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On similarity classes of well-rounded sublattices of $\mathbb{Z}^2$

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ABSTRACT

Text. A lattice is called well-rounded if its minimal vectors span the corresponding Euclidean space. In this paper we study the similarity classes of well-rounded sublattices of $\mathbb{Z}^2$. We relate the set of all such similarity classes to a subset of primitive Pythagorean triples, and prove that it has the structure of a non-commutative infinitely generated monoid. We discuss the structure of a given similarity class, and define a zeta function corresponding to each similarity class. We relate it to Dedekind zeta of $\mathbb{Z}[i]$, and investigate the growth of some related Dirichlet series, which reflect on the distribution of well-rounded lattices. We also construct a sequence of similarity classes of well-rounded sublattices of $\mathbb{Z}^2$, which gives good circle packing density and converges to the hexagonal lattice as fast as possible with respect to a natural metric we define. Finally, we discuss distribution of similarity classes of well-rounded sublattices of $\mathbb{Z}^2$ in the set of similarity classes of all well-rounded lattices in $\mathbb{R}^2$.

Video. For a video summary of this paper, please visit http://www.youtube.com/watch?v=q3LJV4lv0PA.

Contents

1. Introduction and statement of results 2531
2. Parametrization by Pythagorean triples 2538
3. Similarity classes and corresponding zeta functions 2543
4. Weight enumerators $W_d(s)$ and $W_m(s)$ 2548
5. Approximating the hexagonal lattice 2550
6. Diophantine approximation by quotients of Pythagorean triples 2554

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Acknowledgments 2555
Supplementary material 2556
References 2556

1. Introduction and statement of results

Let $N \geqslant 2$ be an integer, and let $\Lambda \subseteq \mathbb{R}^N$ be a lattice of full rank. Define the *minimum* of Λ to be

$$|\Lambda| = \min_{\boldsymbol{x} \in \Lambda \setminus \{\mathbf{0}\}} \|\boldsymbol{x}\|,$$

where $\| \ \|$ stands for the usual Euclidean norm on $\mathbb{R}^N$. Let

$$S(\Lambda) = \left\{\boldsymbol{x} \in \Lambda\colon \ \|\boldsymbol{x}\| = |\Lambda|\right\}$$

be the set of *minimal vectors* of Λ. We say that Λ is a *well-rounded* lattice (abbreviated WR) if $S(\Lambda)$ spans $\mathbb{R}^N$. WR lattices come up in a wide variety of different contexts, including discrete optimization (e.g. sphere packing, covering, and kissing number problems), coding theory, and the linear Diophantine problem of Frobenius, just to name a few. In particular, the classical discrete optimization problems on lattices can usually be reduced to WR lattices in every dimension. Distribution of unimodular WR lattices in $\mathbb{R}^N$ has been studied by C. McMullen in [17]. Also, the distribution of full-rank WR sublattices of $\mathbb{Z}^2$ has been recently studied in [10]. The goal of this paper is to continue this investigation from a somewhat different perspective. In particular, in [10] the zeta function $\zeta_{\mathrm{WR}(\mathbb{Z}^2)}(s)$ of WR sublattices of $\mathbb{Z}^2$ has been introduced, and we proved that it is analytic in the half-plane $\Re(s) > 1$ with a pole of order *at least two* at $s = 1$. In Theorem 1.5 we establish that in fact the order of the pole is *exactly* two, where the notion of the order of the pole we use here is defined by (13) below. To obtain this result we study the structure of the set of similarity classes of WR sublattices of $\mathbb{Z}^2$ (Theorems 1.1–1.3) and use it to provide a simple analytic description for the Dirichlet series corresponding to each such similarity class (Theorem 1.4). We then decompose $\zeta_{\mathrm{WR}(\mathbb{Z}^2)}(s)$ over similarity classes to prove Theorem 1.5. We also discuss sphere packing density of similarity classes of WR sublattices of $\mathbb{Z}^2$ (Theorem 1.6 and Corollary 1.7), as well as their distribution among *all* WR similarity classes in $\mathbb{R}^2$ (Theorem 1.8).

We start out with a few words of motivation for the problems we study here. The similarity classes of the integer lattice $\mathbb{Z}^2$ and the hexagonal lattice Λ_h (defined in (20) below) are very special in dimension two: these are the only two strongly eutactic similarity classes in $\mathbb{R}^2$, and $\langle \Lambda_h \rangle$ is the only strongly perfect similarity class (we define the notions of strong eutaxy and perfection at the end of Section 5, see (61) in particular; also see [16], especially Chapter 16, for a detailed discussion of strongly eutactic and strongly perfect lattices and their properties). The distribution of sublattices of Λ_h is studied in [6], while the distribution of *all* sublattices of $\mathbb{Z}^2$ is well understood (see for instance [10], especially (52) and the beginning of Section 8, for a discussion of this). Studying the distribution of WR sublattices of these lattices is arguably even more important, since the WR property is vital in lattice theory. The goal of [10] and the current paper is to carry out this investigation for $\mathbb{Z}^2$. We now introduce necessary notation and describe our results in more details.

Recall that two lattices $\Lambda_1, \Lambda_2 \subseteq \mathbb{R}^N$ of rank N are said to be *similar* if there exist a matrix A in $O_N(\mathbb{R})$, the group of $N \times N$ real orthogonal matrices, and a real constant α such that $\Lambda_1 = \alpha A \Lambda_2$. This is an equivalence relation, which we will denote by writing $\Lambda_1 \sim \Lambda_2$, and the equivalence classes of lattices under this relation in $\mathbb{R}^N$ are called *similarity classes*. The distribution of sublattices of $\mathbb{Z}^N$ among similarity classes has been investigated by W.M. Schmidt in [21].

The first trivial observation we can make is that WR property is preserved under similarity. In other words, if two full-rank lattices $\Lambda_1, \Lambda_2 \subseteq \mathbb{R}^N$ are similar, say $\Lambda_1 = \alpha A \Lambda_2$ for some $\alpha \in \mathbb{R}$ and $A \in O_N(\mathbb{R})$, then

$$\det(\Lambda_1) = |\alpha|^N \det(\Lambda_2), \qquad |\Lambda_1| = |\alpha||\Lambda_2|,$$

and Λ_1 is WR if and only if Λ_2 is WR. Therefore we can talk about similarity classes of well-rounded lattices in $\mathbb{R}^N$. From now on we will write $\mathrm{WR}(\Omega)$ for the set of all full-rank WR sublattices of a lattice Ω; we will concentrate on $\mathrm{WR}(\mathbb{Z}^N)$, so let us write $\mathcal{D}_N$ and $\mathfrak{M}_N$ for the sets of determinant and squared minima values, respectively, of lattices from $\mathrm{WR}(\mathbb{Z}^N)$. We will also write $\mathcal{C}_N$ for the set of all similarity classes of lattices in $\mathrm{WR}(\mathbb{Z}^N)$: this is a slight abuse of notation, since elements of $\mathcal{C}_N$ are really nonempty intersections of similarity classes of lattices in $\mathbb{R}^N$ with $\mathrm{WR}(\mathbb{Z}^N)$, as indicated in (15) below when $N = 2$.

In this paper we study the case $N = 2$. It is known that for every $\Lambda \in \mathrm{WR}(\mathbb{Z}^2)$ the set $S(\Lambda)$ has cardinality 4, and contains a *minimal basis* for Λ, which is unique up to $\pm$ signs and reordering (see Lemma 3.2 of [10]). For each $q \in \mathbb{Z}_{>0}$, define

$$\mathcal{S}_q = \left\{ \frac{p}{q} \in \mathbb{Q} \cap \left(\frac{\sqrt{3}}{2}, 1 \right) : \ \gcd(p,q) = 1, \ \sqrt{q^2 - p^2} \in \mathbb{Z} \right\}, \tag{1}$$

and let

$$\mathcal{S} = \left(\bigcup_{q \in \mathbb{Z}_{>0}} \mathcal{S}_q \right) \cup \{1\}, \tag{2}$$

where 1 is also thought of as p/q with $p = q = 1$. It is easy to see that the union in (2) is disjoint, and each $\mathcal{S}_q$ is a subset of the set of Farey fractions of order q in the interval $(\frac{\sqrt{3}}{2}, 1)$. In Section 2 we show that the similarity classes of lattices in $\mathrm{WR}(\mathbb{Z}^2)$ are in bijective correspondence with fractions $p/q \in \mathcal{S}$. From now on, for each $p/q \in \mathcal{S}$, we will write $C(p,q)$ for the corresponding similarity class in $\mathcal{C}_2$, the set of all similarity classes of lattices in $\mathrm{WR}(\mathbb{Z}^2)$; a formal definition of $C(p,q)$ is given by (25). The class $C(1,1)$ plays a special role: it is precisely the similarity class of all *orthogonal* well-rounded lattices, i.e. lattices of the form $\left(\begin{smallmatrix} a & -b \\ b & a \end{smallmatrix}\right)\mathbb{Z}^2$ for some $a, b \in \mathbb{Z}$. The set $\mathcal{C}_2$ has interesting algebraic and combinatorial structure. It is not difficult to notice that the set $\mathcal{S}$, which parametrizes $\mathcal{C}_2$, is in bijective correspondence with the set of primitive Pythagorean triples whose shortest leg is less than half of the hypotenuse. In Section 2 we explore this connection in details and use it to prove the following result.

Theorem 1.1. *The set $\mathcal{C}_2$ of similarity classes of lattices in $\mathrm{WR}(\mathbb{Z}^2)$ has the algebraic structure of an infinitely generated free non-commutative monoid with the class $C(1,1)$ of orthogonal well-rounded lattices serving as identity. As a combinatorial object, $\mathcal{C}_2$ has the structure of a regular rooted infinite tree, where each vertex has infinite degree, which is precisely the Cayley digraph of this monoid.*

Remark 1.1. If G is a monoid with a generating set X, then we define its *Cayley digraph* to be a directed graph with vertices corresponding to the elements of G, and with a directed edge between vertices g and h if $h = gx$ for some $x \in X$ (see for instance [19] for details and related terminology).

We explicitly construct the monoid and the corresponding tree structure for $\mathcal{C}_2$ in Section 2. Notice that due to Theorem 1.1 it makes sense to think of $\mathcal{C}_2$ as the moduli space of lattices in $\mathrm{WR}(\mathbb{Z}^2)$.

In Section 3, we discuss a more explicit parametrization of $\mathcal{C}_2$, which allows to see the structure of each similarity class $C(p,q)$. It turns out that, although most well-rounded lattices are not orthogonal, all similarity classes in $\mathcal{C}_2$ can be parametrized by a subset of lattices from $C(1,1)$. More precisely, let us define a subset of $\mathbb{Z}^2$

$$\mathcal{A} = \big\{(a,b) \in \mathbb{Z}^2 \colon\ 0 < b < a,\ \gcd(a,b) = 1,\ 2 \nmid (a+b),$$
$$\text{and either } b < a < \sqrt{3}b,\ \text{or } (2+\sqrt{3})b < a\big\}, \tag{3}$$

and consider the corresponding subset of $C(1,1)$

$$C'(1,1) = \left\{ \begin{pmatrix} a & -b \\ b & a \end{pmatrix} \mathbb{Z}^2 \in C(1,1) \colon\ (a,b) \in \mathcal{A} \right\}. \tag{4}$$

In Section 3 we prove the following theorem.

