Sphere packing, lattices, and Epstein zeta function

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The sphere packing problem

The **sphere packing problem** in $\mathbb{R}^N$, $N \geq 2$, is the question of how large a proportion of the entire space $\mathbb{R}^N$ can be filled by non-overlapping spheres (= balls) of equal radius, and which particular arrangement of spheres provides this maximal proportion (= density)?

More precisely, if $C^N(a)$ is a cube of side-length a centered at the origin in $\mathbb{R}^N$, then density of a sphere packing is

$$\delta = \lim_{a \to \infty} \frac{\text{volume of the balls in } C^N(a)}{\text{volume of } C^N(a)},$$

and the sphere packing problem is to find an arrangement of spheres in $\mathbb{R}^N$ that maximizes δ.

In order to define a sphere packing, it is sufficient to define an infinite arrangement of points in $\mathbb{R}^N$, and then use these points as centers of the spheres of radius equal to one half of the minimal distance between two such points.

Lattice packing

A **lattice** in $\mathbb{R}^N$ is a free $\mathbb{Z}$-module of rank N; equivalently, it is a discrete co-compact subgroup of $\mathbb{R}^N$.

Every lattice Λ in $\mathbb{R}^N$ has a basis $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \mathbb{R}^N$, so that

$$\Lambda = \left\{ \sum_{i=1}^{N} a_i \boldsymbol{x}_i \ : \ a_1, \ldots, a_n \in \mathbb{Z} \right\} = X\mathbb{Z}^N,$$

where $X = (\boldsymbol{x}_1 \ldots \boldsymbol{x}_N)$ is the corresponding $N \times N$ basis matrix, whose columns are these basis vectors.

A sphere packing in $\mathbb{R}^N$ is called a **lattice packing** if the set of centers of spheres is a lattice.

Kepler's conjecture

The maximal possible sphere packing density in $\mathbb{R}^3$ is that of the **face-centered cubic** (fcc) lattice

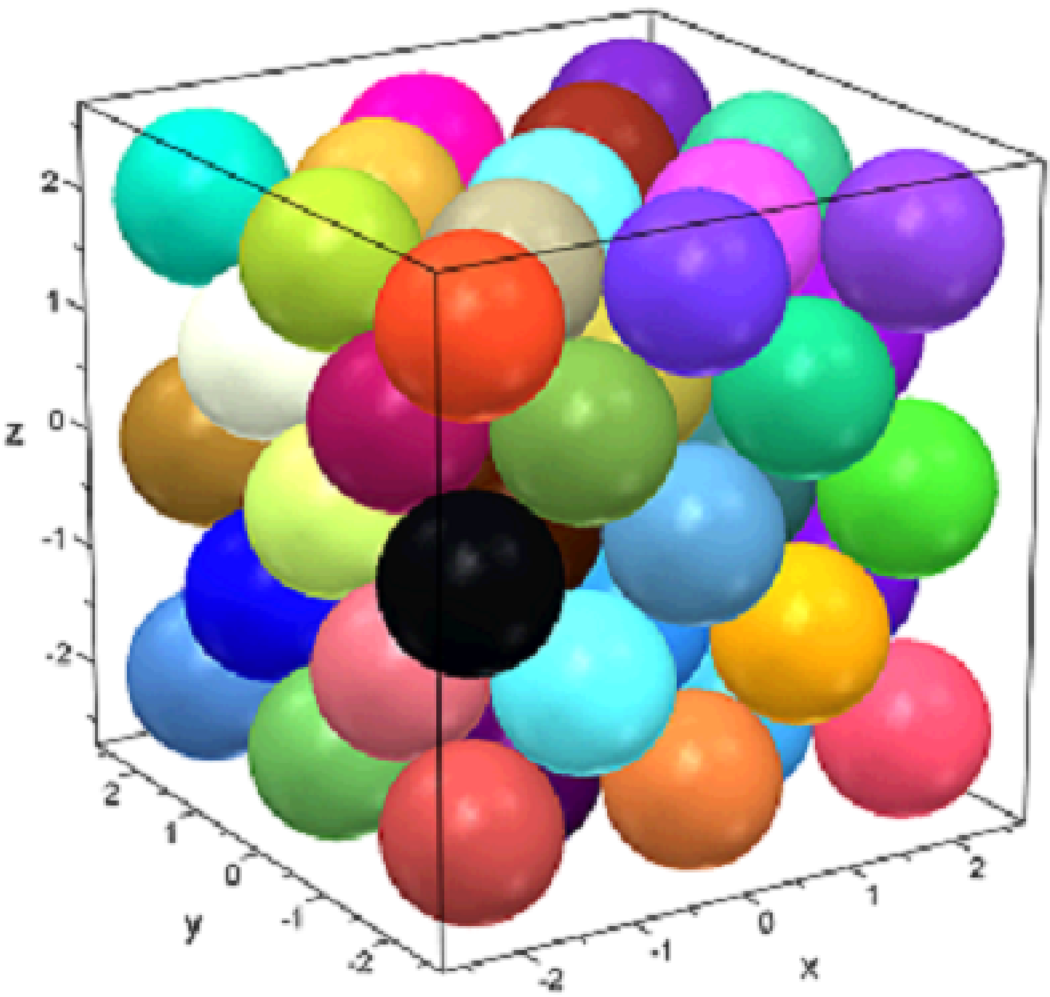
$$\Lambda_{fcc} = \begin{pmatrix} -1 & 1 & 0 \\ -1 & -1 & 1 \\ 0 & 0 & -1 \end{pmatrix} \mathbb{Z}^3,$$

