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# COINCIDENCE ROTATIONS OF THE ROOT LATTICE $A_4$

MICHAEL BAAKE, UWE GRIMM, MANUELA HEUER, AND PETER ZEINER

ABSTRACT. The coincidence site lattices of the root lattice  $A_4$  are considered, and the statistics of the corresponding coincidence rotations according to their indices is expressed in terms of a Dirichlet series generating function. This is possible via an embedding of  $A_4$  into the icosian ring with its rich arithmetic structure, which recently [6] led to the classification of the similar sublattices of  $A_4$ .

Dedicated to Ludwig Danzer on the occasion of his 80th birthday

## 1. INTRODUCTION AND GENERAL SETTING

Consider a lattice  $\Gamma$  in Euclidean  $d$ -space, i.e., a cocompact discrete subgroup of  $\mathbb{R}^d$ . An element  $R \in O(d, \mathbb{R})$  is called a (linear) *coincidence isometry* of  $\Gamma$  when  $\Gamma$  and  $R\Gamma$  are commensurate, written as  $\Gamma \sim R\Gamma$ , which means that they share a common sublattice. The intersection  $\Gamma \cap R\Gamma$  is then called the *coincidence site lattice* (CSL) for the isometry  $R$ . When this is the case, the corresponding *coincidence index*  $\Sigma(R)$  is defined as

$$\Sigma(R) = [\Gamma : (\Gamma \cap R\Gamma)],$$

and it is set to  $\infty$  otherwise. The index satisfies  $[\Gamma : (\Gamma \cap R\Gamma)] = [R\Gamma : (\Gamma \cap R\Gamma)]$ , as  $\Gamma$  and  $R\Gamma$  possess fundamental domains of the same volume, compare [11] for general background on lattice theory. Moreover,

$$\text{OC}(\Gamma) := \{R \in O(d, \mathbb{R}) \mid \Sigma(R) < \infty\}$$

is a group, and one also has  $\Sigma(R^{-1}) = \Sigma(R)$ , see [1] for a general survey and several typical examples. The subgroup  $\text{SOC}(\Gamma)$  consists of all rotations within  $\text{OC}(\Gamma)$ .

Coincidence site lattices play an important role in crystallography, in the description and understanding of grain boundaries, compare [1] and references given there. In recent years, they have also found applications in lattice discretisation problems [26]. From a more theoretical angle, they show up in various lattice and tiling problems, such as Danzer's 'Ein-Stein-Tiling' [14, 15, 2] or the analysis of the pinwheel tilings of the plane [20, 5]. Apart from that, several attempts have been made to get further insight into the theory, see [4, 8, 28, 31] and references given there for recent publications.

Another relevant object in this context, with  $\mathbb{R}_+ := \{\alpha \in \mathbb{R} \mid \alpha > 0\}$ , is the set

$$\text{OS}(\Gamma) := \{R \in O(d, \mathbb{R}) \mid \alpha R\Gamma \subset \Gamma \text{ for some } \alpha \in \mathbb{R}_+\}.$$

It consists of all linear isometries that emerge from similarity mappings of  $\Gamma$  into itself, while  $\text{SOS}(\Gamma)$  is then the subset of rotations of that kind. A sublattice of  $\Gamma$  of the form  $\alpha R\Gamma$  is called a *similar sublattice* of  $\Gamma$ , or SSL for short.

**Fact 1.** *If  $\Gamma \subset \mathbb{R}^d$  is a lattice,  $\text{OS}(\Gamma)$  and  $\text{SOS}(\Gamma)$  are subgroups of  $\text{O}(d, \mathbb{R})$ .*

*Proof.* It suffices to verify the subgroup property for  $\text{OS}(\Gamma)$ . If  $R$  and  $S$  are isometries in  $\text{OS}(\Gamma)$ , with attached positive numbers  $\alpha$  and  $\beta$  say, then so is  $RS$ , because  $\alpha\beta RST = \alpha R(\beta S\Gamma) \subset \alpha R\Gamma \subset \Gamma$ .

