}(B_R^n)g(1)$ and $\widehat{f}(0) = \text{vol}(B_R^n)^2 \mathbb{E}[g(\langle \pi(u), \pi(v) \rangle)]$, where u and v are independent uniform random points in B_1^n . The inequality on the mean from [KL78] says that the average of a positive-definite kernel with respect to a

probability distribution on its inputs must be at least as large as that with respect to the uniform distribution. Thus, $\mathbb{E}[g(\langle \pi(u), \pi(v) \rangle)] \geq \bar{g}$ and

$$\text{vol}(B_1^n) \frac{f(0)}{\widehat{f}(0)} \leq \sin^n(\theta/2) \frac{g(1)}{\bar{g}}.$$

However, we cannot conclude that $\widehat{f}(0) = \text{vol}(B_R^n)^2 \bar{g}$, so the version of this argument in Theorem 3.4 is more elegant.

4. HYPERBOLIC SPHERE PACKING

Hyperbolic sphere packing is far more subtle than Euclidean sphere packing. In both hyperbolic and Euclidean spaces, one must deal with the infinite volume of space available. The Euclidean solution is fairly straightforward: restrict to a large but bounded region, and then let the size of this region tend to infinity. The boundary effects have negligible influence on the global density. However, these arguments become much trickier in hyperbolic space, since the exponential volume growth means the limiting behavior is dominated by what happens near the boundary. Troubling phenomena occur, such as packings that have different densities when one uses regions centered at different points. There are numerous other pathological examples (see, for example, Section 1 of [BR04]), and it is only recently that a widely accepted definition of density has been proposed by Bowen and Radin [BR03, BR04]. Before this definition, some density bounds were proved using Voronoi cell arguments that would apply to any reasonable definition of density, and indeed they apply to the Bowen-Radin definition (see Proposition 3 in [BR03]).

The best bound known is due to Böröczky [B78], who gave an upper bound for the fraction of each Voronoi cell that could be covered in a hyperbolic sphere packing. The bound depends on the radius of the spheres in the packing (the curvature of hyperbolic space sets a distance scale, so density is no longer scaling-invariant, as it is in Euclidean space). At least in sufficiently high dimensions, the Böröczky bound is an increasing function of radius [M99], so it is never better than the radius-zero limit. In that limit it degenerates to the Rogers bound [R58], which in dimension n is asymptotic to $2^{-n/2} \cdot n/e$ as $n \rightarrow \infty$.

Here, we improve the density bound to the Kabatiansky-Levenshtein bound, regardless of the radius. Let $\Delta_{\mathbb{H}^n}(r)$ denote the optimal packing density for balls of radius r in \mathbb{H}^n (we will define this density precisely in Section 4.1). We can bound the packing density of balls in hyperbolic space by the packing density of spherical caps on a sphere, as in the Euclidean setting discussed in Section 2. The next result is analogous to Proposition 2.1.

Theorem 4.1. *For all $n \geq 2$, $\pi/3 \leq \theta \leq \pi$, and $r > 0$, we have*

$$\Delta_{\mathbb{H}^n}(r) \leq \sin^{n-1}(\theta/2) A(n, \theta).$$

More precisely, one could replace $\sin^{n-1}(\theta/2)$ with the hyperbolic volume ratio $\text{vol}(B_r^n) / \text{vol}(B_R^n)$, where R is defined by $\sinh R = (\sinh r) / \sin(\theta/2)$. That would slightly improve the inequality without changing the proof, at the cost of making the statement more cumbersome.

As in the Euclidean case (2.4), this theorem implies that

$$(4.1) \quad \sup_{r>0} \frac{1}{n} \log \Delta_{\mathbb{H}^n}(r) \lesssim \frac{1}{n} \log \Delta_{S^{n-1}}(\theta).$$

By using the Kabatiansky-Levenshtein bound on $\Delta_{S^{n-1}}$, i.e., (2.6) with $\theta \approx 0.35\pi$, we obtain the following new bound on $\Delta_{\mathbb{H}^n}(r)$. It is an exponential improvement over the Böröczky bound, which was previously the best bound known, and the new bound is independent of the radius of the balls used in the packing.

Corollary 4.2. *We have*

$$\sup_{r>0} \Delta_{\mathbb{H}^n}(r) \leq 2^{-(0.5990\dots+o(1))n}.$$

4.1. The Bowen-Radin theory of hyperbolic packings. The Bowen-Radin approach to hyperbolic packing is based on ergodic theory, but our argument is elementary. All we need is the following fact: for every $R > 0$, there exists a ball \mathcal{B} of radius R containing a subset of at least

$$\Delta_{\mathbb{H}^n}(r) \frac{\text{vol}(B_R^n)}{\text{vol}(B_r^n)}$$

points at distance $2r$ or more from each other and not equal to the center of \mathcal{B} . Naively, this should follow from a simple averaging argument, since if we place \mathcal{B} at random in a dense packing, then this is the expected number of sphere centers it will contain, and the probability that one of them will hit the center of \mathcal{B} is zero. Before turning to the proof of Theorem 4.1, we will briefly explain the Bowen-Radin definition and why this fact is true.

In the Bowen-Radin theory, instead of focusing on individual packings one studies measures on the space of packings. Let S_r be the space of relatively dense packings of \mathbb{H}^n with balls of radius r (i.e., packings in which any additional such ball would intersect one from the packing). Bowen and Radin give a natural metric to S_r , under which it is compact, and they study the action of the isometry group G of \mathbb{H}^n on S_r . They define random packings by G -invariant Borel probability measures μ on S_r , and they define the density of μ to be the probability that some fixed origin is contained in one of the balls in the packing (by G -invariance, it is independent of the choice of origin). The optimal packing density $\Delta_{\mathbb{H}^n}(r)$ is defined to be the least upper bound for the density of such measures.

Although restricting attention to G -invariant measures may sound overly limiting, it encompasses the reasonable examples that were known before. For example, if a packing is invariant under a discrete subgroup of G with finite covolume, then the Haar measure on G descends to a probability distribution on the G -orbit of the packing. However, the space of measures is better behaved than the space of discrete subgroups.

Bowen and Radin show that the optimal packing density is achieved by some measure, and they show how to obtain well-behaved dense sphere packings by sampling from such a distribution. Their papers make a convincing case that this ergodic approach is the right framework for studying hyperbolic packing density. See also [R04] for intuition and background.

The fact we need for Theorem 4.1 is the following lemma, which says that the sphere centers in a random packing are uniformly distributed with point density $\delta/\text{vol}(B_r^n)$:

Lemma 4.3. *Let μ be a G -invariant probability measure on S_r with density δ . Then for every Borel set A in \mathbb{H}^n , the expected number of sphere centers in A for a*

μ -random packing is

$$\delta \frac{\text{vol}(A)}{\text{vol}(B_r^n)}.$$

Proof. Let $\nu(A)$ be the expected number of sphere centers in a Borel set A . Then ν is a G -invariant Borel measure on \mathbb{H}^n , and the definition of density can be reformulated as $\nu(B_r^n) = \delta$. Thus, ν is locally finite and therefore proportional to the hyperbolic volume measure. (Recall that Haar measure on G/K is unique up to scaling, for any locally compact group G and compact subgroup K ; see Chapter III of [N65].) The constant of proportionality is determined by $\nu(B_r^n) = \delta$. \square

4.2. Proof of Theorem 4.1. The proof of Theorem 4.1 is analogous to the Euclidean case. The heart of the proof is the following lemma.