which is

$$\delta_{fcc} = \frac{\pi}{\sqrt{18}} = 0.7405\ldots$$

This packing density is also achieved by the hexagonal close-packing in $\mathbb{R}^3$, which is *not* a lattice packing: it is the union of a lattice and its translate. In fact, there are infinitely many nonlattice packings in $\mathbb{R}^3$ which achieve the same density as Λ_{fcc}.

Face-centered cubic lattice packing:



mathPAD Online, vol. 15 (2006)

Historical note

From **Wikipedia**:

The conjecture is named after **Johannes Kepler**, *who stated the conjecture in* **1611** *in Strena sue de nive sexangula (On the Six-Cornered Snowflake). Kepler had started to study arrangements of spheres as a result of his correspondence with the English mathematician and astronomer* **Thomas Harriot** *in 1606. Harriot was a friend and assistant of* **Sir Walter Raleigh**, *who had set Harriot the problem of determining how best to stack cannon balls on the decks of his ships. Harriot published a study of various stacking patterns in 1591, and went on to develop an early version of atomic theory.*

• In 1831, C. F. Gauss proved that Λ_{fcc} gives optimal packing density among lattices, i.e. *best lattice packing* in $\mathbb{R}^3$

• In 1953, L. F. Toth proved that the proof of Kepler's conjecture can be reduced to a finite (albeit very large) number of computations

• **"Symmetric Bilinear Forms" by J. Milnor and D. Husemoller, 1973, p. 35:**

... according to [C. A.] Rogers, "many mathematicians believe and all physicists know that the density cannot exceed $\frac{\pi}{\sqrt{18}}$*"*

(from Wikipedia)

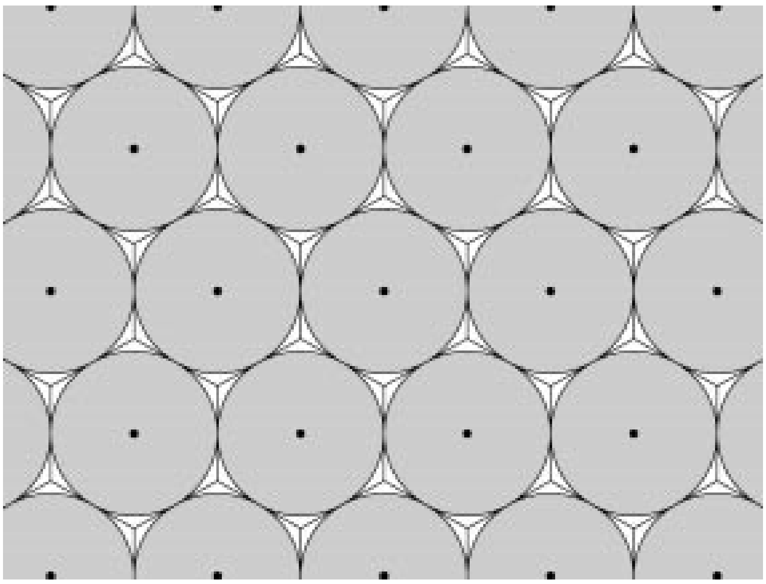
• In 1998, T. C. Hales announced the proof, which was checked by a team of mathematicians, and finally published in 2005/2006 in the *Annals of Mathematics* (overview: 120 pages) and *Discrete and Computational Geometry* (full version: 265 pages); a part of it was done in collaboration with (Hales' graduate student at the time) S. P. Ferguson

