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CSLs of the root lattice $\mathbf{A_4}$

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Abstract. Recently, the group of coincidence isometries of the root lattice A_4 has been determined providing a classification of these isometries with respect to their coincidence indices. A more difficult task is the classification of all CSLs, since different coincidence isometries may generate the same CSL. In contrast to the typical examples in dimensions $d \leq 3$, where coincidence isometries generating the same CSL can only differ by a symmetry operation, the situation is more involved in 4 dimensions. Here, we find coincidence isometries that are not related by a symmetry operation but nevertheless give rise to the same CSL. We indicate how the classification of CSLs can be obtained by making use of the icosian ring and provide explicit criteria for two isometries to generate the same CSL. Moreover, we determine the number of CSLs of a given index and encapsulate the result in a Dirichlet series generating function.

1. Introduction

In crystallography, CSLs are a well established tool for the description and classification of grain boundaries, see [1] and references given there. CSLs have been studied for several decades in dimensions $d \leq 3$. In higher dimensions they became interesting after the discovery of quasicrystals. Here, we discuss a 4-dimensional lattice, namely the root lattice A_4, which is intimately related to quasicrystals with fivefold symmetry and the Penrose tiling in particular.

Let us recall some basic notions first. A *lattice* $\varGamma$ in the Euclidean space $\mathbb{R}^d$, can be described as the set of all integer linear combinations of a basis $\{b_1, \ldots, b_d\}$ of $\mathbb{R}^d$, which is denoted by $\varGamma = \langle b_1, \ldots, b_d \rangle_{\mathbb{Z}}$. A *coincidence site lattice* (CSL) of a lattice $\varGamma$ is defined as $\varGamma \cap R\varGamma$, where R is a linear isometry and the corresponding *coincidence index* $\varSigma(R) = [\varGamma : (\varGamma \cap R\varGamma)]$ is finite, i.e. R and $R\varGamma$ share a common sublattice. The orthogonal group, i.e. the group of all linear isometries of $\mathbb{R}^d$, is denoted by $\mathrm{O}(d, \mathbb{R})$. We define the set of all *coincidence isometries* as

$$\mathrm{OC}(\varGamma) := \{R \in \mathrm{O}(d, \mathbb{R}) \mid \varSigma(R) < \infty\}$$

and its restriction to rotations as $\mathrm{SOC}(\varGamma)$. According to [1–3], $\mathrm{OC}(\varGamma)$ and $\mathrm{SOC}(\varGamma)$ are not only subgroups of $\mathrm{O}(d, \mathbb{R})$, but subgroups of the group of all similarity isometries which is defined as $\mathrm{OS}(\varGamma) := \{R \in \mathrm{O}(d, \mathbb{R}) \mid \alpha R\varGamma \subset \varGamma \text{ for some } \alpha \in \mathbb{R}^+\}$. A sublattice of $\varGamma$ of the form $\alpha R\varGamma$ is called a *similar sublattice* (SSL) of $\varGamma$. If we denote the *denominator* of a matrix $R \in \mathrm{OS}(\varGamma)$ relative to the lattice $\varGamma$ as $\mathrm{den}_{\varGamma}(R) := \min\{\alpha \in \mathbb{R}^+ \mid \alpha R\varGamma \subset \varGamma\}$, we have the following characterisation, see [2] for details:

$$\mathrm{OC}(\Gamma) = \{R \in \mathrm{OS}(\Gamma) \mid \mathrm{den}_\Gamma(R) \in \mathbb{N}\} \tag{1}$$

In the following sections we first describe the root lattice A_4 in a suitable setting. Then, we briefly introduce the key objects required for the analysis of its CSLs, as well as their relations to each other. We continue by reviewing some parts of the classification of the coincidence rotations of the root lattice A_4, see [2, 4] for details, and extend this analysis by providing explicit criteria for two coincidence isometries to generate the same CSL. Finally, we classify the CSLs of the root lattice A_4 with respect to their coincidence indices and encapsulate the result in a Dirichlet series generating function which gives the number of CSLs for every index.