Theorem 1.2. *For each $p/q \in \mathcal{S}$, there exists a unique lattice*

$$\Omega = \begin{pmatrix} a & -b \\ b & a \end{pmatrix} \mathbb{Z}^2 \in C'(1,1),$$

where $a, b \in \mathbb{Z}_{>0}$ are given by

$$p = \max\big\{a^2 - b^2, 2ab\big\}, \quad \text{and} \quad q = a^2 + b^2, \tag{5}$$

such that $\Lambda \in C(p,q)$ if and only if

$$\Lambda = \operatorname{span}_{\mathbb{Z}} \left\{ \boldsymbol{x},\ \begin{pmatrix} \frac{\sqrt{q^2-p^2}}{q} & -\frac{p}{q} \\ \frac{p}{q} & \frac{\sqrt{q^2-p^2}}{q} \end{pmatrix} \boldsymbol{x} \right\} \tag{6}$$

for some $\boldsymbol{x} \in \Omega$. Moreover, every lattice in the set $C'(1,1)$ parametrizes some similarity class $C(p,q)$ with p, q as in (5) *in this way.*

An easy consequence of Theorem 1.2 is the existence of a lattice in each similarity class $C(p,q)$ which, in a sense to be described below, generates $C(p,q)$. First let us recall that given a full-rank lattice Λ in $\mathbb{R}^2$, its Epstein zeta function is defined by

$$E_\Lambda(s) = {\sum_{\boldsymbol{x} \in \Lambda}}' \|\boldsymbol{x}\|^{-2s},$$

where $s \in \mathbb{C}$, and $'$ indicates that the sum is taken over all $\boldsymbol{x} \in (\Lambda/\{\pm 1\}) \setminus \{\boldsymbol{0}\}$. For each such Λ, this Dirichlet series is known to converge for all s with $\Re(s) > 1$. Moreover, $E_\Lambda(s)$ has analytic continuation to $\mathbb{C}$ except for a simple pole at $s = 1$. For more information on $E_\Lambda(s)$ and its properties see [20]. In Section 3 we also prove the following theorem.

Theorem 1.3. *Let $C(p,q) \in \mathcal{C}_2$. There exists a lattice $\Lambda_{p,q} \in C(p,q)$, satisfying the following properties*:

(1) $|\Lambda_{p,q}| = \min\{|\Lambda| \colon\ \Lambda \in C(p,q)\} = \sqrt{q}$.
(2) $\det(\Lambda_{p,q}) = \min\{\det(\Lambda) \colon\ \Lambda \in C(p,q)\} = p$.
(3) *The norm form of $\Lambda_{p,q}$ with respect to its minimal basis is*

$$Q_{p,q}(x,y) = qx^2 + 2xy\sqrt{q^2 - p^2} + qy^2.$$

(4) *For each $\Lambda \in C(p,q)$ there exists $U \in O_2(\mathbb{R})$ such that $\Lambda = \sqrt{\frac{\det(\Lambda)}{p}}\, U \Lambda_{p,q}$; the quadratic form $(\frac{\det(\Lambda)}{p}) Q_{p,q}(x,y)$ is therefore the norm form for Λ with respect to its minimal basis.*

(5) *The Epstein zeta function of any lattice $\Lambda \in C(p,q)$ is of the form*

$$E_\Lambda(s) = \left(\frac{p}{\det(\Lambda)}\right)^s \sum_{(x,y)\in\mathbb{Z}^2}{}' \frac{1}{Q_{p,q}(x,y)^s},$$

and so $\Lambda_{p,q}$ maximizes $E_\Lambda(s)$ on $C(p,q)$ for each real value of $s > 1$.

We call $\Lambda_{p,q}$ a minimal lattice of its similarity class $C(p,q)$; it is unique up to a rational rotation.

Lattices $\Lambda_{p,q}$ also determine zeta functions of corresponding similarity classes $C(p,q)$. Namely, with each $C(p,q) \in \mathcal{C}_2$ we can now associate two Dirichlet series, which incorporate information about the determinants and the minima of lattices in this similarity class, respectively. Specifically, define

$$Z^d_{p,q}(s) = \sum_{\Lambda\in C(p,q)} \big(\det(\Lambda)\big)^{-s}, \qquad Z^m_{p,q}(s) = \sum_{\Lambda\in C(p,q)} |\Lambda|^{-2s},$$

where $s \in \mathbb{C}$. Our next goal is to investigate the properties of $Z^d_{p,q}(s)$ and $Z^m_{p,q}(s)$ for each $C(p,q) \in \mathcal{C}_2$, which we do by relating them to the Epstein zeta function of the lattice Ω parametrizing $C(p,q)$, as in Theorem 1.2.

We will also write $\zeta_K(s)$ for the Dedekind zeta function of a number field K. It is known to be analytic for all $s \in \mathbb{C}$ with $\Re(s) > 1 - 1/d$, where $d = [K:\mathbb{Q}]$, except for a simple pole at $s = 1$. For more information on properties of $\zeta_K(s)$ see [15]. There is a standard relation between Dedekind zeta of imaginary quadratic fields and lattices of rank two, a special case of which we exploit here; see [23] for more details.

Theorem 1.4. *For each $C(p,q) \in \mathcal{C}_2$,*

$$Z^d_{p,q}(s) = \frac{1}{p^s}\zeta_{\mathbb{Q}(i)}(s) = \frac{1}{(\det(\Lambda_{p,q}))^s}\zeta_{\mathbb{Q}(i)}(s), \tag{7}$$

and

$$Z^m_{p,q}(s) = \frac{1}{q^s}\zeta_{\mathbb{Q}(i)}(s) = \frac{1}{|\Lambda_{p,q}|^{2s}}\zeta_{\mathbb{Q}(i)}(s). \tag{8}$$

We prove Theorem 1.4 in Section 3, as well. Notice in particular that $C(1,1)$, the similarity class of all lattices coming from ideals in $\mathbb{Z}[i]$, has $Z^d_{1,1}(s) = Z^m_{1,1}(s) = \zeta_{\mathbb{Q}[i]}(s)$, since $\Lambda_{1,1} = \mathbb{Z}^2$. This fact is also discussed in [10].

In [10] we studied basic properties of the zeta function of *all* well-rounded lattices

$$\zeta_{\mathrm{WR}(\mathbb{Z}^2)}(s) = \sum_{\Lambda\in\mathrm{WR}(\mathbb{Z}^2)} \big(\det(\Lambda)\big)^{-s}.$$

It also makes sense to define

$$\zeta^m_{\mathrm{WR}(\mathbb{Z}^2)}(s) = \sum_{\Lambda\in\mathrm{WR}(\mathbb{Z}^2)} |\Lambda|^{-2s}.$$

These two Dirichlet series carry information about the distribution of lattices in $\mathrm{WR}(\mathbb{Z}^2)$ with respect to their determinant and minima values. For each similarity class $C(p,q) \in \mathcal{C}_2$, let us call p its *determinant weight* and q its *minima weight*. Theorem 1.4 immediately implies that

$$\zeta_{\mathrm{WR}(\mathbb{Z}^2)}(s) = \sum_{C(p,q)\in\mathcal{C}_2} \sum_{\Lambda\in C(p,q)} \big(\det(\Lambda)\big)^{-s}$$
$$= \sum_{C(p,q)\in\mathcal{C}_2} Z^d_{p,q}(s) = \zeta_{\mathbb{Q}(i)}(s) \sum_{\substack{p:\ p/q\in\mathcal{S} \\ \text{for some } q\in\mathbb{Z}_{>0}}} \frac{a_p}{p^s}, \tag{9}$$

and similarly

$$\zeta^m_{\mathrm{WR}(\mathbb{Z}^2)}(s) = \zeta_{\mathbb{Q}(i)}(s) \sum_{\substack{q:\ p/q\in\mathcal{S} \\ \text{for some } p\in\mathbb{Z}_{>0}}} \frac{b_q}{q^s}, \tag{10}$$

where a_p is the number of similarity classes in $\mathcal{C}_2$ with determinant weight p, and b_q is the number of similarity classes in $\mathcal{C}_2$ with minima weight q; notice that $b_q = |\mathcal{S}_q|$, where $\mathcal{S}_q$ is as in (1). In fact, let us write

$$W_d(s) = \sum_{C(p,q)\in\mathcal{C}_2} \frac{1}{p^s} = \sum_{\substack{p:\ p/q\in\mathcal{S} \\ \text{for some } q\in\mathbb{Z}_{>0}}} \frac{a_p}{p^s}, \tag{11}$$

and

$$W_m(s) = \sum_{C(p,q)\in\mathcal{C}_2} \frac{1}{q^s} = \sum_{\substack{q:\ p/q\in\mathcal{S} \\ \text{for some} p\in\mathbb{Z}_{>0}}} \frac{b_q}{q^s}. \tag{12}$$

We will call $W_d(s)$ and $W_m(s)$ *determinant* and *minima weight enumerators*, respectively. Therefore the question of distribution of lattices in $\mathrm{WR}(\mathbb{Z}^2)$ is linked to understanding the basic analytic properties of $W_d(s)$ and $W_m(s)$. In Section 4 we use an approach different from that of [10] to prove the following result.

Theorem 1.5. *Let the notation be as above, then $W_d(s)$ and $W_m(s)$ both have simple poles at $s = 1$ and are analytic for all $s \in \mathbb{C}$ with $\Re(s) > 1$. Therefore $\zeta_{\mathrm{WR}(\mathbb{Z}^2)}(s)$ and $\zeta^m_{\mathrm{WR}(\mathbb{Z}^2)}(s)$ both have poles of order two at $s = 1$ and are analytic for all $s \in \mathbb{C}$ with $\Re(s) > 1$.*

We should point out that we are using the notion of a pole here *not* in a sense that would imply the existence of an analytic continuation, but only to reflect on the growth of the coefficients. More precisely, for a Dirichlet series $\sum_{n=1}^{\infty} c_n n^{-s}$, we say that it has a *pole of order* μ at $s = s_0$, where μ and s_0 are positive real numbers, if

$$0 < \lim_{s\to s_0^+} |s - s_0|^{\mu} \sum_{n=1}^{\infty} \big|c_n n^{-s}\big| < \infty. \tag{13}$$

Notice that Theorem 1.5 in particular improves slightly on the result of Theorem 1.5 of [10]. The approach we use in Section 4 to prove Theorem 1.5 uses bounds on coefficients of weight enumerators $W_d(s)$ and $W_m(s)$ by coefficients of Dirichlet series associated with the set of primitive Pythagorean triples, which have Euler product expansions.

A standard object of lattice theory is a sphere packing associated with a lattice, and a classical problem is to determine the optimal packing density among lattices in a given dimension (see [9]). This problem has been solved in dimension two; in fact, it is not difficult to show that maximization of packing density can be restricted to WR lattices. Here we will discuss the circle packing density corresponding to lattices in $\mathrm{WR}(\mathbb{Z}^2)$, investigating how "close" can one come to the optimal packing

density in dimension two with such lattices. For these purposes, let us write $\langle \Lambda \rangle$ for the similarity class of any lattice Λ in $\mathbb{R}^2$, so that

$$\langle \Lambda \rangle = \{\alpha U \Lambda \colon\ \alpha \in \mathbb{R}_{>0},\ U \in O_2(\mathbb{R})\}. \tag{14}$$

Then for each $p/q \in \mathcal{S}$,

$$C(p,q) = \langle \Lambda_{p,q} \rangle \cap \mathrm{WR}(\mathbb{Z}^2). \tag{15}$$

For a lattice Λ in $\mathbb{R}^2$ define

$$\theta(\Lambda) = \min\left\{ \arcsin\left(\frac{|\boldsymbol{x}^t \boldsymbol{y}|}{\|\boldsymbol{x}\| \|\boldsymbol{y}\|} \right) \colon\ \boldsymbol{x}, \boldsymbol{y} \text{ is a shortest basis for } \Lambda \right\}. \tag{16}$$

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. By a well-known lemma of Gauss, $\theta(\Lambda) \in [\frac{\pi}{3}, \frac{\pi}{2}]$ (see [10]). It is easy to notice that $\theta(\Lambda)$ remains constant on $\langle \Lambda \rangle$, so we can also write $\theta(\langle \Lambda \rangle)$. 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