• The two-dimensional analogue of Kepler's conjecture states that the best circle packing is given by the **hexagonal lattice**

$$\Lambda_h = \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} \end{pmatrix} \mathbb{Z}^2,$$

which gives density $\delta_h = \frac{\pi}{\sqrt{12}} = 0.9069\dots$. The optimality of Λ_h among all lattice packings in $\mathbb{R}^2$ was proved by C. F. Gauss, and among all packings in $\mathbb{R}^2$ - by Thue in 1910 (a different proof was also given by L. F. Toth in 1940).

Here is a picture of the circle packing, given by the hexagonal lattice:



Lattices, Linear Codes, and Invariants, Part I, N. D. Elkies, AMS Notices, vol. 47 no. 10

Back to lattice packings

The sphere packing problem has not been solved in any dimension > 3. However, the optimal lattice packing is known in dimensions ≤ 8 and dimension 24 (the famous Leech lattice - recent result by H. Cohn and A. Kumar (2004)).

For the rest of this talk we will restrict to lattice packings only.

Given a lattice Λ, define its **minimum** to be

$$|\Lambda| = \min\{\|\boldsymbol{x}\| \ : \ \boldsymbol{x} \in \Lambda, \ \boldsymbol{x} \neq \boldsymbol{0}\}.$$

This is precisely the diameter of a sphere in the corresponding packing.

Also, **determinant** of $\Lambda = A\mathbb{Z}^N$, where A is a basis matrix, is

$$\det(\Lambda) = |\det(A)|.$$

This is the volume of a fundamental domain of Λ.

Density of a packing associated with Λ is equal to the volume of one ball of radius $\frac{|\Lambda|}{2}$ divided by the volume of a fundamental domain of Λ, i.e.

$$\delta(\Lambda) = \frac{(\sqrt{\pi}\ |\Lambda|)^N}{2^N \Gamma\left(\frac{N}{2}+1\right) \det(A)}.$$

Maximization problem: Find lattices at which δ achieves local maxima.

Question: How does one search for such lattices in a given dimension? In particular, which properties should a lattice have to be a potential candidate for maximizer of the density function?

Similarity

All the properties that we will discuss below (unless stated otherwise) are preserved under **similarity**: $\Lambda_1 \sim \Lambda_2$ if

$$\Lambda_1 = \alpha A \Lambda_2,$$

for some $\alpha \in \mathbb{R}$ and $A \in O_N(\mathbb{R})$. This is an equivalence relation. In particular, it is easy to see that $\delta(\Lambda_1) = \delta(\Lambda_2)$, so we can talk about packing density of a similarity class, and search for a similarity class of lattices with optimal packing density.

From now on when we say that some lattice has a given property, we will usually mean that its entire similarity class has this property.

Epstein zeta function: a related problem

For a lattice Λ in $\mathbb{R}^N$, define

$$\zeta_\Lambda(s) = \sum_{\boldsymbol{x} \in \Lambda \setminus \{\boldsymbol{0}\}} \frac{1}{\|\boldsymbol{x}\|^{2s}},$$

where $s \in \mathbb{R}_{>0}$. This function has a meromorphic continuation to the entire complex plane with only a simple pole at $s = \frac{N}{2}$.

Minimization problem: Find *unimodular* lattices (i.e. with determinant = 1) which minimize $\zeta_\Lambda(s)$ for *all* $s > 0$.

The maximization problem for the packing density function is closely related to the minimization problem for the Epstein zeta function.

Theorem 1 (Ryshkov, 1973)**.** *A lattice in* $\mathbb{R}^N$ *that maximizes the packing density is a stationary point of* $\zeta_\Lambda(s)$ *as* $s \to \infty$ *if and only if it is the absolute minimum of* $\zeta_\Lambda(s)$ *as* $s \to \infty$*.*

Remarks

Notice that when we say that a lattice "maximizes packing density", we mean that its entire similarity class does that; when we say that a lattice "minimizes Epstein zeta function" for some value(s) of s, we mean that a unimodular lattice from its similarity class does that.

Although these two problems are closely related, they do not imply each other. For instance, in $\mathbb{R}^2$ it is known that Λ_h solves both of these problems, but in $\mathbb{R}^3$ the packing density maximizer Λ_{fcc} does not minimize the Epstein zeta function *for all* $s > 0$ (Sarnak, Strömbergsson (2005)). Nevertheless, developments in the direction of one of these problems usually lead to progress toward the other.