Lemma 4.4. *Let $r \leq R \leq 2r$ and $\sin \frac{\theta}{2} = \frac{\sinh r}{\sinh R}$. In a packing of spheres of radius r in \mathbb{H}^n , every ball of radius R contains at most $A(n, \theta)$ sphere centers other than its own center.*

Proof. We use the same projection argument as in the proof of Proposition 2.1. Project the sphere centers from the packing onto the surface of the ball of radius R using rays starting from the center of the ball. By the next lemma, the projections are separated by angles of at least θ , so there can be at most $A(n, \theta)$ of them. \square

The next lemma is the hyperbolic analogue of Lemma 2.2.

Lemma 4.5. *Consider a hyperbolic triangle with side lengths a, b, c and the angle opposite to c having measure γ . If $0 < a, b \leq R \leq 2r \leq c$, then*

$$\sin \frac{\gamma}{2} \geq \frac{\sinh r}{\sinh R}.$$

Proof. By hyperbolic law of cosines,

$$\cos \gamma = \frac{\cosh a \cosh b - \cosh c}{\sinh a \sinh b}.$$

Let

$$f(a, b, c) = \frac{\cosh a \cosh b - \cosh c}{\sinh a \sinh b}.$$

We wish to maximize $f(a, b, c)$ in the domain $0 < a, b \leq R \leq 2r \leq c$. Since f is monotonically decreasing in c , it is maximized by setting $c = 2r$. We have

$$\frac{\partial f}{\partial a} = \frac{\cosh a \cosh c - \cosh b}{\sinh^2 a \sinh b}$$

which is nonnegative since $\cosh c \geq \cosh b$ and $\cosh a \geq 1$. Thus $f(a, b, c)$ is nondecreasing in a , and it is maximized by setting $a = R$. The same is true for b by symmetry, and so

$$\cos \gamma = f(a, b, c) \leq \frac{\cosh^2 R - \cosh 2r}{\sinh^2 R} = 1 - \frac{2 \sinh^2 r}{\sinh^2 R}.$$

Therefore

$$\sin^2 \frac{\gamma}{2} = \frac{1 - \cos \gamma}{2} \geq \frac{\sinh^2 r}{\sinh^2 R},$$

and the result follows. \square

Proof of Theorem 4.1. Define R to satisfy $\sin \frac{\theta}{2} = \frac{\sinh r}{\sinh R}$. Since $\pi/3 \leq \theta \leq \pi$, we have $r \leq R \leq 2r$. (Note that the inequality $R \leq 2r$ does not always hold when $\theta < \pi/3$. It fails in the limit as $r \rightarrow 0$ but holds for large r .)

Let μ be a Bowen-Radin measure with density $\Delta_{\mathbb{H}^n}(r)$, and let A be a ball of radius R with its center omitted. By Lemma 4.3, the expected number of sphere centers in A from a μ -random packing is $\Delta_{\mathbb{H}^n}(r) \frac{\text{vol}(B_R^n)}{\text{vol}(B_r^n)}$, and thus there exists a packing in which there are at least this many. By Lemma 4.4,

$$\Delta_{\mathbb{H}^n}(r) \leq \frac{\text{vol}(B_r^n)}{\text{vol}(B_R^n)} A(n, \theta),$$

and so all that remains is to bound $\text{vol}(B_r^n)/\text{vol}(B_R^n)$. The volume of a ball in \mathbb{H}^n is given by

$$\text{vol}(B_r^n) = \Omega_n \int_0^r \sinh^{n-1} x \, dx,$$

where $\Omega_n = 2\pi^{n/2}/\Gamma(n/2)$ is the surface volume of the unit Euclidean $(n-1)$ -sphere. Thus

$$\begin{aligned} \Delta_{\mathbb{H}^n}(r) &\leq \frac{\int_0^r \sinh^{n-1} x \, dx}{\int_0^R \sinh^{n-1} x \, dx} A(n, \theta) \\ (4.2) \quad &\leq \left(\frac{\sinh r}{\sinh R} \right)^{n-1} A(n, \theta) \\ &= \sin^{n-1}(\theta/2) A(n, \theta), \end{aligned}$$

where the second inequality follows from Lemma 4.6 below. \square

If we fix the ratio $\frac{\sinh r}{\sinh R}$, then the ratio of the integrals in (4.2) is almost determined by the following lemma (the lower bound is sharp as $r \rightarrow 0$ and the upper bound is sharp as $r \rightarrow \infty$). We do not need the lower bound, but it shows that (4.1) cannot be substantially improved by a more careful analysis of the volume of hyperbolic balls.

Lemma 4.6. *For $0 < r \leq R$,*

$$\left(\frac{\sinh r}{\sinh R} \right)^n \leq \frac{\int_0^r \sinh^{n-1} x \, dx}{\int_0^R \sinh^{n-1} x \, dx} \leq \left(\frac{\sinh r}{\sinh R} \right)^{n-1}.$$

Proof. These inequalities amount to saying that

$$\frac{\int_0^r \sinh^{n-1} x \, dx}{\sinh^{n-1} r}$$

is an increasing function of r , while

$$\frac{\int_0^r \sinh^{n-1} x \, dx}{\sinh^n r}$$

is a decreasing function of r .

The derivative of the former function is

$$1 - \frac{(n-1) \cosh r}{\sinh^n r} \int_0^r \sinh^{n-1} x \, dx,$$

so we must prove that

$$\frac{\sinh^n r}{(n-1) \cosh r} - \int_0^r \sinh^{n-1} x \, dx \geq 0.$$

The left side of this inequality vanishes when $r = 0$, and its derivative with respect to r is

$$\frac{\sinh^{n-1} r}{(n-1) \cosh^2 r},$$

so it is increasing and hence nonnegative.

To show that

$$\frac{\int_0^r \sinh^{n-1} x \, dx}{\sinh^n r}$$

is decreasing, note that its derivative is

$$\frac{1}{\sinh r} - \frac{n \cosh r}{\sinh^{n+1} r} \int_0^r \sinh^{n-1} x \, dx,$$

so we must prove that

$$\int_0^r \sinh^{n-1} x \, dx - \frac{\sinh^n r}{n \cosh r} \geq 0.$$

Again the left side vanishes when $r = 0$, and this time its derivative is

$$\frac{\sinh^{n+1} r}{n \cosh^2 r},$$

so it is increasing and hence nonnegative. This completes the proof. \square

5. LINEAR PROGRAMMING BOUNDS IN HYPERBOLIC SPACE

It is natural to try to extend the results of Section 3 on linear programming bounds to hyperbolic space, but one runs into technical difficulties.

Given a function $f: [0, \infty) \rightarrow \mathbb{R}$, we view it as a function of hyperbolic distance and define the corresponding kernel $f: \mathbb{H}^n \times \mathbb{H}^n \rightarrow \mathbb{R}$ by $f(x, y) = f(d(x, y))$, where d denotes the metric on \mathbb{H}^n . (Using the same symbol for both functions is an abuse of notation, but it is convenient not to have to write the metric d repeatedly, and the number of arguments makes it unambiguous.) We say f is *positive definite* if for all N and all $x_1, \dots, x_N \in \mathbb{H}^n$, the matrix $(f(x_i, x_j))_{1 \leq i, j \leq N}$ is positive semidefinite, and we say it is *integrable* on \mathbb{H}^n if $x \mapsto f(x, y)$ is an integrable function on \mathbb{H}^n (of course this is independent of y), in which case we write $\int_{\mathbb{H}^n} f$ for the integral.