Also, one has  $\Gamma \subset \frac{1}{\alpha}R^{-1}\Gamma$ , so that  $[\frac{1}{\alpha}R^{-1}\Gamma : \Gamma] = [\Gamma : \alpha R\Gamma] =: m \in \mathbb{N}$ . By standard lattice theory, compare [11], this means that  $\frac{m}{\alpha}R^{-1}\Gamma \subset \Gamma$ , which shows that also  $R^{-1}$  is an element of  $\text{OS}(\Gamma)$ .  $\square$

Let us start with a general observation on the connection between the similarities and the coincidence isometries.

**Lemma 1.** *If  $R$  is a coincidence isometry for the lattice  $\Gamma \subset \mathbb{R}^d$ , there exists some  $\alpha \in \mathbb{R}_+$  so that  $\alpha R\Gamma \subset \Gamma$ . In other words,  $\text{OC}(\Gamma)$  is a subgroup of  $\text{OS}(\Gamma)$ .*

*Proof.*  $R \in \text{OC}(\Gamma)$  means  $\Sigma(R) = [\Gamma : (\Gamma \cap R\Gamma)] = [R\Gamma : (\Gamma \cap R\Gamma)] = n \in \mathbb{N}$ . This implies  $nR\Gamma \subset (\Gamma \cap R\Gamma) \subset \Gamma$  by standard lattice theory.  $\square$

The converse is not true in general, meaning that *not* all rotations and reflections from similar sublattices will give rise to coincidence isometries. It is precisely one of our goals later on to find the distinction for the case of the root lattice  $A_4$ .

In view of Lemma 1, it is reasonable to define the *denominator* of a matrix  $R \in \text{OS}(\Gamma)$  relative to the lattice  $\Gamma$  as

$$(1) \quad \text{den}_\Gamma(R) = \min\{\alpha \in \mathbb{R}_+ \mid \alpha R\Gamma \subset \Gamma\}.$$

Clearly, as  $R$  is an isometry, one always has  $\text{den}_\Gamma(R) \geq 1$ , and from  $\text{den}_\Gamma(R)R\Gamma \subset \Gamma$  one concludes that  $(\text{den}_\Gamma(R))^d$  must be an integer. Consequently,  $\text{den}_\Gamma(R)$  is either a positive integer or an irrational number, but still algebraic. Moreover, by standard arguments, one has

$$(2) \quad \{\alpha \in \mathbb{R}_+ \mid \alpha R\Gamma \subset \Gamma\} = \text{den}_\Gamma(R)\mathbb{N}.$$

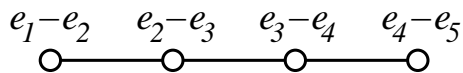
This gives rise to the following refinement of Lemma 1.

**Lemma 2.** *Let  $\Gamma \subset \mathbb{R}^d$  be a lattice, with groups  $\text{OS}(\Gamma)$  and  $\text{OC}(\Gamma)$  as defined above. With the denominator from (1), one has  $\text{OC}(\Gamma) = \{R \in \text{OS}(\Gamma) \mid \text{den}_\Gamma(R) \in \mathbb{N}\}$ .*

*Proof.* If  $\text{den}_\Gamma(R) \in \mathbb{N}$ , one has  $\text{den}_\Gamma(R)R\Gamma \subset (\Gamma \cap R\Gamma)$ . Consequently, the lattices  $\Gamma$  and  $R\Gamma$  are commensurate, so that the inclusion  $\{R \in \text{OS}(\Gamma) \mid \text{den}_\Gamma(R) \in \mathbb{N}\} \subset \text{OC}(\Gamma)$  is clear.