It should also be remarked that the notion of local extrema for packing density function and for Epstein zeta function makes sense, since the space of similarity classes of lattices in a given dimension, as well as the space of similarity classes of *unimodular* lattices (i.e. intersections of similarity classes with the set of unimodular lattices), can be endowed with a metric; we give an example of such a metric in dimension two further below.

The minimizer of Epstein zeta function for all $s > 0$ in $\mathbb{R}^N$ is known in dimensions $N = 2, 4, 8, 24$, the last three being recent work (2005) of Sarnak and Strömbergsson.

Special classes of lattices

Well-rounded (WR): A lattice Λ in $\mathbb{R}^N$ is called well-rounded if its set of minimal vectors

$$S(\Lambda) = \{\boldsymbol{x} \in \Lambda \ : \ \|\boldsymbol{x}\| = |\Lambda|\}$$

spans $\mathbb{R}^N$.

Fact 2. *The maximization problem for packing density can be restricted to WR lattices without loss of generality.*

Perfect: Let $S(\Lambda)$ be the set of minimal vectors of Λ, as before, written as column vectors. Λ is perfect if the set of $N \times N$ matrices

$$\{\boldsymbol{x}\boldsymbol{x}^t \ : \ \boldsymbol{x} \in S(\Lambda)\}$$

spans the group $\mathcal{S}_N(\mathbb{R})$ of all $N \times N$ symmetric real matrices in the sense that

$$\mathcal{S}_N(\mathbb{R}) = \sum_{\boldsymbol{x} \in S(\Lambda)} \mathbb{R}\boldsymbol{x}\boldsymbol{x}^t.$$

Fact 3. *Perfect lattices are WR, and perfection is a necessary condition for a lattice to maximize packing density.*

Spherical designs

A finite subset X of a sphere (not a ball) $\Sigma^{N-1}(r)$ of radius r centered at the origin in $\mathbb{R}^N$ is called a **spherical t-design**, where $t \in \mathbb{Z}_{>0}$ if for every polynomial $f(x_1, \ldots, x_N) \in \mathbb{R}[x_1, \ldots, x_N]$ of degree $\leq t$

$$\int_{\Sigma^{N-1}(r)} f(\boldsymbol{x}) d\boldsymbol{x} = \frac{1}{|X|} \sum_{\boldsymbol{x} \in X} f(\boldsymbol{x}).$$

We will say that a lattice Λ in $\mathbb{R}^N$ **holds a spherical t-design** if its set of minimal vectors $S(\Lambda)$ is a spherical t-design. A lattice is called **strongly perfect** if it holds a spherical 4-design; this implies perfection.

Theorem 4 (Venkov, 2001)**.** *If a lattice Λ in $\mathbb{R}^N$ is strongly perfect, then the packing density function δ has a local maximum at Λ.*

There usually are only finitely many strongly perfect (or even perfect) lattices in a given dimension. However, the number of strongly perfect ones is much smaller: in dimension 8 there is one (up to similarity) strongly perfect lattice, but nearly 11,000 perfect lattices.

Layers of a lattice

We now discuss a condition in terms of spherical designs, analogous to Venkov's theorem, which ensures that a lattice minimizes Epstein zeta-function in a given dimension.

Define the k-**th layer** of a lattice Λ in $\mathbb{R}^N$ as

$$S_k(\Lambda) = \{\boldsymbol{x} \in \Lambda \ : \ \|\boldsymbol{x}\| = a_k\},$$

where a_k is the k-th smallest non-zero value of Euclidean norm assumed by vectors on Λ. So, for instance, the set of minimal vectors $S(\Lambda) = S_1(\Lambda)$.

Theorem 5 (Coulangeon, 2006). *If a unimodular lattice Λ in $\mathbb{R}^N$ is such that $S_k(\Lambda)$ is a spherical 4-design for all $k \geq 1$, then the Epstein zeta function has a strict local minimum at Λ.*

The hexagonal lattice Λ_h

We will now concentrate on the situation in $\mathbb{R}^2$, which is well understood. Here the hexagonal lattice

$$\Lambda_h = \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} \end{pmatrix} \mathbb{Z}^2$$

solves both, the maximization problem for the packing density and minimization problem for the Epstein zeta function for all $s > 0$ (this was proved by Rankin (1953), Cassels (1959), Diananda (1964), and Ennola (1964)).