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

and so if Λ is well-rounded, then $\|\boldsymbol{x}\| = \|\boldsymbol{y}\| = |\Lambda|$, and so

$$\det(\Lambda) = |\Lambda|^2 \sin\theta(\Lambda). \tag{17}$$

It is easy to see that two well-rounded lattices $\Lambda_1, \Lambda_2 \subseteq \mathbb{R}^2$ are similar if and only if $\theta(\Lambda_1) = \theta(\Lambda_2)$, i.e. if and only if

$$\sin\theta(\Lambda_1) = \sin\theta(\Lambda_2) \in \left[\frac{\sqrt{3}}{2}, 1 \right],$$

and so similarity classes of well-rounded lattices in $\mathbb{R}^2$ are indexed by real numbers in the interval $[\frac{\sqrt{3}}{2}, 1]$. Let $\mathrm{Sim}(\mathbb{R}^2)$ be the set of all similarity classes of well-rounded lattices in $\mathbb{R}^2$, and for every two $\langle \Lambda_1 \rangle, \langle \Lambda_2 \rangle \in \mathrm{Sim}(\mathbb{R}^2)$ define

$$d_s(\Lambda_1, \Lambda_2) = \left| \sin\theta(\Lambda_1) - \sin\theta(\Lambda_2) \right|. \tag{18}$$

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

$$\delta(\Lambda) = \frac{\pi |\Lambda|^2}{4 \det(\Lambda)} = \frac{\pi}{4 \sin\theta(\Lambda)}, \tag{19}$$

by (17), and so it depends not on the particular lattice Λ, but on its similarity class $\langle \Lambda \rangle$. Moreover, (19) implies that the smaller is $\sin\theta(\Lambda)$ the bigger is $\delta(\Lambda)$. Indeed, it is a well-known fact that the similarity class $\langle \Lambda_h \rangle$ gives the optimal circle packing in dimension two, where

$$\Lambda_h = \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} \end{pmatrix} \mathbb{Z}^2 \tag{20}$$

is the two-dimensional hexagonal lattice, and $\sin\theta(\Lambda_h) = \frac{\sqrt{3}}{2}$. The lattice Λ_h also has the largest minimum among all lattices in $\mathbb{R}^2$ with the same determinant, and minimizes Epstein zeta function

for all real values of $s > 1$ (see [7]). However, $\langle \Lambda_h \rangle \cap \mathrm{WR}(\mathbb{Z}^2) = \emptyset$. How well, with respect to the metric d_s on $\mathrm{Sim}(\mathbb{R}^2)$, can we approximate the similarity class $\langle \Lambda_h \rangle$ with similarity classes of the form $\langle \Lambda_{p,q} \rangle$, i.e. with similarity classes that have a nonempty intersection with the set $\mathrm{WR}(\mathbb{Z}^2)$? This question is especially interesting since, in contrast to the two-dimensional situation, the three-dimensional counterpart of Λ_h, the face-centered cubic (fcc) lattice which maximizes sphere packing density in $\mathbb{R}^3$, is in $\mathrm{WR}(\mathbb{Z}^3)$. Our next result addresses this question.

Theorem 1.6. *There exists an infinite sequence of similarity classes $\langle \Lambda_{p_k,q_k} \rangle$ such that*

$$\langle \Lambda_{p_k,q_k} \rangle \to \langle \Lambda_h \rangle, \quad \text{as } k \to \infty,$$

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

$$\frac{1}{3\sqrt{3}q_k} < d_s(\Lambda_h, \Lambda_{p_k,q_k}) < \frac{1}{2\sqrt{3}q_k}, \tag{21}$$

where $q_k = O(14^k)$ as $k \to \infty$. Moreover, the inequality (21) is sharp in the sense that

$$\frac{1}{3\sqrt{3}q} < d_s(\Lambda_h, \Lambda_{p,q}), \tag{22}$$

for every similarity class of the form $\langle \Lambda_{p,q} \rangle \neq \langle \Lambda_{1,1} \rangle$. For the similarity class of orthogonal well-rounded lattices $\langle \Lambda_{1,1} \rangle = \langle \mathbb{Z}^2 \rangle$, we clearly have $d_s(\Lambda_h, \mathbb{Z}^2) = \frac{2-\sqrt{3}}{2}$.

Corollary 1.7. *Each similarity class $\langle \Lambda_{p_k,q_k} \rangle$ of Theorem 1.6 gives circle packing density δ_{p_k,q_k} such that*

$$\delta(\Lambda_h)\left(\frac{1}{1+\frac{1}{723\times(13.928)^{k-1}}}\right) < \delta_{p_k,q_k} < \delta(\Lambda_h)\left(\frac{1}{1+\frac{0.92}{723\times(13.947)^{k-1}}}\right), \tag{23}$$

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

We prove Theorem 1.6 and Corollary 1.7 in Section 5. Notice that a well-rounded lattice in $\mathbb{R}^2$ has a rational basis, i.e. a basis consisting of vectors with rational coordinates, if and only if it belongs to a similarity class $\langle \Lambda_{p,q} \rangle$ for some p, q. Therefore results of Theorem 1.6 and Corollary 1.7 can be interpreted as statements on best approximation to Λ_h (and hence best circle packing) by well-rounded lattices in $\mathbb{R}^2$ with rational bases. As we will see in Section 5, this just comes down to finding best approximations to $\frac{\sqrt{3}}{2}$ by fractions $\frac{p}{q}$ where $(p, \sqrt{q^2-p^2}, q)$ is a primitive Pythagorean triple with $\sqrt{q^2-p^2} \leqslant q/2$. In fact, a similar approximation result holds for all WR lattices in $\mathbb{R}^2$, not just Λ_h.

Theorem 1.8. *The similarity classes of WR sublattices of $\mathbb{Z}^2$ are dense in the set of all similarity classes of WR lattices in $\mathbb{R}^2$, in other words the set $\{\langle \Lambda_{p,q} \rangle\colon\ p/q \in \mathcal{S}\}$ is dense in $\mathrm{Sim}(\mathbb{R}^2)$ with respect to the metric d_s. Moreover, for every $\Lambda \in \mathrm{Sim}(\mathbb{R}^2)$, there exist infinitely many non-similar lattices $\Lambda_{p,q} \in \mathrm{WR}(\mathbb{Z}^2)$ such that*

$$d_s(\Lambda, \Lambda_{p,q}) \leqslant \frac{2\sqrt{2}}{q}. \tag{24}$$

We derive Theorem 1.8 in Section 6 as an easy corollary of a theorem of Hlawka on Diophantine approximation with quotients of Pythagorean triples, and discuss equidistribution of $\{\langle \Lambda_{p,q} \rangle\colon\ p/q \in \mathcal{S}\}$ in $\mathrm{Sim}(\mathbb{R}^2)$. As a side remark in Section 6, we also use Hlawka's result to approximate points on

a rational ellipse by rational points on the same ellipse. Notice that Theorem 1.8 does not include Theorem 1.6 as a special case, since the approximating constants in Theorem 1.6 are sharper and the proof is constructive unlike that of Theorem 1.8. We are now ready to proceed.

2. Parametrization by Pythagorean triples

Notice that if a lattice $\Lambda \in \mathrm{WR}(\mathbb{Z}^2)$, then $\cos\theta(\Lambda), \sin\theta(\Lambda) \in \mathbb{Q}_{>0}$, where $\theta(\Lambda)$ is defined in (16), and therefore we can index similarity classes of lattices in $\mathrm{WR}(\mathbb{Z}^2)$ by fractions $p/q \in \mathcal{S}$, where $\mathcal{S}$ is as in (2), so for each such p/q the corresponding similarity class $C(p,q) \in \mathcal{C}_2$ is a set of the form

$$C(p,q) = \left\{ \Lambda \in \mathrm{WR}(\mathbb{Z}^2) \colon \ \sin\theta(\Lambda) = \frac{p}{q} \right\}. \tag{25}$$

For each $p/q \in \mathcal{S}$, define $t = \sqrt{q^2 - p^2} \in \mathbb{Z}$. Then it is easy to notice that

$$0 \leqslant t < \frac{q}{2} < \frac{\sqrt{3}q}{2} < p \leqslant q,$$

and $t^2 + p^2 = q^2$ with $\gcd(t,p,q) = 1$. In other words, the set $\mathcal{S}$, and therefore the set $\mathcal{C}_2$ of similarity classes of lattices in $\mathrm{WR}(\mathbb{Z}^2)$, is in bijective correspondence with the set of primitive Pythagorean triples with the shortest leg being less than half of the hypotenuse.

Let

$$\mathfrak{P} = \left\{ (x,y,z) \colon \ x,y,z \in \mathbb{Z}_{>0},\ 2|y,\ \gcd(x,y,z) = 1,\ x^2 + y^2 = z^2 \right\}$$

be the set of all primitive Pythagorean triples, and let

$$\mathcal{P} = \left\{ (x,y,z) \in \mathfrak{P} \colon \ \min\{x,y\} < z/2 \right\} \cup \left\{ (1,0,1) \right\}.$$

Notice that we include $(1,0,1)$ in $\mathcal{P}$, although it is traditionally not included in $\mathfrak{P}$. Then $p/q \in \mathcal{S}$ if and only if either $(t,p,q) \in \mathcal{P}$ or $(p,t,q) \in \mathcal{P}$. In other words, elements of $\mathcal{P}$ can be used to enumerate similarity classes of lattices in $\mathrm{WR}(\mathbb{Z}^2)$. We will use this approach to provide a convenient combinatorial description of elements of $\mathcal{C}_2$. Define matrices

$$A = \begin{pmatrix} 1 & -2 & 2 \\ 2 & -1 & 2 \\ 2 & -2 & 3 \end{pmatrix}, \qquad B = \begin{pmatrix} 1 & 2 & 2 \\ 2 & 1 & 2 \\ 2 & 2 & 3 \end{pmatrix}, \qquad C = \begin{pmatrix} -1 & 2 & 2 \\ -2 & 1 & 2 \\ -2 & 2 & 3 \end{pmatrix} \in \mathrm{GL}_3(\mathbb{Z}), \tag{26}$$

and let $G = \langle I_3, A, B, C \rangle$ be the non-commutative monoid generated by A, B, C with the 3×3 identity matrix I_3. Let us think of elements of $\mathfrak{P}$ as vectors in $\mathbb{Z}^3$, and for each $M \in G$ define the corresponding linear transformations

$$M(x,y,z) = M \begin{pmatrix} x \\ y \\ z \end{pmatrix}. \tag{27}$$

It is a well-known fact that for every $(x,y,z) \in \mathfrak{P}$, $A(x,y,z), B(x,y,z), C(x,y,z) \in \mathfrak{P}$. Moreover, every $(x,y,z) \in \mathfrak{P}$ can be obtained in a unique way by applying a sequence of linear transformations A, B, C to $(3,4,5)$, the smallest triple in $\mathfrak{P}$ (this construction is attributed to Barning [4]; also see [1,18]). This means that (27) defines a free action of G on the set $\mathfrak{P}$ of primitive Pythagorean triples by left multiplication. The set $\mathfrak{P}$ has the structure of an infinite rooted ternary tree with respect to this action, as described in [1]; this in particular implies that G is a free monoid. In fact, this tree (see Fig. 1 below) is precisely the Cayley digraph of G with respect to the generating set $\{A, B, C\}$.

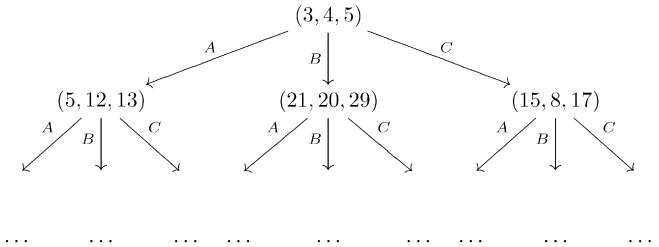

Fig. 1. Ternary tree representation for $\mathfrak{P}$.

We can extend this construction by considering the set $\mathfrak{P}' = \mathfrak{P} \cup \{(1,0,1)\}$ (compare with [2]). It is easy to notice that $A(1,0,1) = B(1,0,1) = (3,4,5)$ and $C(1,0,1) = (1,0,1)$, and hence every $(x,y,z) \in \mathfrak{P}$ can be obtained by applying a sequence of linear transformations A, B, C to $(1,0,1)$. Such a sequence is no longer unique, hence action of G does not extend to $\mathfrak{P}'$, however a *shortest* such sequence is unique up to multiplication on the left by either BA^{-1} or AB^{-1}.