2. The root lattice A_4

The root lattice A_4 is usually defined in a 4-dimensional hyperplane of $\mathbb{R}^5$ as follows:

$$A_4 := \{(x_1, \ldots, x_5) \in \mathbb{Z}^5 \mid x_1 + \ldots + x_5 = 0\}$$

However, this realisation of A_4 in $\mathbb{R}^5$ is not suitable for our purposes. We prefer the following realisation in $\mathbb{R}^4$

$$L := \big\langle (1,0,0,0), \tfrac{1}{2}(-1,1,1,1), (0,-1,0,0), \tfrac{1}{2}(0,1,\tau-1,-\tau) \big\rangle_{\mathbb{Z}}$$

where $\tau = (1+\sqrt{5})/2$ is the golden ratio; see [2, 5, 6] for details. Note that L is just rescaled by a factor $\frac{1}{\sqrt{2}}$ in comparison to A_4. This particular description L is very convenient for our problem, as it enables us to use the arithmetic of the quaternion algebra $\mathbb{H}(\mathbb{Q}(\sqrt{5}\,))$; see [7] for a detailed introduction to Hamilton's quaternions. To simplify the notation we define

$$K := \mathbb{Q}(\sqrt{5}\,) = \{r + s\sqrt{5} \mid r, s \in \mathbb{Q}\},$$

which is a quadratic number field. The algebra $\mathbb{H}(K)$ is explicitly given as

$$\mathbb{H}(K) = K \oplus \mathrm{i}K \oplus \mathrm{j}K \oplus \mathrm{k}K,$$

where the generating elements satisfy Hamilton's relations $\mathrm{i}^2 = \mathrm{j}^2 = \mathrm{k}^2 = \mathrm{ijk} = -1$. It is equipped with a *conjugation* $\bar{\cdot}$ which is the unique mapping that fixes the elements of the centre of the algebra K and reverses the sign on its complement. If we write

$$q = (a,b,c,d) = a + \mathrm{i}b + \mathrm{j}c + \mathrm{k}d, \quad \text{this means} \quad \bar{q} = (a,-b,-c,-d).$$

The reduced norm and trace in $\mathbb{H}(K)$ are defined by

$$\mathrm{nr}(q) := q\bar{q} = |q|^2 \quad \text{and} \quad \mathrm{tr}(q) := q + \bar{q},$$

where we canonically identify an element $\alpha \in K$ with the quaternion $(\alpha,0,0,0)$. For any $q \in \mathbb{H}(K)$, $|q|$ is its Euclidean length, which need not be an element of K. Nevertheless, one has $|rs| = |r||s|$ for arbitrary $r, s \in \mathbb{H}(K)$. Due to the geometric meaning, we use the notations $|q|^2$ and $\mathrm{nr}(q)$ in parallel. An element $q \in \mathbb{H}(K)$ is called *integral* when both $\mathrm{nr}(q)$ and $\mathrm{tr}(q)$ are elements of

$$\mathcal{O} := \mathbb{Z}[\tau] := \{m + n\tau \mid m, n \in \mathbb{Z}\},$$

which is the ring of integers of the quadratic number field K.

The *icosian ring* $\mathbb{I}$ consists of all linear combinations of the vectors

$$(1,0,0,0), (0,1,0,0), \tfrac{1}{2}(1,1,1,1), \tfrac{1}{2}(1-\tau,\tau,0,1)$$

with coefficients in $\mathcal{O}$. The elements of $\mathbb{I}$ are called *icosians*. For more information on this remarkable object, see for example [6, 8–10] and references given there.

An element $p \in \mathbb{I}$ is called $\mathbb{I}$-*primitive* when $\alpha p \in \mathbb{I}$, with $\alpha \in K$, is only possible with $\alpha \in \mathcal{O}$. Similarly, a sublattice Λ of L is called L-*primitive* when $\alpha\Lambda \subset L$, with $\alpha \in \mathbb{Q}$, implies $\alpha \in \mathbb{Z}$. Whenever the context is clear, we simply use the term "primitive" in both cases.

The detailed arithmetic structure of $\mathbb{I}$ plays a key role in the characterisation of the coincidence rotations for L; see [2]. Another important object for this characterisation is the following map, called *twist map*. If $q = (a,b,c,d)$, it is defined by the mapping

$$q \mapsto \widetilde{q} := (a', b', d', c'),$$

where $'$ denotes the algebraic conjugation in K, as defined by the mapping $\sqrt{5} \mapsto -\sqrt{5}$. The algebraic conjugation in K is also needed to define the absolute norm on K, via $\mathrm{N}(\alpha) := |\alpha\alpha'|$. For the various properties of the twist map, e.g. $\widetilde{\widetilde{q}} = q$ and $\widetilde{pq} = \widetilde{q}\widetilde{p}$ where $p, q \in \mathbb{I}$, we refer the reader to [6] and references therein. The most important properties in our present context are summarised in the following Lemma, see [6, Proposition 1] and [2, Lemma 4], which describes the relations between L and $\mathbb{I}$.