Let G be the connected component of the identity in the isometry group of \mathbb{H}^n , and let K be the stabilizer within G of a point $e \in \mathbb{H}^n$. Then (G, K) is a Gelfand pair; i.e., the algebra $L^1(K \backslash G / K)$ of integrable, bi- K -invariant functions on G forms a commutative algebra under convolution. Here G/K is \mathbb{H}^n and functions on $K \backslash G / K$ correspond to radial functions on \mathbb{H}^n . See Chapters 8 and 9 of [W07] for an account of Gelfand pairs and spherical transforms (and see [T82] for a more concrete exposition of Fourier analysis in \mathbb{H}^2). In the setting of \mathbb{H}^n , this theory gives a well-behaved Fourier transform for radial functions. For each $\lambda \geq 0$, let P_λ be the unique radial eigenfunction of the Laplacian on \mathbb{H}^n with eigenvalue λ and $P_\lambda(0) = 1$. These functions are positive definite for all $\lambda \geq 0$ (see Theorem 5.2 in [T63, p. 346]). Given a function $f: [0, \infty) \rightarrow \mathbb{R}$ that is integrable on \mathbb{H}^n , its radial Fourier transform is given by

$$\widehat{f}(\lambda) = \int_{\mathbb{H}^n} f(x, e) P_\lambda(x, e) \, dx,$$

which is of course independent of $e \in \mathbb{H}^n$. As in the Euclidean case, the Fourier transform extends to $L^2(K \backslash G / K)$, and it yields an isomorphism from that space to

$L^2([0, \infty), \mu_P)$, where μ_P is the Plancherel measure. However, unlike the Euclidean case, the Plancherel measure for \mathbb{H}^n is supported just on $[(n-1)^2/4, \infty)$.

Positive-definite functions are characterized by the Bochner-Godement theorem (see Theorems 9.3.4 and 9.4.1 in [W07] or Theorem 12.10 in Chapter III of [H08]). For continuous, integrable functions, it says that f is positive definite if and only if \widehat{f} is nonnegative on the support of the Plancherel measure. However, \widehat{f} can be negative outside of the support, because G is not amenable: Valette [V98] has constructed a continuous, positive-definite function with compact support and negative integral. (His construction works in G , rather than G/K , but it is easy to make it bi- K -invariant.)

In the linear programming bounds, we will assume $\widehat{f} \geq 0$ everywhere, which is a strictly stronger assumption than positive definiteness. We do not know whether the stronger hypothesis is truly needed for the following conjecture, but it will be needed for the proof of Theorem 5.7.

Conjecture 5.1. *Let $f: [0, \infty) \rightarrow \mathbb{R}$ be continuous and integrable on \mathbb{H}^n , and suppose $f(x) \leq 0$ for all $x \geq 2r$ while $\widehat{f}(\lambda) \geq 0$ for all $\lambda > 0$ and $\widehat{f}(0) > 0$. Then*

$$\Delta_{\mathbb{H}^n}(r) \leq \text{vol}(B_r^n) \frac{f(0)}{\widehat{f}(0)}.$$

Here, of course, $\text{vol}(B_r^n)$ denotes the volume of a ball of radius r in \mathbb{H}^n .
Let

$$\Delta_{\mathbb{H}^n}^{\text{LP}}(r) = \inf_f \text{vol}(B_r^n) \frac{f(0)}{\widehat{f}(0)},$$

where the infimum is over all f satisfying the hypotheses of Conjecture 5.1. The conjecture says $\Delta_{\mathbb{H}^n}^{\text{LP}}(r)$ is an upper bound for $\Delta_{\mathbb{H}^n}(r)$. Regardless of whether that is true, $\Delta_{\mathbb{H}^n}^{\text{LP}}(r)$ can be viewed as the solution of an abstract optimization problem.

The following theorem is the hyperbolic analogue of Rodemich's theorem.

Theorem 5.2. *For $\pi/3 \leq \theta \leq \pi$, positive integers $n \geq 2$, and $r > 0$,*

$$\Delta_{\mathbb{H}^n}^{\text{LP}}(r) \leq \sin^{n-1}(\theta/2) A^{\text{LP}}(n, \theta).$$

Proof. The argument is much like the proof of Theorem 3.4. Define R by $\sinh R = (\sinh r)/\sin(\theta/2)$. Given a function g satisfying the hypotheses of Theorem 3.1, define f by

$$f(x, y) = \int_{B_R^n(x) \cap B_R^n(y)} g(\cos \angle xzy) dz,$$

where $\angle xzy$ denotes the angle at z formed by the geodesics to x and y . Of course, this angle is not defined when $x = z$ or $y = z$, but these cases occur with measure zero.

Exactly the same approach as in the proof of Theorem 3.4 shows that f is a positive-definite function and that $f(x, y) \leq 0$ when $d(x, y) \geq 2r$. However, merely being positive definite does not imply that $\widehat{f}(\lambda) \geq 0$ for all $\lambda \geq 0$. To prove that,

we start by fixing $y \in \mathbb{H}^n$ and writing

$$\begin{aligned} \widehat{f}(\lambda) &= \int_{\mathbb{H}^n} P_\lambda(x, y) f(x, y) dx \\ &= \int_{\mathbb{H}^n} \int_{B_R^n(x) \cap B_R^n(y)} P_\lambda(x, y) g(\cos \angle xzy) dz dx \\ &= \int_{B_R^n(y)} \int_{B_R^n(z)} P_\lambda(x, y) g(\cos \angle xzy) dx dz. \end{aligned}$$

The integrand depends only on $d(x, z)$, $d(y, z)$, and $\angle xzy$, because the hyperbolic law of cosines determines $d(x, y)$ using this data, and the integral is proportional to the expected value of $P_\lambda(x, y)g(\cos \angle xzy)$ if we fix y , pick $z \in B_R^n(y)$ uniformly at random, and then pick $x \in B_R^n(z)$. Equivalently, we can fix z and pick $x, y \in B_R^n(z)$, because that induces the same measure on the three parameters $d(x, z)$, $d(y, z)$, and $\angle xzy$. This is obvious for $d(x, z)$ and $d(y, z)$, since they simply follow the radial distance distribution on B_R^n . (Picking $z \in B_R^n(y)$ or $y \in B_R^n(z)$ yields the same distribution on $d(y, z)$.) For $\angle xzy$ it amounts to saying that the angle at z between a random point x and a fixed point y is distributed the same as that between two random points x and y .

Thus, we can change variables to fix z instead of y and integrate over x and y to obtain

$$\widehat{f}(\lambda) = \int_{B_R^n(z)} \int_{B_R^n(z)} P_\lambda(x, y) g(\cos \angle xzy) dx dy.$$

Now we can see that $\widehat{f}(\lambda) \geq 0$, because $(x, y) \mapsto P_\lambda(x, y)g(\cos \angle xzy)$ defines a positive-definite kernel for $x, y \in \mathbb{H}^n \setminus \{z\}$. Specifically, the product of two positive-definite kernels is positive definite by the Schur product theorem (Theorem 7.5.3 in [HJ13]), which says that the set of positive-semidefinite matrices is closed under the Hadamard product.