Notice that $\mathcal{P} \subset \mathfrak{P}'$. Let

$$H = \big\{A^2NB, A^kB, ABNB, C^2NB, C^kB, CBNB, (AC)^kA^2NB, (AC)^kABNB, (AC)^kAB,$$
$$(CA)^kC^2NB, (CA)^kCBNB, (CA)^kCB\colon\ N \in G,\ k \in \mathbb{Z}_{>0}\big\}. \tag{28}$$

It is clear that H is a subsemigroup and $H' = H \cup \{I_3\}$ is a submonoid of G. Let us define the image of $\mathfrak{P}'$ under G to be

$$G\mathfrak{P}' = \big\{M(x,y,z)\colon\ M \in G,\ (x,y,z) \in \mathfrak{P}'\big\},$$

and similarly for the images $G\mathcal{P}$, $H\mathfrak{P}'$, and $H\mathcal{P}$.

Lemma 2.1. $H\mathfrak{P}' = H\mathcal{P} = \mathcal{P} \setminus \{(1,0,1)\}$.

Proof. First we will prove that $H\mathfrak{P}' \subseteq \mathcal{P}$. It is clear that $(1,0,1) \notin H\mathfrak{P}'$. Let $M \in H$, then there exists some $N \in G$ such that one of the following is true:

(1) $M = A^2N$,
(2) $M = ABN$,
(3) $M = C^2N$,
(4) $M = CBN$,
(5) $M = (AC)^kA^2N$, where $k \in \mathbb{Z}_{>0}$,
(6) $M = (AC)^kABN$, where $k \in \mathbb{Z}_{>0}$,
(7) $M = (CA)^kC^2N$, where $k \in \mathbb{Z}_{>0}$,
(8) $M = (CA)^kCBN$, where $k \in \mathbb{Z}_{>0}$.

Let $(x,y,z) \in \mathfrak{P}'$, and write $(x',y',z') = N(x,y,z)$, where N is as above. Then, in case (1)

$$M(x,y,z) = A^2(x',y',z') = \begin{pmatrix} x' - 4y' + 4z' \\ 4x' - 7y' + 8z' \\ 4x' - 8y' + 9z' \end{pmatrix},$$

where

$$\frac{1}{2}(4x' - 8y' + 9z') = 2x' - 4y' + \frac{9}{2}z' > x' - 4y' + 4z',$$

hence $M(x, y, z) \in \mathcal{P}$. In case (2)

$$M(x, y, z) = AB(x', y', z') = \begin{pmatrix} x' + 4y' + 4z' \\ 4x' + 7y' + 8z' \\ 4x' + 8y' + 9z' \end{pmatrix},$$

where

$$\frac{1}{2}(4x' + 8y' + 9z') = 2x' + 4y' + \frac{9}{2}z' > x' + 4y' + 4z',$$

hence $M(x, y, z) \in \mathcal{P}$. In case (3)

$$M(x, y, z) = C^2(x', y', z') = \begin{pmatrix} -7x' + 4y' + 8z' \\ -4x' + y' + 4z' \\ -8x' + 4y' + 9z' \end{pmatrix},$$

where

$$\frac{1}{2}(-8x' + 4y' + 9z') = -4x' + 2y' + \frac{9}{2}z' > -4x' + y' + 4z',$$

hence $M(x, y, z) \in \mathcal{P}$. In case (4)

$$M(x, y, z) = CB(x', y', z') = \begin{pmatrix} 7x' + 4y' + 8z' \\ 4x' + y' + 4z' \\ 8x' + 4y' + 9z' \end{pmatrix},$$

where

$$\frac{1}{2}(8x' + 4y' + 9z') = 4x' + 2y' + \frac{9}{2}z' > 4x' + y' + 4z',$$

hence $M(x, y, z) \in \mathcal{P}$.

For cases (5) and (6), let

$$(x_2, y_2, z_2) = M(x, y, z) = (AC)^k(x_1, y_1, z_1),$$

where

$$(x_1, y_1, z_1) = A^2(x', y', z') = \begin{pmatrix} x' - 4y' + 4z' \\ 4x' - 7y' + 8z' \\ 4x' - 8y' + 9z' \end{pmatrix}$$

in case (5), and

$$(x_1, y_1, z_1) = AB(x', y', z') = \begin{pmatrix} x' + 4y' + 4z' \\ 4x' + 7y' + 8z' \\ 4x' + 8y' + 9z' \end{pmatrix}$$

in case (6). It is not difficult to notice that $x_2 = \min\{x_2, y_2\}$, and

$$\frac{z_2}{2} = x_2 + \left(\frac{z_1}{2} - x_1\right).$$

Therefore $(x_2, y_2, z_2) \in \mathcal{P}$ if and only if $x_1 \leqslant z_1/2$, which is true in both cases, (5) and (6). On the other hand,

$$B(x', y', z') = \begin{pmatrix} x' + 2y' + 2z' \\ 2x' + y' + 2z' \\ 2x' + 2y' + 3z' \end{pmatrix},$$

and

$$C(x', y', z') = \begin{pmatrix} -x' + 2y' + 2z' \\ -2x' + y' + 2z' \\ -2x' + 2y' + 3z' \end{pmatrix},$$

which implies that $(AC)^k B(x', y', z'), (AC)^k C(x', y', z') \notin \mathcal{P}$ for any (x', y', z').

For cases (7) and (8), let

$$(x_2, y_2, z_2) = M(x, y, z) = (CA)^k (x_1, y_1, z_1),$$

where

$$(x_1, y_1, z_1) = C^2(x', y', z') = \begin{pmatrix} -7x' + 4y' + 8z' \\ -4x' + y' + 4z' \\ -8x' + 4y' + 9z' \end{pmatrix}$$

in case (7), and

$$(x_1, y_1, z_1) = CB(x', y', z') = \begin{pmatrix} 7x' + 4y' + 8z' \\ 4x' + y' + 4z' \\ 8x' + 4y' + 9z' \end{pmatrix}$$

in case (8). It is not difficult to notice that $y_2 = \min\{x_2, y_2\}$, and

$$\frac{z_2}{2} = y_2 + \left(\frac{z_1}{2} - y_1\right).$$

Therefore $(x_2, y_2, z_2) \in \mathcal{P}$ if and only if $y_1 \leqslant z_1/2$, which is true in both cases, (7) and (8). On the other hand,

$$B(x', y', z') = \begin{pmatrix} x' + 2y' + 2z' \\ 2x' + y' + 2z' \\ 2x' + 2y' + 3z' \end{pmatrix},$$

and

$$A(x', y', z') = \begin{pmatrix} x' - 2y' + 2z' \\ 2x' - y' + 2z' \\ 2x' - 2y' + 3z' \end{pmatrix},$$

which implies that $(CA)^k B(x', y', z'), (CA)^k A(x', y', z') \notin \mathcal{P}$ for any (x', y', z'). We have shown that $H\mathcal{P} \subseteq H\mathfrak{P}' \subseteq \mathcal{P} \setminus \{(1, 0, 1)\}$.

To finish the proof of the lemma, we will show that $\mathcal{P} \setminus \{(1, 0, 1)\} \subseteq H\mathcal{P}$. Notice that it is in fact sufficient to show that for each $(x, y, z) \in \mathcal{P} \setminus \{(1, 0, 1)\}$ there exists $M \in H$ such that $(x, y, z) = M(1, 0, 1)$. We know that there exists $N \in G$ such that $(x, y, z) = N(3, 4, 5)$, and so

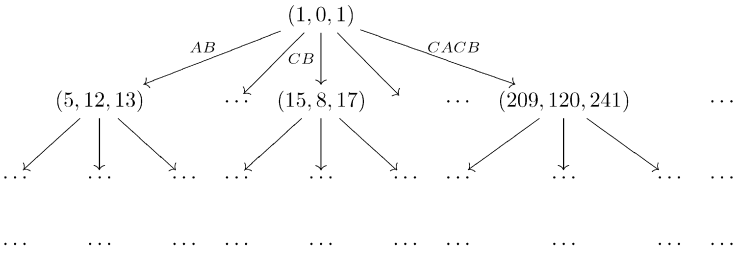

Fig. 2. Infinite-degree tree representation for $\mathcal{P}$.

$(x, y, z) = NB(1, 0, 1)$. First notice that N cannot be of the form BN' for some $N' \in G$. Indeed, suppose it is, then

$$(x, y, z) = B(x', y', z') = \begin{pmatrix} x' + 2y' + 2z' \\ 2x' + y' + 2z' \\ 2x' + 2y' + 3z' \end{pmatrix},$$

where $(x', y', z') = N'(x, y, z) \in \mathfrak{P}'$, but

$$\frac{1}{2}(2x' + 2y' + 3z') = x' + y' + \frac{3}{2}z' < \min\{x' + 2y' + 2z', 2x' + y' + 2z'\},$$

which contradicts the fact that $(x, y, z) \in \mathcal{P}$. Similarly, from the arguments above it follows that N cannot be of the form $(AC)^k BN'$, $(AC)^k CN'$, $(CA)^k BN'$, or $(CA)^k AN'$. The only options left are those described in cases (1)–(8) above, which means that $M = NB \in H$. Therefore $\mathcal{P} \setminus \{(1, 0, 1)\} \subseteq H\mathcal{P}$, which completes the proof. □

Theorem 2.2. *H' is a free infinitely generated monoid, which acts freely on the set $\mathcal{P}$ by left multiplication. With respect to this action, $\mathcal{P}$ has the structure of a regular rooted infinite tree, where each vertex has infinite degree (see Fig. 2 above); this is precisely the Cayley digraph of H'.*

Proof. H' is a submonoid of G, which is a free monoid, hence H' must also be free by the Nielsen–Schreier theorem (see for instance [19]). To see that H' is infinitely generated, consider for instance the set $\{AB^k\colon\ k \in \mathbb{Z}_{>0}\}$ of elements of H'. Since $A, B^k \notin H'$ for any $k \in \mathbb{Z}_{>0}$, it is clear that no finite subset of H' can generate all of the elements of the form AB^k: if this was possible, there would have to be relations between elements of H', contradicting the fact that it is free. Therefore H' must be infinitely generated, and so its Cayley digraph is a regular rooted infinite tree, where each vertex has infinite degree, and the root corresponds to I_3.

By Lemma 2.1 we know that $H'\mathcal{P} = \mathcal{P}$. Moreover, we know that for each $(x, y, z) \in \mathcal{P}$ there exists a unique element $N \in G$ such that $N(3, 4, 5) = (x, y, z)$, and hence NB is the unique element in H such that $NB(1, 0, 1) = (x, y, z)$. This means that H' acts freely on $\mathcal{P}$. Then we can identify $(1, 0, 1) \in \mathcal{P}$ with $I_3 \in H'$, and each $(x, y, z) \in \mathcal{P}$ with the corresponding unique $NB \in H'$ such that $NB(1, 0, 1) = (x, y, z)$, which means that with respect to the action of H' the set $\mathcal{P}$ has the structure of the Cayley digraph of H' with respect to an appropriate generating set. □

Corollary 2.3. *The set $\mathcal{C}_2$ of similarity classes of lattices in* $\mathrm{WR}(\mathbb{Z}^2)$ *has the structure of a non-commutative free infinitely generated monoid. Specifically, it is isomorphic to H'.*

Proof. We will identify $\mathcal{C}_2$ with H' in the following way. From Theorem 2.2 we know that there exists a bijection $\varphi : \mathcal{P} \to H'$, given by

$$\varphi(x, y, z) = M, \quad \text{such that } M(1, 0, 1) = (x, y, z),$$

for each $(x, y, z) \in \mathcal{P}$ with $\varphi^{-1} : H' \to \mathcal{P}$ defined by

$$\varphi^{-1}(M) = M(1, 0, 1),$$

for each $M \in H'$.

On the other hand, there also exists a bijection $\psi : \mathcal{C}_2 \to \mathcal{P}$, given by

$$\psi\big(C(p,q)\big) = \begin{cases} (\sqrt{q^2-p^2}, p, q) & \text{if } 2|p, \\ (p, \sqrt{q^2-p^2}, q) & \text{if } 2 \nmid p, \end{cases}$$

for each $C(p, q) \in \mathcal{C}_2$ with $\psi^{-1} : \mathcal{P} \to \mathcal{C}_2$ defined by

$$\psi^{-1}(x, y, z) = C(p, q), \quad \text{where } p = \max\{x, y\},\ q = z,$$

for each $(x, y, z) \in \mathcal{P}$. Therefore we have bijections $\varphi\psi : \mathcal{C}_2 \to H'$ and $(\varphi\psi)^{-1} = \psi^{-1}\varphi^{-1} : H' \to \mathcal{C}_2$.