Lemma 1. *Within* $\mathbb{H}(K)$*, one has* $\widetilde{\mathbb{I}} = \mathbb{I}$ *and*

$$L = \{x \in \mathbb{I} \mid \widetilde{x} = x\} = \{x + \widetilde{x} \mid x \in \mathbb{I}\} = \phi_+(\mathbb{I}),$$

where the $\mathbb{Q}$*-linear mapping* $\phi_+ \colon \mathbb{H}(K) \longrightarrow \mathbb{H}(K)$*, is defined by* $\phi_+(x) = x + \widetilde{x}$*.*

The dual A_4^* of the the root lattice A_4, here in form of the dual of the lattice L, is given by

$$L^* := \{x \in \mathbb{R}^4 \mid \langle x|y\rangle \in \mathbb{Z} \text{ for all } y \in L\}.$$

3. CSLs

The investigation of CSLs of L can be restricted to rotations only, since $\overline{L} = L$, which means that any orientation reversing operation can be obtained from an orientation preserving one after applying conjugation first. Let $\mathrm{SOS}(L)$ be the group of all similarity rotations of the lattice L. Considering Eq. (1), it is obvious how $\mathrm{SOC}(L)$ and $\mathrm{SOS}(L)$ are related in general. By [6, Corollary 1] we know that any similarity rotation of L is of the form $x \mapsto \frac{1}{|q\widetilde{q}|}\, qx\widetilde{q}$ with $q \in \mathbb{I}$, which we refer to as $R(q)$, or more precisely we define $R(q)x := \frac{1}{|q\widetilde{q}|}\, qx\widetilde{q}$. We denote the denominator of $R(q)$ by $\mathrm{den}(q)$. Among the elements of $\mathrm{SOS}(L)$, we can identify the elements of $\mathrm{SOC}(L)$ as follows; see [2] for the proof.

Proposition 2. *Let* $0 \neq q \in \mathbb{I}$ *be an arbitrary icosian. Then, the lattice* $\frac{1}{|q\widetilde{q}|}\, qL\widetilde{q} \cap L$ *is a CSL of* L *if and only if* $|q\widetilde{q}| \in \mathbb{N}$*. If* q *is primitive, then* $\mathrm{den}(q) = |q\widetilde{q}|$*.*

We call an icosian $q \in \mathbb{I}$ *admissible* when $|q\widetilde{q}| \in \mathbb{N}$. As $\mathrm{nr}(\widetilde{q}) = \mathrm{nr}(q)'$, the admissibility of q implies that $\mathrm{N}\big(\mathrm{nr}(q)\big) = |q\widetilde{q}|^2$ is a square in $\mathbb{N}$. An immediate consequence of Proposition 2 is that

$$\mathrm{SOC}(L) = \{R(p) \mid p \in \mathbb{I} \text{ is primitive and admissible }\}, \tag{2}$$

which delivers the following classification.

Theorem 3. *The CSLs of L are precisely the lattices of the form $L \cap \frac{1}{|q\widetilde{q}|}\, qL\widetilde{q}$ with $q \in \mathbb{I}$ primitive and admissible.*

This is the first step to connect certain primitive right ideals $p\mathbb{I}$ of the icosian ring with the CSLs of L. Before we continue in this direction, let us consider the relation with the coincidence rotations, see [2, Lemma 5].

Lemma 4. *Let $r, s \in \mathbb{I}$ be primitive and admissible quaternions, with $r\mathbb{I} = s\mathbb{I}$. Then, one has $L \cap \frac{rL\tilde{r}}{|r\tilde{r}|} = L \cap \frac{sL\tilde{s}}{|s\tilde{s}|}$.*

The converse statement to Lemma 4 is not true, as the equality of two CSLs does *not* imply the corresponding ideals to be equal. An example is provided by $r = (\tau, 2\tau, 0, 0)$ and $s = (\tau^2, \tau, \tau, 1)$, which define the same CSL, though $s^{-1}r$ is not a unit in $\mathbb{I}$. The CSL is spanned by the basis $\{(1,2,0,0), (2,-1,0,0), (\frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}), (-1, \frac{1}{2}, \frac{\tau-1}{2}, -\frac{\tau}{2})\}$. Note that, as a direct consequence of [6, Lemma 5], two primitive quaternions $r, s \in \mathbb{I}$ are related by a rotation symmetry of L if and only if $r\mathbb{I} = s\mathbb{I}$.