It also follows from this formula and $P_0 = 1$ that

$$\widehat{f}(0) = \text{vol}(B_R^n)^2 \bar{g},$$

and combining this with $f(0) = \text{vol}(B_R^n)g(1)$ yields

$$\text{vol}(B_r^n) \frac{f(0)}{\widehat{f}(0)} = \frac{\text{vol}(B_r^n) g(1)}{\text{vol}(B_R^n) \bar{g}} \leq \sin^{n-1}(\theta/2) \frac{g(1)}{\bar{g}},$$

as desired. □

In the remainder of this section, we explain why a straightforward approach fails to prove Conjecture 5.1 and how to prove it for periodic packings under an admissibility condition on f . The latter proof is based on unpublished work of Cohn, Lurie, and Sarnak.

5.1. Obstacles to proving the conjecture. We have not been able to prove Conjecture 5.1 by imitating the proof of Theorem 3.3. The problem is that the boundary effects when restricting to a ball are not negligible.

Specifically, consider a hyperbolic sphere packing with balls of radius r , and imagine restricting it to a ball of radius R (i.e., looking only at the points within

this large ball). Let S_R be the set of all sphere centers in this ball and μ_R the hyperbolic volume measure on the ball, and consider the signed measure

$$\nu = \sum_{x \in S_R} \delta_x + \lambda \mu_R,$$

where λ is a constant to be specified shortly. Because f is positive definite,

$$\iint f(x, y) d\nu(x) d\nu(y) \geq 0,$$

which implies

$$\lambda^2 \iint f(x, y) d\mu_R(x) d\mu_R(y) + 2\lambda \sum_{x \in S_R} \int f(x, y) d\mu_R(y) + |S_R|f(0) \geq 0,$$

as in the proof of Theorem 3.3.

Now suppose we have a Bowen-Radin measure on packings, with density δ . Averaging over such a measure yields

$$\left(\lambda^2 + \frac{2\delta\lambda}{\text{vol}(B_r^n)} \right) \iint f(x, y) d\mu_R(x) d\mu_R(y) + \delta \frac{\text{vol}(B_R^n)}{\text{vol}(B_r^n)} f(0) \geq 0,$$

because Lemma 4.3 says the sphere centers are uniformly distributed. In particular, taking $\lambda = -\delta/\text{vol}(B_r^n)$ yields

$$\delta \leq \text{vol}(B_r^n) \frac{f(0)}{\iint f(x, y) d\mu_R(x) d\mu_R(y) / \text{vol}(B_R^n)}.$$

This proves a legitimate bound on the density:

Proposition 5.3. *Let $f: [0, \infty) \rightarrow \mathbb{R}$ be continuous and positive definite on \mathbb{H}^n , and suppose $f(x) \leq 0$ for all $x \geq 2r$. Then for each $R > 0$,*

$$\Delta_{\mathbb{H}^n}(r) \leq \text{vol}(B_r^n) \frac{f(0)}{\iint f(x, y) d\mu_R(x) d\mu_R(y) / \text{vol}(B_R^n)},$$

assuming the denominator is not zero.

It is natural to add the assumption that f is integrable and then take the limit as $R \rightarrow \infty$. However, the denominator does not converge to $\widehat{f}(0)$, as it does in the Euclidean case. To see why, let χ_R be the characteristic function of $[0, R]$. Then

$$\iint f(x, y) d\mu_R(x) d\mu_R(y) = \int_{\mathbb{H}^n} (f * \chi_R) \chi_R,$$

where the right side denotes the integral of a radial function on \mathbb{H}^n , and the convolution is defined by

$$(f * g)(x, y) = \int_{\mathbb{H}^n} f(x, z) g(y, z) dz.$$

Because the Fourier transform is unitary,

$$\int_{\mathbb{H}^n} (f * \chi_R) \chi_R = \int \widehat{f * \chi_R} \widehat{\chi_R} d\mu_P,$$

where μ_P is the Plancherel measure, and that simplifies to

$$\int \widehat{f} \widehat{\chi_R}^2 d\mu_P.$$

One can show similarly that $\text{vol}(B_R^n) = \int \widehat{\chi}_R^2 d\mu_P$, and thus

$$\frac{\iint f(x, y) d\mu_R(x) d\mu_R(y)}{\text{vol}(B_R^n)} = \frac{\int \widehat{f\widehat{\chi}_R^2} d\mu_P}{\int \widehat{\chi}_R^2 d\mu_P}.$$

We can already see a problem: we would like the mass of $\widehat{\chi}_R^2$ to be concentrated near 0 as $R \rightarrow \infty$. However, 0 is not even contained within the support of the Plancherel measure μ_P , so this cannot possibly work. To see how badly it fails, we return to radial functions on \mathbb{H}^n via

$$\int \widehat{f\widehat{\chi}_R^2} d\mu_P = \int_{\mathbb{H}^n} f \cdot (\chi_R * \chi_R).$$

(We use \cdot for multiplication here to avoid confusion with f applied to an argument.) The function $(\chi_R * \chi_R) / \text{vol}(B_R^n)$ measures the fraction of overlap between two balls of radius R whose centers are a given distance apart. In the limit as $R \rightarrow \infty$, this function does not converge to 1, as it does in Euclidean space. Instead, when the distance between the centers is z it converges to

$$(5.1) \quad \frac{B\left(\frac{1}{1+e^z}; \frac{n-1}{2}, \frac{n-1}{2}\right)}{B\left(\frac{1}{2}; \frac{n-1}{2}, \frac{n-1}{2}\right)},$$

where

$$B(u; \alpha, \beta) = \int_0^u t^{\alpha-1} (1-t)^{\beta-1} dt$$

is the incomplete beta function. (See Appendix B for the calculation.) Note that (5.1) equals 1 when $z = 0$ and vanishes in the limit as $z \rightarrow \infty$.

Thus,

$$\frac{\iint f(x, y) d\mu_R(x) d\mu_R(y)}{\text{vol}(B_R^n)}$$

converges to the integral of f times a function that takes values between 0 and 1. Variants of this approach, for example replacing χ_R with a smoother function such as the heat kernel, fail for essentially the same reason. In Euclidean space the heat kernel converges to the constant function 1 as time tends to infinity, if we rescale it so its value at the origin is fixed as 1. In other words, flowing heat becomes nearly uniformly distributed over time. However, in hyperbolic space that is not true (heat kernel asymptotics can be found in [DM88]).

5.2. Periodic packings. We can prove a variant of Conjecture 5.1 in the special case of periodic packings, i.e., packings that are invariant under a discrete, finite-covolume group of isometries.² This was first proved by Cohn, Lurie, and Sarnak in unpublished work; here, we give a proof under weaker hypotheses but using the same fundamental approach. It is not known in general whether periodic packings come arbitrarily close to the optimal Bowen-Radin packing density, although this has been proved for the hyperbolic plane [B03]. Maximizing the density for a single-orbit packing in \mathbb{H}^n under a cocompact group is equivalent to maximizing the systolic ratio of an n -dimensional compact hyperbolic manifold (see [K07] for background on systolic geometry), which makes periodic packings a particularly important case.