It is easy to see that $|\Lambda_h| = 1$, $\det(\Lambda_h) = \frac{\sqrt{3}}{2}$, and

$$S(\Lambda_h) = \{\pm \boldsymbol{x}_1, \pm \boldsymbol{x}_2, \pm \boldsymbol{x}_3\},$$

where

$$\boldsymbol{x}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \ \boldsymbol{x}_2 = \begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}, \ \boldsymbol{x}_3 = \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}.$$

In particular Λ_h is WR. Moreover, it is the only lattice in $\mathbb{R}^2$ (up to similarity) which has 6 minimal vectors: the rest have 4 or 2. This is the reason why it is also the only strongly perfect, and the only perfect, lattice in $\mathbb{R}^2$ (up to similarity, again). Indeed, let

$$A = \boldsymbol{x}_1 \boldsymbol{x}_1^t = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

$$B = \frac{2}{3}(\boldsymbol{x}_2 \boldsymbol{x}_2^t + \boldsymbol{x}_3 \boldsymbol{x}_3^t) - \frac{1}{3}\boldsymbol{x}_1 \boldsymbol{x}_1^t = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$

$$C = \frac{2}{\sqrt{3}}(\boldsymbol{x}_2 \boldsymbol{x}_2^t - \boldsymbol{x}_3 \boldsymbol{x}_3^t) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

then any real symmetric 2×2 matrix is of the form

$$M = \begin{pmatrix} a & c \\ c & b \end{pmatrix} = aA + bB + cC,$$

which means that $\boldsymbol{x}_1 \boldsymbol{x}_1^t$, $\boldsymbol{x}_2 \boldsymbol{x}_2^t$, and $\boldsymbol{x}_3 \boldsymbol{x}_3^t$ generate the group $\mathcal{S}_2(\mathbb{R})$ as a real vector space, and so Λ_h is perfect.

Theorem 6 (Venkov (2001)). *A lattice* Λ *in* $\mathbb{R}^N$ *supports a spherical* t*-design if and only if for every* $\boldsymbol{a} \in \mathbb{R}^N$*, there exists a real constant* c *such that*

$$\sum_{\boldsymbol{x} \in S(\Lambda)} (\boldsymbol{a} \cdot \boldsymbol{x})^t = c \|\boldsymbol{a}\|^t.$$

Let $\boldsymbol{a} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \in \mathbb{R}^2$, then it is not difficult to compute that

$$\sum_{\boldsymbol{x} \in S(\Lambda_h)} (\boldsymbol{a} \cdot \boldsymbol{x})^4 = \frac{9}{4}(a_1^4 + a_2^4 + 2a_1^2 a_2^2) = \frac{9}{4} \|\boldsymbol{a}\|^4.$$

Therefore, by Theorem 6, Λ_h is strongly perfect.

The statement that Λ_h is *the only* perfect and strongly perfect lattice in $\mathbb{R}^2$, up to similarity, can be proved with some more work, although we will not do it here.

Approximating the hexagonal lattice

Notice that

$$\Lambda_{fcc} = \begin{pmatrix} -1 & 1 & 0 \\ -1 & -1 & 1 \\ 0 & 0 & -1 \end{pmatrix} \mathbb{Z}^3,$$

which is the maximizer of packing density in $\mathbb{R}^3$, is a WR lattice with an **integral basis**.

On the other hand, it is not difficult to notice that no lattice in the similarity class of Λ_h has an integral (or rational) basis.

Question: How "well" can Λ_h be approximated by WR lattices with rational bases in $\mathbb{R}^2$?

To make this question rigorous, we will need some notation. For a lattice Λ in $\mathbb{R}^2$, we will write $\langle \Lambda \rangle$ for its similarity class, that is

$$\langle \Lambda \rangle = \{\alpha U \Lambda : \alpha \in \mathbb{R}_{>0},\ U \in O_2(\mathbb{R})\}.$$

Also define

$$\theta(\Lambda) = \min \left\{ \arcsin\left(\frac{|\boldsymbol{x}^t \boldsymbol{y}|}{\|\boldsymbol{x}\|\|\boldsymbol{y}\|}\right) : \boldsymbol{x}, \boldsymbol{y} \text{ is a shortest basis for } \Lambda \right\}.$$

By a **shortest basis** $\boldsymbol{x}, \boldsymbol{y}$ of Λ we mean here that $\boldsymbol{x}$ is a minimal vector of Λ, and $\boldsymbol{y}$ is a vector of smallest Euclidean norm such that $\boldsymbol{x}, \boldsymbol{y}$ is a basis for Λ.