We can now define a binary operation $*$ on $\mathcal{C}_2$ as follows: for every $C(p_1, q_1)$ and $C(p_2, q_2)$ in $\mathcal{C}_2$, let

$$C(p_1, q_1) * C(p_2, q_2) = \psi^{-1}\big(\varphi\psi\big(C(p_1, q_1)\big)\varphi\psi\big(C(p_2, q_2)\big)(1, 0, 1)\big). \tag{29}$$

It is easy to see that $\mathcal{C}_2$ is a free non-commutative monoid with respect to $*$, which is isomorphic to H' via the monoid isomorphism $\varphi\psi : \mathcal{C}_2 \to H'$, and $(\varphi\psi)^{-1}(I_3) = C(1, 1) \in \mathcal{C}_2$ is the identity. Hence the tree in Fig. 2 is the Cayley digraph of $\mathcal{C}_2$ with respect to an appropriate generating set. This completes the proof. □

Now Theorem 1.1 follows by combining Theorem 2.2 with Corollary 2.3.

3. Similarity classes and corresponding zeta functions

In this section we discuss the structure of similarity classes $C(p, q)$, as well as the properties of associated zeta functions. Our first goal is to prove Theorem 1.2. For each $p/q \in \mathcal{S}$, define

$$\mathfrak{M}_2(p,q) = \big\{\boldsymbol{x} \in \big(\mathbb{Z}^2/\{\pm 1\}\big) \setminus \{\mathbf{0}\} \colon\ x_1\sqrt{q^2-p^2} \equiv x_2 p \pmod q,\ x_2\sqrt{q^2-p^2} \equiv -x_1 p \pmod q\big\}.$$

Notice that $\boldsymbol{x} \in \mathfrak{M}_2(p, q)$ if and only if

$$\Lambda(\boldsymbol{x}) := \operatorname{span}_{\mathbb{Z}} \left\{ \boldsymbol{x},\ \begin{pmatrix} \frac{\sqrt{q^2-p^2}}{q} & -\frac{p}{q} \\ \frac{p}{q} & \frac{\sqrt{q^2-p^2}}{q} \end{pmatrix} \boldsymbol{x} \right\} \in C(p, q). \tag{30}$$

Hence lattices in the similarity class $C(p, q)$ are in bijective correspondence with points in $\mathfrak{M}_2(p, q)$.

Lemma 3.1. *Let $p/q \in \mathcal{S}$. The congruence relations*

$$x_1\sqrt{q^2-p^2} \equiv x_2 p \pmod q \tag{31}$$

and

$$x_2\sqrt{q^2-p^2} \equiv -x_1 p \pmod q \tag{32}$$

are equivalent, meaning that

$$\mathfrak{M}_2(p,q) = \left\{\boldsymbol{x} \in \left(\mathbb{Z}^2/\{\pm 1\}\right) \setminus \{\mathbf{0}\} \colon x_1\sqrt{q^2-p^2} \equiv x_2 p \pmod{q}\right\}.$$

Proof. Recall that $\gcd(p,q) = 1$. Also $q^2 - p^2 = (p-q)(p+q)$, and

$$\gcd(q-p,q) = \gcd(q+p,q) = \gcd(p,q) = 1,$$

therefore $\gcd(q^2-p^2,q) = \gcd(\sqrt{q^2-p^2},q) = 1$. Hence

$$x_1\sqrt{q^2-p^2} \equiv x_2 p \pmod{q}$$

if and only if

$$x_2 p\sqrt{q^2-p^2} \equiv x_1\left(q^2-p^2\right) \equiv -x_1 p^2 \pmod{q},$$

which happens if and only if $-x_1 p \equiv x_2\sqrt{q^2-p^2} \pmod{q}$. □

For each $p/q \in \mathcal{S}$, define $c(p,q)$ to be the unique integer such that $0 \leqslant c(p,q) \leqslant q-1$ and

$$c(p,q)p \equiv \sqrt{q^2-p^2} \pmod{q}. \tag{33}$$

Then, by Lemma 3.1, for every $\boldsymbol{x} \in \mathfrak{M}_2(p,q)$ we have $x_2 \equiv c(p,q)x_1 \pmod{q}$, meaning that $x_2 = c(p,q)x_1 + yq$ for some $y \in \mathbb{Z}$. In other words, $\mathfrak{M}_2(p,q)$ can be presented as

$$\mathfrak{M}_2(p,q) = \left\{\begin{pmatrix} x \\ c(p,q)x + qy \end{pmatrix} \colon \begin{pmatrix} x \\ y \end{pmatrix} \in \left(\mathbb{Z}^2/\{\pm 1\}\right) \setminus \{\mathbf{0}\}\right\}. \tag{34}$$

Define

$$\Omega(p,q) = \begin{pmatrix} 1 & 0 \\ c(p,q) & q \end{pmatrix}\mathbb{Z}^2, \tag{35}$$

so that $\mathfrak{M}_2(p,q) = (\Omega(p,q)/\{\pm 1\}) \setminus \{\mathbf{0}\}$.

Lemma 3.2. *$\Omega(p,q) \in C(1,1)$, and $|\Omega(p,q)|^2 = \det(\Omega(p,q)) = q$. In fact, each $\Omega(p,q)$ is in the set $C'(1,1)$ as defined by* (4)*. Moreover, every lattice $\left(\begin{smallmatrix} a & -b \\ b & a \end{smallmatrix}\right)\mathbb{Z}^2$ in the set $C'(1,1)$ is of the form $\Omega(p,q)$ for p, q satisfying* (5)*.*

Proof. First fix a lattice $\Omega(p,q)$. It is a well-known fact that there exist unique relatively prime $a > b \in \mathbb{Z}_{>0}$ of different parity such that either $p = a^2 - b^2$ or $p = 2ab$, and $q = a^2 + b^2$ (this is the standard parametrization of primitive Pythagorean triples, see for instance [22]). The fact that $\frac{\sqrt{3}}{2}q < p \leqslant q$ ensures that $(a,b) \in \mathcal{A}$. Then the lattice

$$\Omega = \begin{pmatrix} a & -b \\ b & a \end{pmatrix}\mathbb{Z}^2$$

is in $C'(1,1)$, and $|\Omega|^2 = \det(\Omega) = q$. We will now show that $\Omega(p,q) = \Omega$. Since $\gcd(a,b) = 1$, there exist $g_1, g_2 \in \mathbb{Z}$ such that

$$g_1 a - g_2 b = 1. \tag{36}$$

Let $\gamma = g_1 b + g_2 a$, and notice that

$$\begin{pmatrix} a & -b \\ b & a \end{pmatrix} \begin{pmatrix} g_1 & b \\ g_2 & a \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \gamma & q \end{pmatrix},$$

and $\det\left(\begin{smallmatrix} a & -b \\ b & a \end{smallmatrix}\right) = \det\left(\begin{smallmatrix} 1 & 0 \\ \gamma & q \end{smallmatrix}\right) = q$, so

$$\Omega = \begin{pmatrix} 1 & 0 \\ \gamma & q \end{pmatrix} \mathbb{Z}^2. \tag{37}$$

Notice that $\gamma^2 + 1$ is divisible by q. Indeed, (36) implies that $g_1 = \frac{g_2 b + 1}{a}$, and so

$$\begin{aligned} \gamma^2 + 1 &= (g_1 b + g_2 a)^2 + 1 = g_2^2 a^2 + 2 g_2 b (g_2 b + 1) + \frac{b^2}{a^2} (g_2 b + 1)^2 + 1 \\ &= q\left(\frac{g_2 q + 2 g_2 b + 1}{a^2} \right) = q\left(g_1^2 + g_2^2\right). \end{aligned} \tag{38}$$

Moreover, we can ensure that $0 \leqslant \gamma \leqslant q - 1$ by replacing γ with $\gamma + qm$ for some $m \in \mathbb{Z}$, if necessary: it is easy to see that $\gamma^2 + 1$ will still be divisible by q, and (37) will still hold. We will now show that $\gamma = c(p,q)$. Notice that

$$F_{\gamma,q}(x,y) = \left(\frac{\gamma^2 + 1}{q} \right) x^2 + 2\gamma xy + q y^2 \tag{39}$$

is an integral binary quadratic form with discriminant -4, hence it is equivalent to

$$G(x,y) = x^2 + y^2,$$

since the class number of -4 is one. In fact, it is easy to verify that

$$F_{\gamma,q}(x,y) = G(g_1 x - by, g_2 x - ay), \qquad G(x,y) = F_{\gamma,q}(ax - by, g_2 x - g_1 y).$$

Let us write $t = a^2 - b^2$, so either $p = t$ or $p = \sqrt{q^2 - t^2}$, then

$$q = G(a,b) = F_{\gamma,q}(t,k) = \left(\frac{\gamma^2 + 1}{q} \right) t^2 + 2\gamma tk + qk^2,$$

where $k = g_2 a - g_1 b$. Therefore

$$\gamma^2 t^2 + 2\gamma tk + q^2 k^2 = q^2 - t^2,$$

meaning that

$$\gamma^2 t^2 \equiv q^2 - t^2 \pmod{q}. \tag{40}$$

Notice that $\gcd(\gamma, q) = 1$, since $q|(\gamma^2 + 1)$, so $\gcd(\gamma, q)$ must divide 1. Therefore, if $p = t$, then (40) implies that

$$\gamma p \equiv \sqrt{q^2 - p^2} \pmod{q}. \tag{41}$$

If, on the other hand, $p = \sqrt{q^2 - t^2}$, then (40) implies that $\gamma\sqrt{q^2 - p^2} \equiv p \pmod{q}$, meaning that $\gamma^2\sqrt{q^2 - p^2} \equiv \gamma p \pmod{q}$, but on the other hand $\gamma^2 \equiv -1 \pmod{q}$, and so

$$-\sqrt{q^2 - p^2} \equiv \gamma p \pmod{q}.$$

By Lemma 3.1, this last congruence is equivalent to (41). We conclude that $0 \leqslant \gamma \leqslant q - 1$, and γ satisfies (41), which means that $\gamma = c(p, q)$, and so $\Omega = \Omega(p, q)$.

In the opposite direction, assume that

$$\Omega = \begin{pmatrix} a & -b \\ b & a \end{pmatrix} \mathbb{Z}^2 \in C'(1, 1),$$

and define $q = a^2 + b^2$, $p = \max\{a^2 - b^2, 2ab\}$. Then the fact that $(a, b) \in \mathcal{A}$ ensures that $\frac{\sqrt{3}}{2}q < p \leqslant q$, i.e. $p/q \in \mathcal{S}$. It is not difficult to notice that for $p/q \in \mathcal{S}$, $p = a^2 - b^2$ if and only if $a > (2 + \sqrt{3})b$, and $p = 2ab$ if and only if $b < a < \sqrt{3}b$. The argument identical to the one above now shows that $\Omega = \Omega(p, q)$. This completes the proof. □

Remark 3.1. It is not difficult to conclude from an argument very similar to the one in the proof of Lemma 3.2 that all binary integral quadratic forms of discriminant -4 are of the form $F_{\gamma,q}(x, y)$ as in (39) for some odd positive integer q which is not divisible by any prime of the form $4k + 3$ and an integer γ (positive or negative) such that $\gamma^2 + 1$ is divisible by q. This statement is essentially equivalent to the fact that there is a bijection between ideals of the form $(da + dbi)$ in $\mathbb{Z}[i]$ with $a > b > 0$, $d > 0$, and Pythagorean triples $(d^2(a^2 - b^2), 2d^2ab, d^2(a^2 + b^2))$.