Given a periodic packing with balls of radius r , let $\Gamma \subset G$ be its symmetry group. By assumption, $\Gamma \backslash \mathbb{H}^n$ has finite volume. Suppose the spheres in the packing are

²Note that the definition of “periodic” varies between papers: [BR03] requires a cocompact group, while [B03] does not.

centered on the orbits $\Gamma x_1, \dots, \Gamma x_N$, and let Γ_i be the stabilizer of x_i in Γ . Then the density of the packing is the fraction of a fundamental domain covered by balls. If the stabilizers are trivial, then this fraction is simply $N \operatorname{vol}(B_r^n) / \operatorname{vol}(\Gamma \backslash \mathbb{H}^n)$. More generally, Γ_i preserves the ball centered at x_i , and only a $1/|\Gamma_i|$ fraction of this ball will lie in any given fundamental domain (specifically, one element of each Γ_i -orbit). Thus, the density is

$$\frac{\operatorname{vol}(B_r^n)}{\operatorname{vol}(\Gamma \backslash \mathbb{H}^n)} \sum_{i=1}^N \frac{1}{|\Gamma_i|}.$$

It is the same as the density of the corresponding Bowen-Radin measure.³

The proof of the linear programming bounds is based on the Selberg trace formula [S56]. More precisely, we use a pre-trace formula that plays the role of the Poisson summation formula in [CE03]. To minimize the background required, we derive it from the spectral theory of the Laplacian on $\Gamma \backslash \mathbb{H}^n$. Note that Selberg did not publish a complete proof of the trace formula. For a detailed proof, see [F67] for \mathbb{H}^2 , [V73] for hyperbolic spaces under some mild hypotheses on the discrete group, [EGM98] for the three-dimensional case (using techniques that work in greater generality), and [CS80] for hyperbolic spaces in general.

Call a function $f: [0, \infty) \rightarrow \mathbb{R}$ *admissible* on \mathbb{H}^n if

- (1) it is continuous and integrable on \mathbb{H}^n ,
- (2) for every discrete subgroup $\Gamma \subset G$ for which $\Gamma \backslash \mathbb{H}^n$ has finite volume,

$$\sum_{\gamma \in \Gamma} f(\gamma x, y)$$

converges absolutely for all $x, y \in \mathbb{H}^n$ and uniformly on compact subsets of \mathbb{H}^n , and

- (3) for each fixed y ,

$$x \mapsto \sum_{\gamma \in \Gamma} f(\gamma x, y)$$

is in $L^2(\Gamma \backslash \mathbb{H}^n)$.

All of the functions constructed in the proof of Theorem 5.2 are admissible by the following lemma.

Lemma 5.4. *Every continuous, compactly supported function is admissible.*

Proof. Let $f: [0, \infty) \rightarrow \mathbb{R}$ be continuous, and suppose f vanishes outside $[0, r]$. In the sum

$$\sum_{\gamma \in \Gamma} f(\gamma x, y),$$

the term $f(\gamma x, y)$ is nonzero only if $d(\gamma x, y) \leq r$. Absolute and uniform convergence on compact subsets is easy: if x and y are confined to a compact set K , then there is a finite subset S of Γ such that $d(\gamma x, y) > r$ whenever $\gamma \notin S$, because Γ acts discontinuously on \mathbb{H}^n (see §5.3 in [R06]). Then only the terms with $\gamma \in S$ contribute to the sum.

To complete the proof, we will show that the sum is bounded for fixed y , based on the proof of Lemma 2.6.1 in [EGM98]. Choose $\varepsilon > 0$ so that the balls $B_\varepsilon^n(\gamma^{-1}y)$

³Proposition 1 in [BR03] is stated for the cocompact case, but the proof works for the finite covolume case as well.

form a sphere packing; in other words, the only intersections between them come from the stabilizer Γ_y of y . Then the number of γ for which $d(\gamma x, y) \leq r$ is at most

$$\frac{|\Gamma_y| \operatorname{vol}(B_{r+\varepsilon}^n)}{\operatorname{vol}(B_\varepsilon^n)},$$

because at most $\operatorname{vol}(B_{r+\varepsilon}^n)/\operatorname{vol}(B_\varepsilon^n)$ of the balls $B_\varepsilon^n(\gamma^{-1}y)$ can fit into $B_{r+\varepsilon}^n(x)$, and each occurs for $|\Gamma_y|$ choices of γ . This bound is independent of x , and

$$\sum_{\gamma \in \Gamma} |f(\gamma x, y)| \leq \frac{|\Gamma_y| \operatorname{vol}(B_{r+\varepsilon}^n)}{\operatorname{vol}(B_\varepsilon^n)} \max_{[0,r]} |f|.$$

□

The following lemma provides more examples of admissible functions. It is essentially Lemma 1.4 in [V73], where it is attributed to Selberg, and we include the proof here for completeness.

Lemma 5.5 (Selberg). *Suppose $f: [0, \infty) \rightarrow \mathbb{R}$ is continuous and integrable on \mathbb{H}^n , and there exist constants c_1, c_2 such that for all $x, y \in \mathbb{H}^n$,*

$$|f(x, y)| \leq c_1 \int_{d(z,x) \leq c_2} |f(y, z)| dz.$$

Then f is admissible on \mathbb{H}^n .

Proof. Because Γ acts discontinuously on \mathbb{H}^n , each of the balls $B_{c_2}^n(\gamma x)$ with $\gamma \in \Gamma$ intersects only a finite number of these balls, say $N(x)$ of them (counting itself), and this function N is bounded on compact sets. Then

$$\begin{aligned} \sum_{\gamma \in \Gamma} |f(\gamma x, y)| &\leq c_1 \sum_{\gamma \in \Gamma} \int_{B_{c_2}^n(\gamma x)} |f(y, z)| dz \\ (5.2) \qquad \qquad \qquad &\leq c_1 N(x) \int_{\mathbb{H}^n} |f(y, z)| dz. \end{aligned}$$

The left side is invariant under switching x and y , while the right side is independent of y , from which it follows that

$$\sum_{\gamma \in \Gamma} |f(\gamma x, y)|$$

is bounded for each fixed y . All that remains is to verify uniform convergence on compact sets, which is not hard to check as follows. Suppose x and y are restricted to a compact set K , and let $r > 0$. In the upper bound $\int_{\mathbb{H}^n} |f(y, z)| dz$ from (5.2), all $z \in B_r^n(y)$ come from a finite subset S of Γ depending only on K and r . It follows that

$$\sum_{\gamma \notin S} |f(\gamma x, y)| \leq c_1 N(x) \int_{d(z,y) \geq r} |f(y, z)| dz,$$

and the upper bound tends to zero as $r \rightarrow \infty$. □

The only place where we require the trace formula machinery is the proof of the following lemma:

Lemma 5.6. *Let $f: [0, \infty) \rightarrow \mathbb{R}$ be admissible on \mathbb{H}^n and satisfy $\widehat{f}(\lambda) \geq 0$ for all $\lambda \geq 0$. If Γ is a discrete subgroup in G with finite covolume, then the function F defined by*

$$F(x, y) = \sum_{\gamma \in \Gamma} f(\gamma x, y)$$

is positive definite on $\mathbb{H}^n \times \mathbb{H}^n$. Furthermore, $F - \widehat{f}(0)/\text{vol}(\Gamma \backslash \mathbb{H}^n)$ remains positive definite.