For our further discussion we need to replace the primitive and admissible icosian p, and with it $\tilde{p}$, by certain $\mathcal{O}$-multiples, such that their norms have the same prime divisors in $\mathcal{O}$. In view of the form of the rotation $x \mapsto \frac{1}{|p\widetilde{p}|}\, px\widetilde{p}$, this is actually rather natural because it restores some kind of symmetry of the expressions in relation to the two quaternions involved. For a primitive and admissible icosian $p \in \mathbb{I}$ we choose explicitly

$$\alpha_q \,=\, \sqrt{\frac{\mathrm{lcm}(\mathrm{nr}(q), \mathrm{nr}(\widetilde{q}))}{\mathrm{nr}(q)}} \,\in\, \mathcal{O}\,, \tag{3}$$

where we assume a suitable standardisation for the lcm (least common multiple) of two elements of $\mathcal{O}$; see [2] for details. Moreover, we have the relation $\alpha_{\tilde{q}} = \widetilde{\alpha_q} = \alpha_q'$. The icosian $\alpha_q q$ is called the *extension* of the primitive admissible element $q \in \mathbb{I}$, and $(\alpha_q q, \alpha_q' \widetilde{q})$ the corresponding *extension pair*. Since α_q and α_q' are central, the extension does not change the rotation, i.e.

$$\frac{qx\widetilde{q}}{|q\widetilde{q}|} \,=\, \frac{q_\alpha x \widetilde{q_\alpha}}{|q_\alpha \widetilde{q_\alpha}|}$$

holds for all quaternions x. Note that the definition of the extension pair is unique up to units of $\mathcal{O}$, and that one has the relation

$$\mathrm{nr}(q_\alpha) \,=\, \mathrm{lcm}\big(\mathrm{nr}(q), \mathrm{nr}(\widetilde{q})\big) \,=\, \mathrm{nr}(\widetilde{q_\alpha}) \,=\, |q_\alpha \widetilde{q_\alpha}| \,\in\, \mathbb{N}\,.$$

Following [2] we define the set

$$L(q) \,=\, \{qx + \widetilde{x}\widetilde{q} \mid x \in \mathbb{I}\} \,=\, \phi_+(q\mathbb{I})\,.$$

Note that, due to $\widetilde{\mathbb{I}} = \mathbb{I}$, one has $L(q) = \widetilde{L(q)}$. This leads to the following parametrisation of the CSLs of L, compare [2, Theorem 2].

Theorem 5. *Let $q \in \mathbb{I}$ be admissible and primitive, and let $q_\alpha = \alpha_q q$ be its extension. Then, the CSL defined by q is given by*

$$L \cap \frac{1}{|q\widetilde{q}|} qL\widetilde{q} \,=\, L(q_\alpha) \,=\, (q_\alpha \mathbb{I} + \mathbb{I}\widetilde{q_\alpha}) \cap L.$$

and its index is $\Sigma_L(q) \,=\, \mathrm{nr}(q_\alpha) \,=\, \mathrm{lcm}(\mathrm{nr}(q), \mathrm{nr}(q)')\,.$

4. The Number of CSLs of each Index

Until now we have followed the argumentation in [2], which lead to the classification of all coincidence rotations of the lattice L. In order to obtain a classification of the actual CSLs, we make use of the corresponding classification for the icosian ring $\mathbb{I}$ and its submodul $L[\tau]$, which can either be seen as $\mathcal{O}$-modules of rank 4 or as lattices in $\mathbb{R}^8$, so all our definitions of the introductory section apply. Since any coincidence rotation of L is a coincidence rotation of $L[\tau]$ and $\mathbb{I}$, we can start our analysis from the classification of the CSLs of $\mathbb{I}$, which directly gives a first sufficient condition when two CSLs of L are equal, see [11] for details.