Proof of Theorem 1.2. Fix a similarity class $C(p, q) \in \mathcal{C}_2$ for some $p/q \in \mathcal{S}$. For each $\Lambda \in C(p, q)$, we have $\Lambda = \Lambda(\boldsymbol{x})$ as defined by (30) for some $\boldsymbol{x} = \binom{x}{c(p,q)x+qy}$ where $x, y \in \mathbb{Z}$, hence $\boldsymbol{x} \in \Omega(p, q)$. On the other hand, for each $\boldsymbol{x} \in \Omega(p, q)$, the corresponding lattice $\Lambda(\boldsymbol{x})$ is easily seen to be in $C(p, q)$. Combining this observation with Lemma 3.2 completes the proof of the theorem. □

Proof of Theorem 1.3. We first introduce the notion of a minimal lattice in each similarity class $C(p, q)$. Let $\boldsymbol{x}(p, q) \in \Omega(p, q)$ be such that $\|\boldsymbol{x}(p, q)\| = |\Omega(p, q)|$, and let $\Lambda(\boldsymbol{x}(p, q))$ be defined by (30); we will call this lattice a *minimal lattice* of the similarity class $C(p, q)$ and will denote it by $\Lambda_{p,q}$. By Lemma 3.2, we have

$$\big|\Omega(p, q)\big| = \big\|\boldsymbol{x}(p, q)\big\| = \sqrt{q}. \tag{42}$$

On the other hand, since $\sqrt{3}/2 < p/q \leqslant 1$, meaning that the angle between $\boldsymbol{x}(p, q)$ and the other minimal basis vector given in (30) is $\arcsin(p/q) \in (\pi/3, \pi/2)$, a well-known lemma of Gauss (see [3] or [10]) implies that $|\Lambda_{p,q}| = \|\boldsymbol{x}(p, q)\|$, and so $|\Lambda_{p,q}| = \sqrt{q}$. Therefore

$$\det(\Lambda_{p,q}) = |\Lambda_{p,q}|^2 \frac{p}{q} = p = \min\big\{\det(\Lambda):\ \Lambda \in C(p, q)\big\}. \tag{43}$$

Moreover, a straight-forward computation shows that the norm form of $\Lambda_{p,q}$ with respect to its minimal basis is

$$Q_{p,q}(x, y) = (x, y)\begin{pmatrix} q & \sqrt{q^2 - p^2} \\ \sqrt{q^2 - p^2} & q \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = qx^2 + 2xy\sqrt{q^2 - p^2} + qy^2. \tag{44}$$

Notice that the minimal lattice of a similarity class may not in general be unique, however it is unique up to a rational rotation, and so for our purposes it suffices to pick any one of them.

Next, let $\Lambda \in C(p,q)$, then $\Lambda \sim \Lambda_{p,q}$, and so there must exist $\alpha \in \mathbb{R}_{>0}$ and $U \in O_2(\mathbb{R})$ such that $\Lambda = \alpha U \Lambda_{p,q}$. Then $\det(\Lambda) = \alpha^2 p$, and so $\alpha = \sqrt{\frac{\det(\Lambda)}{p}} > 1$. If we write A and $A_{p,q}$ for the minimal basis matrices of Λ and $\Lambda_{p,q}$, respectively, then $A = \sqrt{\frac{\det(\Lambda)}{p}} U A_{p,q}$, and the norm form of Λ with respect to this minimal basis is

$$Q_\Lambda(x,y) = (x,y)A^t A \begin{pmatrix} x \\ y \end{pmatrix} = \frac{\det(\Lambda)}{p}(x,y)A_{p,q}^t A_{p,q} \begin{pmatrix} x \\ y \end{pmatrix} = \frac{\det(\Lambda)}{p} Q_{p,q}(x,y).$$

Epstein zeta function of Λ is therefore given by

$$E_\Lambda(s) = \sum_{\boldsymbol{x} \in \Lambda}{}' \|\boldsymbol{x}\|^{-2s} = \sum_{(x,y)\in\mathbb{Z}^2}{}' Q_\Lambda(x,y)^{-s} = \left(\frac{p}{\det(\Lambda)}\right)^s \sum_{(x,y)\in\mathbb{Z}^2}{}' Q_{p,q}(x,y)^{-s}.$$

Then (43) implies that for every fixed real value of $s > 1$, $E_\Lambda(s)$ achieves its maximum on $C(p,q)$ when $\Lambda = \Lambda_{p,q}$, and it does not achieve a minimum since there exist lattices in $C(p,q)$ with arbitrarily large determinants. This completes the proof of the theorem. □

Proof of Theorem 1.4. We now derive the properties of the Dirichlet series corresponding to each $C(p,q)$. Fix a similarity class $C(p,q) \in \mathcal{C}_2$. By Theorem 1.2, each $\Lambda \in C(p,q)$ is of the form $\Lambda(\boldsymbol{x})$ for some $\boldsymbol{x} \in \Omega(p,q)$. As in the proof of Theorem 1.3 above, a well-known lemma of Gauss (see [3] or [10]) implies that $|\Lambda(\boldsymbol{x})| = \|\boldsymbol{x}\|$. Since also, by Lemma 3.2 of [10], the set of minimal vectors of $\Lambda(\boldsymbol{x})$ is precisely

$$\left\{ \pm\boldsymbol{x}, \pm \begin{pmatrix} \frac{\sqrt{q^2-p^2}}{q} & -\frac{p}{q} \\ \frac{p}{q} & \frac{\sqrt{q^2-p^2}}{q} \end{pmatrix} \boldsymbol{x} \right\},$$

it follows that $\Lambda(\boldsymbol{x}_1) = \Lambda(\boldsymbol{x}_2)$ if and only if $\boldsymbol{x}_1 = \pm\boldsymbol{x}_2$. Therefore

$$Z_{p,q}^m(s) = \sum_{\Lambda \in C(p,q)} |\Lambda|^{-2s} = \sum_{\boldsymbol{x}\in\Omega(p,q)}{}' \|\boldsymbol{x}\|^{-2s} = E_{\Omega(p,q)}(s).$$

Now Theorem 1.2 readily implies that there exists $U \in O_2(\mathbb{R})$ such that

$$\Omega(p,q) = U \begin{pmatrix} \sqrt{q} & 0 \\ 0 & \sqrt{q} \end{pmatrix} \mathbb{Z}^2,$$

which means that $E_{\Omega(p,q)}(s)$ is equal to the Epstein zeta function of $\left(\begin{smallmatrix} \sqrt{q} & 0 \\ 0 & \sqrt{q} \end{smallmatrix}\right)\mathbb{Z}^2$. Hence

$$Z_{p,q}^m(s) = E_{\Omega(p,q)}(s) = \frac{1}{q^s} \sum_{\boldsymbol{x}\in\mathbb{Z}^2}{}' \|\boldsymbol{x}\|^{-2s} = \frac{1}{q^s}\zeta_{\mathbb{Q}(i)}(s),$$

which proves (8). Now recall that for each $\Lambda \in C(p,q)$,

$$\det(\Lambda) = |\Lambda|^2 \sin\theta(\Lambda) = |\Lambda|^2 \frac{p}{q}.$$

Then (7) follows. □

4. Weight enumerators $W_d(s)$ and $W_m(s)$

In this section we will discuss in more details some properties of the Dirichlet series $W_d(s)$ and $W_m(s)$ as defined in (11) and (12), respectively, and will prove Theorem 1.5. Recall that we write a_p and b_q for the coefficients of $W_d(s)$ and $W_m(s)$, respectively, as defined in Section 1. The following formulas for a_p and b_q are immediate from Theorem 1.2 and the definition of the set $\mathcal{A}$ in (3).

Lemma 4.1. *For each p such that $p/q \in \mathcal{S}$ for some $q \in \mathbb{Z}_{>0}$,*

$$a_p = \left|\left\{(m,n) \in \mathcal{A}\colon\ p = \max\left\{m^2 - n^2, 2mn\right\}\right\}\right|,$$

and for each q such that $p/q \in \mathcal{S}$ for some $p \in \mathbb{Z}_{>0}$,

$$b_q = \left|\left\{(m,n) \in \mathcal{A}\colon\ q = m^2 + n^2\right\}\right|.$$

Notice that the expression for a_p in Lemma 4.1 is similar in spirit to the function β defined in [10], in particular it can also be bounded in terms of Hooley's Δ-function. On the other hand, we can obtain simple explicit bounds for a_p and b_q from our Pythagorean tree construction in Section 3. For each $p, q \in \mathbb{Z}_{>0}$, define $L(p)$ to be the number of primitive Pythagorean triples with a leg p, and $H(q)$ to be the number of primitive Pythagorean triples with the hypotenuse q. There are well-known formulas for $L(p)$ and $H(q)$ (see [5, p. 116]): if $p, q > 1$, then

$$L(p) = \begin{cases} 0 & \text{if } p \equiv 2 \pmod 4, \\ 2^{\omega(p)-1} & \text{otherwise,} \end{cases}$$

where $\omega(p)$ is the number of distinct prime divisors of p, and

$$H(q) = \begin{cases} 0 & \text{if } 2|q, \text{ or if } q \text{ has a prime factor } l \equiv 3 \pmod 4, \\ 2^{\omega(q)-1} & \text{otherwise.} \end{cases}$$

For convenience, we also set $L(1) = H(1) = \frac{1}{2}$. It is clear that $a_p \leqslant L(p)$ and $b_q \leqslant H(q)$ when $p, q > 1$, and $a_1 = b_1 = 1$. One can ask how good are these bounds? We will now show that the correct order of magnitude of the bound for both, a_p and b_q, in the sense that the corresponding Dirichlet series has the same behavior at $s = 1$ as $W_d(s)$ and $W_m(s)$, is given by H and not by L. Namely, define

$$\mathcal{L}(s) = \sum_{n=1}^{\infty} \frac{L(n)}{n^s}, \qquad \mathcal{H}(s) = \sum_{n=1}^{\infty} \frac{H(n)}{n^s}.$$

Lemma 4.2. *$\mathcal{H}(s)$ has a simple pole at $s = 1$ and is analytic for all $s \in \mathbb{C}$ with $\Re(s) > 1$. Moreover when $\Re(s) > 1$, $\mathcal{H}(s)$ has an Euler product type expansion*

$$\mathcal{H}(s) = \frac{1}{2} \prod_{l \equiv 1 \pmod 4} \frac{l^s + 1}{l^s - 1}, \tag{45}$$

where the product is over primes l.