In other words, for all $x_1, \dots, x_N \in \mathbb{H}^n$, the $N \times N$ matrix with entries $F(x_i, x_j) - \widehat{f}(0)/\text{vol}(\Gamma \backslash \mathbb{H}^n)$ is positive semidefinite.

Proof. First, suppose $\Gamma \backslash \mathbb{H}^n$ is compact, so the spectrum of the Laplacian is discrete. Let v_0, v_1, \dots be the orthonormal eigenfunctions of the Laplacian on $\Gamma \backslash \mathbb{H}^n$, viewed as periodic functions on \mathbb{H}^n , and let $\lambda_0 \leq \lambda_1 \leq \dots$ be the corresponding eigenvalues. The sum

$$\sum_{\gamma \in \Gamma} f(\gamma x, y)$$

is periodic modulo Γ as a function of x (or y), so we can expand it in terms of the eigenfunctions of the Laplacian. We have

$$\sum_{\gamma \in \Gamma} f(\gamma x, y) \simeq \sum_{i=0}^{\infty} v_i(x) \int_{\Gamma \backslash \mathbb{H}^n} \left(\sum_{\gamma \in \Gamma} f(\gamma z, y) \right) \overline{v_i(z)} dz,$$

where \simeq denotes L^2 convergence. The coefficients unfold to

$$\int_{\mathbb{H}^n} f(z, y) \overline{v_i(z)} dz,$$

and we can rotationally symmetrize about y , which turns $v_i(z)$ into $v_i(y)P_{\lambda_i}(z, y)$ and the coefficient into

$$\overline{v_i(y)} \int_{\mathbb{H}^n} f(z, y) \overline{P_{\lambda_i}(z, y)} dz = \overline{v_i(y)} \widehat{f}(\lambda_i).$$

(The conjugate on P_{λ_i} does not matter, because this function is real-valued.) Thus,

$$\sum_{\gamma \in \Gamma} f(\gamma x, y) \simeq \sum_{i=0}^{\infty} \widehat{f}(\lambda_i) v_i(x) \overline{v_i(y)}.$$

The functions $(x, y) \mapsto v_i(x) \overline{v_i(y)}$ are clearly positive definite, and the coefficients $\widehat{f}(\lambda_i)$ are nonnegative. Furthermore, positive definiteness is preserved under pointwise convergence. However, this expansion may not converge pointwise. Fortunately, L^2 convergence implies that a subsequence converges pointwise almost everywhere (see, for example, Theorem 3.12 in [R87]). Thus, for almost all $x_1, \dots, x_N \in \mathbb{H}^n$, the matrix with entries $F(x_i, x_j)$ is positive semidefinite, and the same holds for all x_1, \dots, x_N by continuity. Furthermore, v_0 is the constant eigenfunction, so $v_0 \overline{v_0}$ must be $1/\text{vol}(\Gamma \backslash \mathbb{H}^n)$ by orthonormality, and thus $F - \widehat{f}(0)/\text{vol}(\Gamma \backslash \mathbb{H}^n)$ is also positive definite.

All that remains is to deal with the case when $\Gamma \backslash \mathbb{H}^n$ has finite volume but is not compact. Harmonic analysis on the quotient is quite a bit more involved, because of continuous spectrum coming from the cusps, but a completely analogous argument works. Suppose $\Gamma \backslash \mathbb{H}^n$ has h cusps. For $1 \leq k \leq h$ and $s \in \mathbb{C}$ with $\Re(s) = (n-1)/2$, there is an Eisenstein series $x \mapsto E_k(x, s)$, which is an eigenfunction with eigenvalue

$s(n-1-s)$. Note that these Eisenstein series are not in $L^2(\Gamma \backslash \mathbb{H}^n)$. When $s = (n-1)/2 + it$, the eigenvalue becomes $(n-1)^2/4 + t^2$, so it is contained in the support $[(n-1)^2/4, \infty)$ of the Plancherel measure. The spectral resolution is now

$$\begin{aligned} \sum_{\gamma \in \Gamma} f(\gamma x, y) &\simeq \sum_{j=0}^{\infty} \widehat{f}(\lambda_j) v_j(x) \overline{v_j(y)} \\ &+ \frac{1}{4\pi} \sum_{k=1}^h \int_{-\infty}^{\infty} \widehat{f} \left(\frac{(n-1)^2}{4} + t^2 \right) \\ &E_k \left(x, \frac{n-1}{2} + it \right) \overline{E_k \left(y, \frac{n-1}{2} + it \right)} dt. \end{aligned}$$

See (7.30) in [CS80, p. 75] for the underlying decomposition of $L^2(\Gamma \backslash \mathbb{H}^n)$, although that formula is missing the factor of $1/(4\pi)$. This expansion means that the left side is the L^2 limit of

$$\begin{aligned} &\sum_{j=0}^N \widehat{f}(\lambda_j) v_j(x) \overline{v_j(y)} \\ &+ \frac{1}{4\pi} \sum_{k=1}^h \int_{-T}^T \widehat{f} \left(\frac{(n-1)^2}{4} + t^2 \right) E_k \left(x, \frac{n-1}{2} + it \right) \overline{E_k \left(y, \frac{n-1}{2} + it \right)} dt \end{aligned}$$

as N and T tend to infinity. Now the proof proceeds as in the compact case. \square

The proof of Lemma 5.6 depends on the hypothesis that $\widehat{f} \geq 0$ everywhere, not just on the support $[(n-1)^2/4, \infty)$ of the Plancherel measure, because the eigenvalues of the Laplacian on $\Gamma \backslash \mathbb{H}^n$ need not be contained in the support: 0 is always an eigenvalue, and there can be others between 0 and $(n-1)^2/4$. Selberg's eigenvalue conjecture [S65, S95] says there are no nonzero eigenvalues in $(0, 1/4)$ for congruence subgroups of $\mathrm{SL}_2(\mathbb{Z})$, but that is a special arithmetic property not shared by more general groups.

Theorem 5.7 (Cohn, Lurie, and Sarnak). *Let $f: [0, \infty) \rightarrow \mathbb{R}$ be admissible on \mathbb{H}^n , and suppose $f(x) \leq 0$ for all $x \geq 2r$ while $\widehat{f}(\lambda) \geq 0$ for all $\lambda > 0$ and $\widehat{f}(0) > 0$. Then every periodic packing in \mathbb{H}^n using balls of radius r has density at most*

$$\mathrm{vol}(B_r^n) \frac{\widehat{f}(0)}{\widehat{f}(0)}.$$

Proof. Consider a periodic packing consisting of orbits $\Gamma x_1, \dots, \Gamma x_N$ of a finite-covolume group Γ , and let Γ_i be the stabilizer of x_i in Γ . Recall that the density of the packing is

$$\frac{\mathrm{vol}(B_r^n)}{\mathrm{vol}(\Gamma \backslash \mathbb{H}^n)} \sum_{i=1}^N \frac{1}{|\Gamma_i|}.$$

Let

$$F(x, y) = \sum_{\gamma \in \Gamma} f(\gamma x, y).$$

By Lemma 5.6,

$$\sum_{i,j=1}^N \frac{1}{|\Gamma_i| |\Gamma_j|} \left(F(x_i, x_j) - \frac{\widehat{f}(0)}{\mathrm{vol}(\Gamma \backslash \mathbb{H}^n)} \right) \geq 0,$$

which amounts to

$$\sum_{i,j=1}^N \frac{F(x_i, x_j)}{|\Gamma_i| |\Gamma_j|} \geq \left(\sum_{i=1}^N \frac{1}{|\Gamma_i|} \right)^2 \frac{\widehat{f}(0)}{\text{vol}(\Gamma \backslash \mathbb{H}^n)}.$$