Lemma 6. *Let $p_1, p_2 \in \mathbb{I}$ be primitive and admissible, such that*

$$|p_1|^2 = |p_2|^2 \quad \textit{and} \quad \operatorname{glcd}(p_1, |p_1\widetilde{p}_1|) = \operatorname{glcd}(p_2, |p_2\widetilde{p}_2|).$$

Then $L \cap \frac{1}{|p_1\widetilde{p}_1|} p_1 L\widetilde{p}_1 = L \cap \frac{1}{|p_2\widetilde{p}_2|} p_2 L\widetilde{p}_2$.

In fact, the converse holds only if $|p_1|^2 = |p_2|^2$ is not divisible by the splitting prime $p = 5$. For the general situation we have the following

Theorem 7. *Let $p_1, p_2 \in \mathbb{I}$ be primitive and admissible. Then*

$$L \cap \tfrac{1}{|p_1\widetilde{p}_1|} p_1 L\widetilde{p}_1 = L \cap \tfrac{1}{|p_2\widetilde{p}_2|} p_2 L\widetilde{p}_2$$

if and only if

$$|p_1|^2 = |p_2|^2 \quad \textit{and} \quad \operatorname{glcd}(p_1, \tfrac{|p_1\widetilde{p}_1|}{c}) = \operatorname{glcd}(p_2, \tfrac{|p_2\widetilde{p}_2|}{c}), \tag{4}$$

where $c = \sqrt{5}$, if $|p_1|^2 = |p_2|^2$ is divisible by 5 and $c = 1$ otherwise.

Note that $|p_1|^2 = |p_2|^2$ directly implies that the coincidence indices and denominators coincide, which is clearly necessary for the CSLs to be equal. The second condition of (4) tells us how much p_1 and p_2 are allowed to differ in terms of their decomposition in irreducible elements of $\mathbb{I}$. If $|p_1|^2 = |p_2|^2$ is not divisible by 5 and $\operatorname{nr}(p_1) = \operatorname{nr}(p_1)'$, then (and only then) the second condition is equivalent to $p_1 = p_2\epsilon$ where ϵ is a unit of $\mathbb{I}$, which means that R_1 and R_2 are symmetry related. Hence, in this special case, and only then, we can deduce from two equal CSLs that they are generated by coincidence rotations which are symmetry related, whereas in all other cases there are at least two rotations that are not symmetry related but give the same CSL.

Now, we can conclude with the derivation of the Dirichlet series for the number of CSLs of L of a given index, see [12] for a introduction to Dirichlet series. Note, that by [1, Lemma 2.5, Theorem 2.2] the number of CSLs of a given index n is the same for the lattices A_4 and L as well as their dual lattice L^*. Let $f(n)$ be the number of CSLs of index n. Then, $f(n)$ is a multiplicative arithmetic function, given at prime powers p^r with $r \geq 1$ by

$$f(p^r) = \begin{cases} 6 \cdot 5^{2r-2} & \text{for } p = 5 \\ (p^2+1)p^{2r-2} & \text{for } p \equiv \pm 2 \pmod 5 \\ \frac{(p+1)^2}{p^3-1}(p^{2r+1} + p^{2r-2} - 2p^{\frac{(r-1)}{2}}) & \text{for } p \equiv \pm 1 \pmod 5, r \text{ odd}, \\ \frac{(p+1)^2}{p^3-1}\left(p^{2r+1} + p^{2r-2} - 2\frac{(p^2+1)}{p+1}p^{\frac{(r-2)}{2}}\right) & \text{for } p \equiv \pm 1 \pmod 5, r \text{ even}. \end{cases}$$

Finally elementary calculations involving geometric series yield its Dirichlet series generating function compare [11, 13]:

$$D(s) = \sum_{n=1}^{\infty} \frac{f(n)}{n^s} = \left(1 + 6\tfrac{5^{-s}}{1-5^{2-s}}\right) \prod_{p\equiv\pm1\,(5)} \tfrac{1+p^{-s}+2p^{1-s}+2p^{-2s}+p^{1-2s}+p^{1-3s}}{(1-p^{2-s})\,(1-p^{1-2s})} \prod_{p\equiv\pm2\,(5)} \tfrac{1+p^{-s}}{1-p^{2-s}}$$
$$= 1 + \tfrac{5}{2^s} + \tfrac{10}{3^s} + \tfrac{20}{4^s} + \tfrac{6}{5^s} + \tfrac{50}{6^s} + \tfrac{50}{7^s} + \tfrac{80}{8^s} + \tfrac{90}{9^s} + \tfrac{30}{10^s} + \tfrac{144}{11^s} + \ldots$$

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