Proof. Let us define

$$V_1 = \left\{n \in \mathbb{Z}_{>0}\colon\ n \text{ is only divisible by primes which are } \equiv 1 \pmod 4\right\}.$$

Then notice that, as in the proof of Lemma 8.1 of [10],

$$2\mathcal{H}(s) = \sum_{n\in V_1} \frac{2^{\omega(n)}}{n^s} = \prod_{l\equiv 1 \pmod 4} \left(\sum_{k=0}^{\infty} 2^{\omega(l^k)} l^{-ks} \right) = \prod_{l\equiv 1 \pmod 4} \left(1 + 2\sum_{k=1}^{\infty} l^{-ks} \right)$$
$$= \prod_{l\equiv 1 \pmod 4} \left(\frac{2}{1-l^{-s}} - 1 \right) = \prod_{l\equiv 1 \pmod 4} \frac{l^s+1}{l^s-1},$$

whenever this product is convergent, where l is always prime. The fact that $\mathcal{H}(s)$ has a simple pole at $s=1$ and is analytic for all $s\in\mathbb{C}$ with $\Re(s)>1$ then follows immediately from Lemma 8.1 of [10]. □

Proof of Theorem 1.5. First of all notice that since $\frac{\sqrt{3}}{2}q \leqslant p \leqslant q$, we have

$$\left|\left(\frac{\sqrt{3}}{2}\right)^s\right| \sum_{C(p,q)\in\mathcal{C}_2} \left|\frac{1}{p^s}\right| \leqslant \sum_{C(p,q)\in\mathcal{C}_2} \left|\frac{1}{q^s}\right| \leqslant \sum_{C(p,q)\in\mathcal{C}_2} \left|\frac{1}{p^s}\right|,$$

meaning that $W_d(s)$ and $W_m(s)$ must have poles of the same order and the same half-plane of convergence. Since $b_q \leqslant H(q)$, Lemma 4.2 implies that $W_m(s)$ has at most a simple pole at $s=1$, and is analytic when $\Re(s)>1$. On the other hand, Theorem 1.5 of [10] implies that $\zeta_{\mathrm{WR}(\mathbb{Z}^2)}(s)$ has at least a pole of order two at $s=1$, meaning that, by (9), $W_d(s)$ must have at most a simple pole at $s=1$. This means that both, $W_d(s)$ and $W_m(s)$, have simple poles at $s=1$ and are analytic when $\Re(s)>1$, and therefore, by (9) and (10), $\zeta_{\mathrm{WR}(\mathbb{Z}^2)}(s)$ and $\zeta^m_{\mathrm{WR}(\mathbb{Z}^2)}(s)$ both have poles of order two at $s=1$ and are analytic when $\Re(s)>1$. This completes the proof. □

Remark 4.1. Notice that Theorem 1.5 combined with Lemma 4.2 implies that the Dirichlet series $\sum_{(x,y,z)\in\mathcal{P}} \frac{1}{\max\{x,y\}^s}$ and $\sum_{(x,y,z)\in\mathfrak{P}'} \frac{1}{\max\{x,y\}^s}$ have poles of the same order 1 at $s=1$. This fact could be roughly interpreted to mean that the sets $\mathcal{P}$ and $\mathfrak{P}'$ are comparable in size, i.e. that "most" primitive Pythagorean triples correspond to similarity classes of lattices from $\mathrm{WR}(\mathbb{Z}^2)$. In other words, the imposed condition that the shortest leg of a primitive Pythagorean triple is no longer than half of the hypotenuse is not particularly restrictive. Moreover, we can roughly think of $H(n)$ as a bound on the average orders of a_n and b_n for each $n\in\mathbb{Z}_{>0}$.

On the other hand, we have the following.

Lemma 4.3. *Let the notation be as above, then $\mathcal{L}(s)$ has a pole of order two at $s=1$ and is analytic for all $s\in\mathbb{C}$ with $\Re(s)>1$. Moreover when $\Re(s)>1$, $\mathcal{L}(s)$ has an Euler product type expansion*

$$\mathcal{L}(s) = \frac{1}{2}\left(\frac{4^s-2^s+2}{4^s-2^s}\right) \prod_{l\neq 2 \text{ prime}} \frac{l^s+1}{l^s-1} = \frac{1}{2}\left(\frac{4^s-2^s+2}{4^s+2^s}\right) \frac{\zeta(s)^2}{\zeta(2s)}, \tag{46}$$

where $\zeta(s)$ is the Riemann zeta function.

Proof. Let us consider the Dirichlet series $2\mathcal{L}(s)$, then

$$2\mathcal{L}(s) = \sum_{n=1}^{\infty} \frac{2L(n)}{n^s} = \sum_{2\nmid n} \frac{2^{\omega(n)}}{n^s} + \sum_{4|n} \frac{2^{\omega(n)}}{n^s} = \sum_{2\nmid n} \frac{2^{\omega(n)}}{n^s} + \frac{1}{4^s}\sum_{n=1}^{\infty} \frac{2^{\omega(2n)}}{n^s}$$
$$= \sum_{2\nmid n} \frac{2^{\omega(n)}}{n^s} + \frac{1}{4^s}\left(2\sum_{2\nmid n} \frac{2^{\omega(n)}}{n^s} + \sum_{2|n} \frac{2^{\omega(n)}}{n^s}\right)$$
$$= \left(1+\frac{2}{4^s}\right)\sum_{2\nmid n} \frac{2^{\omega(n)}}{n^s} + \frac{1}{4^s}\sum_{2|n} \frac{2^{\omega(n)}}{n^s}. \tag{47}$$

On the other hand,

$$\sum_{2|n} \frac{2^{\omega(n)}}{n^s} = \frac{1}{2^s} \sum_{n=1}^{\infty} \frac{2^{\omega(2n)}}{n^s} = \frac{1}{2^s} \left(2 \sum_{2\nmid n} \frac{2^{\omega(n)}}{n^s} + \sum_{2|n} \frac{2^{\omega(n)}}{n^s} \right),$$

and so

$$\sum_{2|n} \frac{2^{\omega(n)}}{n^s} = \frac{2}{2^s - 1} \sum_{2\nmid n} \frac{2^{\omega(n)}}{n^s}. \tag{48}$$

Combining (47) and (48), we obtain

$$2\mathcal{L}(s) = \left(\frac{4^s - 2^s + 2}{4^s - 2^s} \right) \sum_{2\nmid n} \frac{2^{\omega(n)}}{n^s}. \tag{49}$$

Now define

$$L_1(n) = \begin{cases} 0 & \text{if } 2|n, \\ 2^{\omega(n)} & 2\nmid n. \end{cases}$$

It is easy to see that $L_1(1) = 1$ and L_1 is multiplicative, i.e. if $\gcd(m, n) = 1$ then $L_1(mn) = L_1(m)L_1(n)$. Therefore, by Theorem 286 of [11],

$$\begin{aligned} \sum_{2\nmid n} \frac{2^{\omega(n)}}{n^s} &= \sum_{n=1}^{\infty} \frac{L_1(n)}{n^s} = \prod_{l \text{ prime}} \left(\sum_{k=0}^{\infty} \frac{L_1(l^k)}{l^{ks}} \right) = \prod_{l \neq 2 \text{ prime}} \left(1 + 2 \sum_{k=1}^{\infty} l^{-ks} \right) \\ &= \prod_{l \neq 2 \text{ prime}} \left(\frac{2}{1 - l^{-s}} - 1 \right) = \prod_{l \neq 2 \text{ prime}} \frac{l^s + 1}{l^s - 1}, \end{aligned} \tag{50}$$

when $\Re(s) > 1$. Moreover, by Theorem 301 of [11],

$$\frac{\zeta(s)^2}{\zeta(2s)} = \sum_{n=1}^{\infty} \frac{2^{\omega(n)}}{n^s} = \prod_{l \text{ prime}} \frac{l^s + 1}{l^s - 1}. \tag{51}$$

Now (46) follows by combining (49), (50), and (51). Moreover, $\zeta(s)^2/\zeta(2s)$ clearly has a pole of order two at $s = 1$, and is analytic for all $s \in \mathbb{C}$ with $\Re(s) > 1$. This completes the proof. □

Remark 4.2. Since $\mathcal{L}(s)$ is the sum over *all* the legs of primitive Pythagorean triples, short and long, and it is easy to see that for each $(x, y, z) \in \mathfrak{P}'$, $\max\{x, y\} \geqslant \frac{1}{\sqrt{2}} z$, Lemma 4.3 combined with Remark 4.1 imply that $\sum_{(x,y,z)\in\mathfrak{P}'} \frac{1}{\min\{x,y\}^s}$ must have a pole of order 2 at $s = 1$.

5. Approximating the hexagonal lattice

In this section we will talk about circle packing density corresponding to similarity classes of lattices in $\mathrm{WR}(\mathbb{Z}^2)$. Our goal is to prove Theorem 1.6. We do it by first proving the following slightly more technical lemma, from which the theorem follows easily.

Lemma 5.1. *Let A, B, C be matrices as in* (26)*. For each $k \in \mathbb{Z}_{>0}$, let*

$$(p_k, t_k, q_k) = (CA)^k CB(1,0,1) \in \mathcal{P}, \tag{52}$$

then $p_k > t_k$, $2|t_k$, and $C(p_k, q_k) \in \mathcal{C}_2$. Moreover,

$$t_k = \sqrt{q_k^2 - p_k^2} = \frac{q_k - 1}{2}, \tag{53}$$

and so

$$\frac{1}{(2+\sqrt{3})q_k} - \frac{2}{(2+\sqrt{3})q_k^2} < \left| \frac{\sqrt{3}}{2} - \frac{p_k}{q_k} \right| < \frac{1}{2\sqrt{3}q_k} \to 0, \quad \text{as } k \to \infty, \tag{54}$$

and more precisely

$$241(7+4\sqrt{3})^{k-1} = 241 \times (13.928\ldots)^{k-1} < q_k < 241 \times (13.947)^{k-1}. \tag{55}$$

Hence, by (19)*, for each such $C(p_k, q_k)$ the corresponding circle packing density is*

$$\frac{\pi}{\sqrt{12}} \left(\frac{1}{1 + \frac{1}{723(7+4\sqrt{3})^{k-1}}} \right) < \delta_{p_k,q_k} = \frac{\pi q_k}{4p_k} < \frac{\pi}{\sqrt{12}} \left(\frac{1}{1 + \frac{0.920\ldots}{723 \times (13.947)^{k-1}}} \right), \tag{56}$$

so $\delta_{p_k,q_k} \to \frac{\pi}{\sqrt{12}} = 0.9069\ldots = \delta(\Lambda_h)$ as $k \to \infty$, and the quadratic form $Q_{p_k,q_k}(x,y)$ as in (44) *satisfies*

$$\frac{1}{q_k} Q_{p_k,q_k}(x,y) = x^2 + \left(\frac{q_k - 1}{q_k} \right) xy + y^2 \ \to \ Q_h(x,y) := x^2 + xy + y^2, \quad \text{as } k \to \infty, \tag{57}$$

where $Q_h(x,y)$ is the norm form of Λ_h with respect to the basis matrix as in (20)*.* □

Proof. We start by proving (53). Let (p_k, t_k, q_k) be given by (52), then

$$\begin{pmatrix} p_k \\ t_k \\ q_k \end{pmatrix} = \begin{pmatrix} 7 & -4 & 8 \\ 4 & -1 & 4 \\ 8 & -4 & 9 \end{pmatrix}^k \begin{pmatrix} 15 \\ 8 \\ 17 \end{pmatrix}. \tag{58}$$

We argue by induction on k. First notice that $p_1 = 209$, $t_1 = 120$, and $q_1 = 241$, so that $p_1 > t_1$, $2|t_1$, and (53) is satisfied. Now assume this holds for $(p_{k-1}, t_{k-1}, q_{k-1})$. By (58),

$$\begin{pmatrix} p_k \\ t_k \\ q_k \end{pmatrix} = \begin{pmatrix} 7p_{k-1} - 4t_{k-1} + 8q_{k-1} \\ 4p_{k-1} - t_{k-1} + 4q_{k-1} \\ 8p_{k-1} - 4t_{k-1} + 9q_{k-1} \end{pmatrix}, \tag{59}$$

and so

$$p_k = t_k + (3p_{k-1} - 3t_{k-1} + 4q_{k-1}) > t_k,$$

since $p_{k-1} > t_{k-1}$, as well as

$$t_k = 4(p_{k-1} + q_{k-1}) - t_{k-1}$$

is divisible by 2, since $2|t_{k-1}$, and finally

$$\frac{q_k-1}{2} = 4p_{k-1} - t_{k-1} + 4q_{k-1} + \left(\frac{q_{k-1}-1}{2} - t_{k-1}\right) = t_k,$$

since $\frac{q_{k-1}-1}{2} = t_{k-1}$. The conclusion follows by induction.

Next we derive (54) from (53). Notice that by squaring both sides of (53) and rearranging terms, we immediately obtain

$$\left(\frac{p_k}{q_k} - \frac{\sqrt{3}}{2}\right)\left(\frac{p_k}{q_k} + \frac{\sqrt{3}}{2}\right) = \frac{q_k-2}{2q_k^2}, \tag{60}$$

and since $\frac{p_k}{q_k} < 1$, we have

$$\left|\frac{p_k}{q_k} - \frac{\sqrt{3}}{2}\right| > \frac{q_k-2}{(2+\sqrt{3})q_k^2},$$

which is the lower bound of (54). For the upper bound, we rewrite (60) as

$$\left|\frac{p_k}{q_k} - \frac{\sqrt{3}}{2}\right| = \frac{q_k-2}{q_k(2p_k+\sqrt{3}q_k)} < \frac{1}{2p_k+\sqrt{3}q_k} < \frac{1}{2\sqrt{3}q_k},$$

since $\sqrt{3}q_k < 2p_k$. It is also clear that $q_k \to \infty$ as $k \to \infty$.