On the other hand, $F(x_i, x_j) \leq 0$ for $i \neq j$, because all the terms in the sum defining F are nonpositive in that case, and $F(x_i, x_i) \leq |\Gamma_i| f(0)$, because there are $|\Gamma_i|$ group elements γ for which $\gamma x_i = x_i$. Thus,

$$\sum_{i=1}^N \frac{|\Gamma_i| f(0)}{|\Gamma_i|^2} \geq \left(\sum_{i=1}^N \frac{1}{|\Gamma_i|} \right)^2 \frac{\widehat{f}(0)}{\text{vol}(\Gamma \backslash \mathbb{H}^n)}.$$

We conclude that

$$\frac{\text{vol}(B_r^n)}{\text{vol}(\Gamma \backslash \mathbb{H}^n)} \sum_{i=1}^N \frac{1}{|\Gamma_i|} \leq \text{vol}(B_r^n) \frac{f(0)}{\widehat{f}(0)},$$

as desired. \square

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APPENDIX A. NUMERICAL COMPUTATION OF EUCLIDEAN DENSITY BOUNDS

Before the Cohn-Elkies paper [CE03], the three best upper bounds known for sphere packing in \mathbb{R}^n with $n > 3$ were those of Rogers [R58], Levenshtein [L79], and Kabatiansky and Levenshtein [KL78]. The Rogers bound was the best known for $4 \leq n \leq 95$, the Levenshtein bound for $96 \leq n \leq 114$, and the Kabatiansky-Levenshtein bound for $n \geq 115$. See Table A.1 for numerical data. Note that the asymptotic decay rates are not apparent from the behavior in low dimensions.

Table A.1 differs from the bounds presented in Table 1.3 of [CS99]. Specifically, [CS99, p. 20] says that the Kabatiansky-Levenshtein bound improves on the Rogers bound for $n \geq 43$, and Table 1.3 lists some special cases, but our computations of the Kabatiansky-Levenshtein bound disagree. To help resolve this discrepancy, we will specify how we computed all these bounds.

The Rogers bound is conceptually simple: it is the fraction of a regular simplex covered by congruent balls centered at its vertices and tangent to each other. However, it is somewhat complicated to compute explicitly. Based on Chapter 7 of [Z99], we used the formula

$$\frac{(n+1)!}{(n/2)!} \cdot \frac{\pi^{(n-1)/2}}{2^{3n/2}} \int_{-\infty}^{\infty} e^{(n+1)(n/2 - \sqrt{2n}ui - u^2)} \left(1 - \text{erf}\left(\sqrt{n/2} - ui\right)\right)^n du$$

for the Rogers bound in \mathbb{R}^n , where erf denotes the error function

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt.$$

The Levenshtein bound in \mathbb{R}^n equals

$$\frac{j_{n/2}^n}{(n/2)!^2 4^n},$$

where $j_{n/2}$ is the first positive root of the Bessel function $J_{n/2}$.

TABLE A.1. Upper bounds for sphere packing density in \mathbb{R}^n . The last column gives the new bound from Proposition 2.1, applied using the Kabatiansky-Levenshtein bound for $A(n, \theta)$. All numbers are rounded up.

n	Rogers	Levenshtein	K.-L.	Prop. 2.1
12	8.759×10^{-2}	1.065×10^{-1}	1.038×10^0	9.666×10^{-1}
24	2.456×10^{-3}	3.420×10^{-3}	2.930×10^{-2}	2.637×10^{-2}
36	5.527×10^{-5}	8.109×10^{-5}	5.547×10^{-4}	4.951×10^{-4}
48	1.128×10^{-6}	1.643×10^{-6}	8.745×10^{-6}	7.649×10^{-6}
60	2.173×10^{-8}	3.009×10^{-8}	1.223×10^{-7}	1.046×10^{-7}
72	4.039×10^{-10}	5.135×10^{-10}	1.550×10^{-9}	1.322×10^{-9}
84	7.315×10^{-12}	8.312×10^{-12}	1.850×10^{-11}	1.574×10^{-11}
96	1.300×10^{-13}	1.291×10^{-13}	2.111×10^{-13}	1.786×10^{-13}
108	2.277×10^{-15}	1.937×10^{-15}	2.320×10^{-15}	1.942×10^{-15}
120	3.940×10^{-17}	2.826×10^{-17}	2.452×10^{-17}	2.051×10^{-17}
240	6.739×10^{-35}	4.888×10^{-36}	1.542×10^{-37}	1.267×10^{-37}
360	8.726×10^{-53}	3.522×10^{-55}	3.689×10^{-58}	3.003×10^{-58}
480	1.007×10^{-70}	1.643×10^{-74}	5.536×10^{-79}	4.484×10^{-79}
600	1.090×10^{-88}	5.847×10^{-94}	6.233×10^{-100}	5.036×10^{-100}

For the Kabatiansky-Levenshtein bound, let $t_{n,k}$ denote the largest root of the Gegenbauer polynomial $C_k^{n/2-1}$ of degree k . Kabatiansky and Levenshtein proved that

$$A(n, \theta) \leq \frac{4 \binom{k+n-2}{k}}{1 - t_{n,k+1}}$$

whenever $\cos \theta \leq t_{n,k}$. Combining this bound for $A(n+1, \theta)$ with (2.1) and taking $\cos \theta = t_{n+1,k}$ to minimize $\sin(\theta/2)$, we obtain a sphere packing density bound of

$$\inf_k \left(\frac{1 - t_{n+1,k}}{2} \right)^{n/2} \frac{4 \binom{k+n-1}{k}}{1 - t_{n+1,k+1}}$$

in \mathbb{R}^n . We have not rigorously analyzed how this bound depends on k , but the infimum appears to be achieved, in fact at a unique local minimum. In our numerical calculations, we search consecutively through $k = 1, 2, \dots$ until we find the first local minimum.

Our new bound in this paper (Proposition 2.1, applied using the Kabatiansky-Levenshtein bound on $A(n, \theta)$) is given by

$$\min_k \left(\frac{1 - t_{n,k}}{2} \right)^{n/2} \frac{4 \binom{k+n-2}{k}}{1 - t_{n,k+1}},$$

where the minimum is over k satisfying $t_{n,k} \leq 1/2$ (which corresponds to $\theta \geq \pi/3$). Note that $t_{n,k}$ is an increasing function of k and $t_{n,k} \rightarrow 1$ as $k \rightarrow \infty$.

Using the above formulas, we have computed these bounds for $2 \leq n \leq 128$ and several larger values of n using MATHEMATICA 9.0.1 [W13], to obtain the cross-over points listed above and the data in Table A.1. Strictly speaking, our calculations are not rigorous, because we have not proved bounds for floating-point error. Furthermore, we have not proved that the bounds never cross again. There is

no theoretical reason why these issues could not be addressed, but it would take some work.