Theorem 7 (Gauss)**.** $\theta(\Lambda) \in \left[\frac{\pi}{3}, \frac{\pi}{2}\right]$.

It is easy to notice that $\theta(\Lambda)$ remains constant on $\langle \Lambda \rangle$. If $\boldsymbol{x}, \boldsymbol{y}$ is a shortest basis for Λ with the angle between $\boldsymbol{x}$ and $\boldsymbol{y}$ equal to $\theta(\Lambda)$, then

$$\det(\Lambda) = \|\boldsymbol{x}\|\|\boldsymbol{y}\| \sin \theta(\Lambda).$$

Hence if Λ is WR, then $\|\boldsymbol{x}\| = \|\boldsymbol{y}\| = |\Lambda|$, and so

$$\det(\Lambda) = |\Lambda|^2 \sin\theta(\Lambda).$$

Let $\mathrm{Sim}(\mathbb{R}^2)$ be the set of all similarity classes of WR lattices in $\mathbb{R}^2$, then

$$\sin\theta(\Lambda) : \mathrm{Sim}(\mathbb{R}^2) \to \sin\left[\frac{\pi}{3}, \frac{\pi}{2}\right] = \left[\frac{\sqrt{3}}{2}, 1\right]$$

is a bijection. For every two $\langle\Lambda_1\rangle$ and $\langle\Lambda_2\rangle$ in $\mathrm{Sim}(\mathbb{R}^2)$, define

$$d_s(\Lambda_1, \Lambda_2) = \left|\sin\theta(\Lambda_1) - \sin\theta(\Lambda_2)\right|.$$

It is easy to see that d_s is a metric on $\mathrm{Sim}(\mathbb{R}^2)$. If Λ is a WR lattice in $\mathbb{R}^2$, then the density of circle packing given by Λ is

$$\delta(\Lambda) = \frac{\pi|\Lambda|^2}{4\det(\Lambda)} = \frac{\pi}{4\sin\theta(\Lambda)}.$$

This implies that the smaller is $\sin\theta(\Lambda)$ the bigger is $\delta(\Lambda)$, which again explains why Λ_h maximizes δ: it represents the only similarity class with $\sin\theta(\Lambda) = \frac{\sqrt{3}}{2}$, the smallest possible value.

Theorem 8 (F. (2007))**.** *There exists an infinite sequence of non-similar WR sublattices of* $\mathbb{Z}^2$*,* $\{\Lambda_k\}_{k=1}^{\infty}$*, such that*

$$\langle \Lambda_k \rangle \longrightarrow \langle \Lambda_h \rangle, \text{ as } k \to \infty,$$

with respect to the metric d_s *on* $\mathrm{Sim}(\mathbb{R}^2)$*. The rate of this convergence for all* $k > 1$ *can be expressed by*

$$\frac{1}{3\sqrt{3}\ |\Lambda_k|^2} < d_s(\Lambda_h, \Lambda_k) < \frac{1}{2\sqrt{3}\ |\Lambda_k|^2},$$

where $|\Lambda_k|^2 = O(14^k)$ *as* $k \to \infty$*. Moreover, this inequality is sharp in the sense that*

$$\frac{1}{3\sqrt{3}\ |\Lambda|^2} < d_s(\Lambda_h, \Lambda),$$

for every WR sublattice $\Lambda \subsetneq \mathbb{Z}^2$*. For the case of* $\Lambda = \mathbb{Z}^2$*, which is precisely* Λ_1 *in our sequence, we clearly have* $d_s(\Lambda_h, \mathbb{Z}^2) = \frac{2-\sqrt{3}}{2}$*.*

Corollary 9. *Each similarity class* $\langle \Lambda_k \rangle$ *of Theorem 8 gives circle packing density* $\delta(\Lambda_k)$ *such that*

$$\begin{aligned}
& \delta(\Lambda_h)\left(\frac{1}{1+\frac{1}{723\times(13.928)^{k-1}}}\right) \\
< \; & \delta(\Lambda_k) \\
< \; & \delta(\Lambda_h)\left(\frac{1}{1+\frac{0.92}{723\times(13.947)^{k-1}}}\right),
\end{aligned}$$

where $\delta(\Lambda_h) = \frac{\pi}{\sqrt{12}} = 0.9069...$ *is the circle packing density of* Λ_h.