To prove (55), we first notice that $q_1 = 241$. Moreover, by (54), the sequence p_k/q_k is monotone decreasing and converges to $\sqrt{3}/2$, therefore

$$\frac{\sqrt{3}}{2} \leqslant \frac{p_k}{q_k} \leqslant \frac{p_1}{q_1} = \frac{209}{241},$$

for every $k \geqslant 1$. Then, by (59) and (53),

$$q_k = 8p_{k-1} - 4t_{k-1} + 9q_{k-1} \geqslant (7+4\sqrt{3})q_{k-1} + 2 > (7+4\sqrt{3})q_{k-1},$$

and

$$q_k = 8p_{k-1} - 4t_{k-1} + 9q_{k-1} \leqslant \left(7 + \frac{8\times 209}{241}\right)q_{k-1} + 2 < 13.947 \times q_{k-1}.$$

The inequalities (55) follow by induction on k.

To prove (56), notice that upper bound (54) implies that

$$\frac{p_k}{q_k} < \frac{\sqrt{3}}{2} + \frac{1}{2\sqrt{3}q_k} = \frac{\sqrt{3}}{2}\left(1 + \frac{1}{3q_k}\right) < \frac{\sqrt{3}}{2}\left(1 + \frac{1}{723(7+4\sqrt{3})^{k-1}}\right),$$

where the last inequality is obtained by applying by the lower bound of (55). Then the lower bound of (56) follows. To obtain the upper bound of (56), combine the lower bound of (54) with the upper bound of (55) in a similar manner.

Finally notice that (57) follows immediately from (53) and the fact that $q_k \to \infty$ as $k \to \infty$, and this completes the proof. □

Proof of Theorem 1.6. Let $\langle \Lambda_{p_k,q_k} \rangle$ be the sequence of similarity classes corresponding to the triples (p_k, t_k, q_k) as defined in (52), then (54) guarantees convergence of this sequence to the similarity class $\langle \Lambda_h \rangle$ with respect to the metric d_s on $\mathrm{Sim}(\mathbb{R}^2)$, and also implies (21), since $q_k \geqslant q_1 = 241$. The fact that $q_k = O(14^k)$ follows immediately from (55). To prove (22), assume that there exists some similarity class $\langle \Lambda_{p,q} \rangle \neq \langle \Lambda_{1,1} \rangle$ such that

$$d_s(\Lambda_h, \Lambda_{p,q}) = \frac{p}{q} - \frac{\sqrt{3}}{2} \leqslant \frac{1}{3\sqrt{3}q},$$

which implies that $(3\sqrt{3}p - 1)^2 \leqslant \frac{81}{4}q^2$, and therefore

$$q^2 - p^2 \geqslant \left(\frac{1}{2}\right)^2 \frac{27q^2 - 24\sqrt{3}p + 4}{27},$$

where

$$\frac{27q^2 - 24\sqrt{3}p + 4}{27} > q^2 - \frac{8p}{3\sqrt{3}} > q(q - \sqrt{3}) > 1,$$

since if $q > 1$, then $q \geqslant 13$. Hence

$$\sqrt{q^2 - p^2} > \frac{1}{2},$$

which contradicts the fact that either $(p, \sqrt{q^2 - p^2}, q)$ or $(\sqrt{q^2 - p^2}, p, q)$ is in $\mathcal{P}$, and so (22) must be true for each similarity class of the form $\langle \Lambda_{p,q} \rangle$. This completes the proof of the theorem. □

Finally, Corollary 1.7 follows immediately from (56).

The approximation result of Theorem 1.6 is also interesting since the similarity class $\langle \Lambda_h \rangle$ has a number of important properties: besides providing the optimal circle packing and minimizing Epstein zeta function, as mentioned in Section 1, it also solves the related minimization problem for the height of flat tori in dimension 2 (see [8] for details), as well as the quantizer problem in dimension 2 (see [9] for details). Let us also recall that a lattice Λ is called *perfect* if any real symmetric matrix A in the corresponding dimension can be represented as

$$A = \sum_{\boldsymbol{x} \in S(\Lambda)} \alpha_{\boldsymbol{x}} \boldsymbol{x}\boldsymbol{x}^t,$$

where $S(\Lambda)$ is the set of minimal vectors of Λ as in Section 1, each $\boldsymbol{x}$ is written as a column vector, and each $\alpha_{\boldsymbol{x}}$ is a real number. It is not difficult to see that for a lattice Λ in $\mathbb{R}^2$ to be perfect, the cardinality of $S(\Lambda)$ must be six, meaning that the only perfect lattices in $\mathbb{R}^2$ come from $\langle \Lambda_h \rangle$. Moreover, $\langle \Lambda_h \rangle$ is *strongly perfect*, meaning that it supports a spherical 5-design: we say that a lattice Λ in $\mathbb{R}^N$ (and hence its similarity class) supports a *spherical t-design* for $t \in \mathbb{Z}_{>0}$ if for every homogeneous polynomial $f(\boldsymbol{x})$ of degree $\leqslant t$ with real coefficients

$$\int_{\mathfrak{S}^{N-1}} f(\boldsymbol{x})\, d\boldsymbol{x} = \frac{1}{|S(\Lambda)|} \sum_{\boldsymbol{x} \in S(\Lambda)} f(\boldsymbol{x}), \tag{61}$$

where $\mathfrak{S}^{N-1}$ is the unit sphere in $\mathbb{R}^N$ with the canonical measure $d\boldsymbol{x}$ on it, normalized so that $\int_{\mathfrak{S}^{N-1}} d\boldsymbol{x} = 1$. No other similarity class in $\mathrm{Sim}(\mathbb{R}^2)$ supports a spherical 5-design (or 4-design), and $\langle \Lambda_{1,1} \rangle$ is the only other similarity class that supports a spherical 3-design (or 2-design); such similarity classes are called *strongly eutactic* (clearly, every lattice supports a 1-design). For detailed

information on perfect and eutactic lattices see [16], especially Chapter 16 for connections to spherical designs.

6. Diophantine approximation by quotients of Pythagorean triples

In this section we first prove Theorem 1.8. It follows immediately from the following direct consequence of a theorem of Hlawka [12] on simultaneous Diophantine approximation by quotients of Pythagorean triples, which we state here.

Theorem 6.1. *Let $x \in (0,1)$ be a real number. Then there exist infinitely many Pythagorean triples $(p, \sqrt{q^2-p^2}, q)$ such that*

$$\left| x - \frac{p}{q} \right| \leqslant \frac{2\sqrt{2}}{q}. \tag{62}$$

Proof of Theorem 1.8. Recall that

$$d_s(\Lambda, \Lambda_{p,q}) = \left|\sin\theta(\Lambda) - \sin\theta(\Lambda_{p,q})\right| = \left|\sin\theta(\Lambda) - \frac{p}{q}\right|,$$

and apply Theorem 6.1 with $x = \sin\theta(\Lambda)$. □

Moreover, we can say that the set $\{\langle \Lambda_{p,q}\rangle\colon\ p/q \in \mathcal{S}\}$ of similarity classes of WR sublattices of $\mathbb{Z}^2$ is equidistributed in the set $\mathrm{Sim}(\mathbb{R}^2)$ of similarity classes of all WR lattices in $\mathbb{R}^2$ in the following sense. It is a well-known fact that the map

$$t \mapsto \left(\frac{1-t^2}{1+t^2}, \frac{t}{t^2-1}\right)$$

is a bijection from the set of rational numbers onto the set of all rational points on the unit circle. Ordering $\mathbb{Q}$ as the set of Farey fractions induces an ordering on the set of rational points on the unit circle, and hence on the set $\mathcal{S}$ of y-coordinates of such points that fall in the interval $[\frac{\sqrt{3}}{2}, 1]$. Now, it is a well-known fact that Farey fractions are uniformly distributed (mod 1).

As a side remark, we can also use Theorem 6.1 to approximate points on a unit circle with rational points on the same circle.

Corollary 6.2. *Let (x, y) be a point on the unit circle. Then either $x, y \in \{0, \pm 1\}$, or there exist infinitely many rational points $(p/q, r/q)$ on the same circle such that*

$$\max\left\{\left|x - \frac{p}{q}\right|, \left|y - \frac{r}{q}\right|\right\} \leqslant \frac{2\sqrt{2}}{q}. \tag{63}$$

Proof. First notice that it suffices to prove the statement of this corollary for the case $0 < x, y < 1$, namely the case when the point in question lies in the first quadrant, since any other point on the circle can be obtained from those in the first quadrant by a rational rotation. Let c be an arbitrary real number in the interval $(0,1)$, then either

$$0 < x \leqslant \sqrt{1-c^2} < 1, \quad c \leqslant y < 1, \tag{64}$$

or

$$0 < y \leqslant \sqrt{1-c^2} < 1, \quad c \leqslant x < 1. \tag{65}$$

First assume that (64) holds. By Theorem 6.1, there exist infinitely many Pythagorean triples (p, r, q) with $r = \sqrt{q^2 - p^2}$ which satisfy (62). Then:

$$\frac{2\sqrt{2}}{q} \geqslant \left|x - \frac{p}{q}\right| = \left|\sqrt{1-y^2} - \sqrt{1-\frac{r^2}{q^2}}\right| = \frac{|\frac{r^2}{q^2} - y^2|}{\sqrt{1-y^2}+\sqrt{1-\frac{r^2}{q^2}}}$$
$$= \frac{\frac{r}{q}+y}{\sqrt{1-y^2}+\sqrt{1-\frac{r^2}{q^2}}}\left|y - \frac{r}{q}\right| \geqslant \frac{c(1+\frac{n}{n+1})}{2\sqrt{1-\frac{n^2}{(n+1)^2}c^2}}\left|y - \frac{r}{q}\right|. \tag{66}$$

The last inequality is true because $\frac{w+z}{\sqrt{1-w^2}+\sqrt{1-z^2}}$ is an increasing function in both variables for $0 < z, w < 1$; since $y \geqslant c$, we can pick q large enough so that r/q would have to be sufficiently close to y so that $r/q \geqslant \frac{n}{n+1}c$ for some $n \in \mathbb{Z}_{>0}$, then $r/q + y \geqslant c(1+\frac{n}{n+1})$, and $\sqrt{1-y^2}+\sqrt{1-\frac{r^2}{q^2}} \leqslant 2\sqrt{1-\frac{n^2}{(n+1)^2}c^2}$. Then (66) implies

$$\left|y - \frac{r}{q}\right| \leqslant \frac{\sqrt{1-\frac{n^2}{(n+1)^2}c^2}}{c(1+\frac{n}{n+1})} \times \frac{4\sqrt{2}}{q}. \tag{67}$$

Since our choice of $c \in (0,1)$ and positive integer n was arbitrary, we can for instance choose

$$c = \frac{2n+2}{\sqrt{8n^2+4n+1}}, \tag{68}$$

and take $n = 2$, in which case, combining (62), (67), and (68), we obtain (63).

If, on the other hand, (65) holds instead of (64), simply repeat the above argument interchanging x with y and p/q with r/q. This completes the proof. □

A related result has also been obtained by Kopetzky in [13] (also see [14]), however his bounds are different in flavor in the sense that the constants in the upper bounds depend on x and y. Notice that the bound of Corollary 6.2 can be easily extended to any rational ellipse.

Corollary 6.3. *Let (x, y) be a point on the ellipse E, given by the equation*

$$\left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 = 1,$$

where a, b are positive rational numbers. Then either $(x, y) = (\pm a, 0), (0, \pm b)$, or there exist infinitely many rational points $(p/q, r/q)$ on the same ellipse such that

$$\max\left\{\left|x - \frac{p}{q}\right|, \left|y - \frac{r}{q}\right|\right\} \leqslant \frac{2\sqrt{2}\max\{a, b\}}{q}. \tag{69}$$

Proof. Notice that the map $(x, y) \mapsto (x/a, y/b)$ is a bijection between E and the unit circle, which takes rational points to rational points. Now apply Corollary 6.2 to points of the form $(x/a, y/b)$. □

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Supplementary material

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