As we mentioned above, our calculations disagree with those in [CS99]. For example, Table 1.3 of [CS99] says the Kabatiansky-Levenshtein bound for \mathbb{R}^{48} is

$$2^{15.27} \cdot \frac{\pi^{24}}{24!} \approx 5.44 \times 10^{-8},$$

which is substantially less than the 8.745×10^{-6} listed in Table A.1. Page 265 of [CS99] explains that the Kabatiansky-Levenshtein calculations in Table 1.3 were carried out using information about the Gegenbauer polynomial roots from [KL78, p. 12]. The results in [KL78, p. 12] are asymptotic formulas that are not accurate in low dimensions, and we hypothesize that this explains the discrepancy, although we do not know how to obtain the numbers quoted in Table 1.3 of [CS99].

For comparison, the Cohn-Elkies linear programming bound improves on all these bounds for $4 \leq n \leq 128$. Improving on the Kabatiansky-Levenshtein bound is no surprise by Theorem 3.4, and Proposition 6.1 of [CE03] says the linear programming bound is always at least as strong as the Levenshtein bound. Improving on the Rogers bound is the only part we cannot explain conceptually, and it can be verified using an auxiliary function with eight forced double roots in the numerical technique from Section 7 of [CE03]. We do not report linear programming bounds in Table A.1, because we have not completed enough calculations to give truly representative data. As the dimension grows, the number of forced double roots required to optimize the bound grows as well. Using only eight of them substantially weakens the bound, but it already suffices to improve on the other bounds when $4 \leq n \leq 128$. For example, using eight forced double roots leads to a bound of 1.164×10^{-17} when $n = 120$.

APPENDIX B. OVERLAP OF BALLS IN HYPERBOLIC SPACE

Proposition B.1. *If $n \geq 2$ and x_1 and x_2 are points in \mathbb{H}^n at distance r from each other, then*

$$\lim_{R \rightarrow \infty} \frac{\text{vol}(B_R^n(x_1) \cap B_R^n(x_2))}{\text{vol}(B_R^n)} = \frac{B\left(\frac{1}{1+e^r}; \frac{n-1}{2}, \frac{n-1}{2}\right)}{B\left(\frac{1}{2}; \frac{n-1}{2}, \frac{n-1}{2}\right)}.$$

Recall that

$$B(u; \alpha, \beta) = \int_0^u t^{\alpha-1} (1-t)^{\beta-1} dt$$

is the incomplete beta function. To prove Proposition B.1, we will compute the convolution $(\chi_R * \chi_R)(r) / \text{vol}(B_R^n)$ on \mathbb{H}^n , where χ_R is the characteristic function of a ball of radius R , and take the limit as $R \rightarrow \infty$.

First, we observe that given two radial functions f_1 and f_2 on \mathbb{H}^n , their convolution can be computed as follows. Let x_1 and x_2 be two points in \mathbb{H}^n at distance r from each other, and consider a third point z at distances r_1 and r_2 from x_1 and x_2 , respectively. Then $(f_1 * f_2)(r)$ is the integral of $f_1(r_1)f_2(r_2)$ over all $z \in \mathbb{H}^n$. To write it down explicitly, we can use polar coordinates centered at x_1 . Let $u = \cos \angle x_2 x_1 z$. Then

$$(f_1 * f_2)(r) = \frac{2\pi^{(n-1)/2}}{\Gamma((n-1)/2)} \int_0^\infty \int_{-1}^1 f_1(r_1)f_2(r_2)(\sinh^{n-1} r_1)(1-u^2)^{(n-3)/2} du dr_1,$$

where we view r_2 as a function of r_1 and u via the hyperbolic law of cosines. Changing variables from u to r_2 yields

$$(B.1) \quad \frac{2\pi^{(n-1)/2}}{\Gamma((n-1)/2)} \iint f_1(r_1)f_2(r_2) \frac{\sinh r_1 \sinh r_2}{\sinh^{n-2} r} C(r, r_1, r_2)^{(n-3)/2} dr_1 dr_2,$$

where the integral is over all r_1 and r_2 such that r, r_1, r_2 form the side lengths of a triangle, and

$$C(r, r_1, r_2) = 1 - \cosh^2 r - \cosh^2 r_1 - \cosh^2 r_2 + 2 \cosh r \cosh r_1 \cosh r_2.$$

Now we apply (B.1) to $f_1 = f_2 = \chi_R$ and divide by $\text{vol}(B_R^n)$, which is asymptotic to $2\pi^{n/2}e^{(n-1)R}/((n-1)2^{n-1}\Gamma(n/2))$ as $R \rightarrow \infty$. We find that $(\chi_R * \chi_R)(r)/\text{vol}(B_R^n)$ is asymptotic to

$$(B.2) \quad \frac{(n-1)2^{n-1}}{B((n-1)/2, 1/2)} e^{-(n-1)R} \iint_X \frac{\sinh r_1 \sinh r_2}{\sinh^{n-2} r} C(r, r_1, r_2)^{(n-3)/2} dr_1 dr_2,$$

where $B(\alpha, \beta) = B(1; \alpha, \beta) = \Gamma(\alpha)\Gamma(\beta)/\Gamma(\alpha + \beta)$ denotes the beta function and X is the set of $(r_1, r_2) \in [0, R]^2$ for which r, r_1, r_2 form a triangle.

We now change variables in (B.2) from r_1 and r_2 to $x = r_1 - r_2$ and $y = 2R - r_1 - r_2$. In the new variables, the domain X of integration becomes

$$\{(x, y) : |x| \leq r \text{ and } |x| \leq y \leq 2R - r\}.$$

Expanding the hyperbolic trigonometric functions in terms of exponentials shows that

$$\begin{aligned} \sinh r_1 &= \frac{e^{R+(x-y)/2}}{2} + O(1), \\ \sinh r_2 &= \frac{e^{R-(x+y)/2}}{2} + O(1), \end{aligned}$$

and

$$C(r, r_1, r_2) = e^{2R-y} \frac{\cosh r - \cosh x}{2} + O(1),$$

where the $O(1)$ terms depend on r but not x, y , or R . By the mean value theorem,

$$C(r, r_1, r_2)^{(n-3)/2} = \left(e^{2R-y} \frac{\cosh r - \cosh x}{2} \right)^{(n-3)/2} + O\left(e^{(n-5)R - (n-5)y/2} \right),$$

where the constant in the big O term depends only on n and r . Now as $R \rightarrow \infty$, the integral (B.2) converges to

$$\frac{(n-1)2^{(n-5)/2}}{B((n-1)/2, 1/2) \sinh^{n-2} r} \int_{-r}^r \int_{|x|}^{\infty} e^{-(n-1)y/2} (\cosh r - \cosh x)^{(n-3)/2} dy dx.$$

We can evaluate the y integral explicitly, and the remaining integrand is an even function of x . The integral thus equals

$$\frac{2^{(n-1)/2}}{B((n-1)/2, 1/2) \sinh^{n-2} r} \int_0^r e^{-(n-1)x/2} (\cosh r - \cosh x)^{(n-3)/2} dx.$$

Finally, we change to a new variable

$$t = \frac{e^{-x} - e^{-r}}{e^r - e^{-r}}$$

to arrive at

$$\frac{2^{n-1}}{B((n-1)/2, 1/2)} \int_0^{1/(1+e^r)} (t(1-t))^{(n-3)/2} dt.$$

It follows from the duplication formula for the gamma function that this expression equals

$$\frac{\int_0^{1/(1+e^r)} (t(1-t))^{(n-3)/2} dt}{B((n-1)/2, (n-1)/2)/2}.$$

This completes the proof of Proposition B.1.

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