Conversely, if  $R \in \text{OC}(\Gamma)$ ,  $\Gamma$  and  $R\Gamma$  are commensurate by definition. In particular, one has  $\Sigma(R)R\Gamma \subset \Gamma$ , so that  $\Sigma(R) \in \text{den}_\Gamma(R)\mathbb{N}$  by Eq. (2). As  $\Sigma(R) \in \mathbb{N}$ , this is only possible if  $\text{den}_\Gamma(R) \in \mathbb{Q}$ . Since we also know from above that  $(\text{den}_\Gamma(R))^d \in \mathbb{N}$ , we may now conclude that  $\text{den}_\Gamma(R) \in \mathbb{N}$ , whence the claim follows.  $\square$

For later use, we state a factorisation property for coincidence indices from [10].

FIGURE 1. Standard basis representation of the root lattice  $A_4$ .

**Lemma 3.** *Let  $\Gamma \subset \mathbb{R}^d$  be a lattice and  $R_1, R_2 \in \text{OC}(\Gamma)$ . When  $\Sigma(R_1)$  and  $\Sigma(R_2)$  are relatively prime, one has  $\Sigma(R_1 R_2) = \Sigma(R_1) \Sigma(R_2)$ . In general, one has the divisibility relation  $\Sigma(R_1 R_2) \mid \Sigma(R_1) \Sigma(R_2)$ .  $\square$*

When a lattice  $\Gamma$  is given, the set  $\Sigma(\text{OC}(\Gamma))$  is called the *simple coincidence spectrum*. It may or may not possess an algebraic structure. In nice situations,  $\Sigma(\text{OC}(\Gamma))$  is a multiplicative monoid within  $\mathbb{N}$ . On top of the spectrum, one is also interested in the number  $f(m)$  of different CSLs of a given index  $m$ . This arithmetic function is often encapsulated into a Dirichlet series generating function,

$$(3) \quad \Phi_\Gamma(s) := \sum_{m=1}^{\infty} \frac{f(m)}{m^s},$$

which is a natural approach because it permits an Euler product decomposition when  $f$  is multiplicative. Beyond three dimensions, this generating function seems difficult to determine, and  $A_4$  is no exception. In this paper, we thus concentrate on the slightly simpler problem to count the coincidence rotations of  $A_4$  of index  $m$ , which always come in multiples of 120, the order of the rotation symmetry group of  $A_4$ . The latter is the subgroup of  $\text{SOC}(A_4)$  of rotations with coincidence index  $\Sigma = 1$ . If  $120f_{\text{rot}}(m)$  is the number of coincidence rotations with index  $m$ , we define the corresponding generating function as

$$(4) \quad \Phi_\Gamma^{\text{rot}}(s) := \sum_{m=1}^{\infty} \frac{f_{\text{rot}}(m)}{m^s},$$

which will turn out to possess a nice Euler product expansion. Note that  $0 \leq f(m) \leq f_{\text{rot}}(m)$  and that  $f(m) \neq 0$  if and only if  $f_{\text{rot}}(m) \neq 0$ . Asymptotic properties for  $m \rightarrow \infty$  can be extracted from the generating functions via Delange's theorem, see [7] and references therein for details in this context.

## 2. THE ROOT LATTICE $A_4$ AND ITS ARITHMETIC STRUCTURE

The root lattice  $A_4$  is usually defined as a lattice in a 4-dimensional hyperplane of  $\mathbb{R}^5$ , via the Dynkin diagram of Figure 1. Here, the  $e_i$  denote the standard Euclidean basis vectors in 5-space. Though convenient for many purposes, this description does not seem to be optimal for the geometric properties we are after. Since the similar sublattices of  $A_4$  were recently classified [6] by a different 4-dimensional approach, using the arithmetic of the quaternion algebra  $\mathbb{H}(\mathbb{Q}(\sqrt{5}))$ , we use the same setting again in this paper.

From now on, we use the notation  $K = \mathbb{Q}(\sqrt{5})$  for brevity. The algebra  $\mathbb{H}(K)$ , which is a skew field, is explicitly given as  $\mathbb{H}(K) = K \oplus iK \oplus jK \oplus kK$ , where the generating elements satisfy Hamilton's relations  $i^2 = j^2 = k^2 = ijk = -1$ , see [22] for more.  $\mathbb{H}(K)$  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  $q = (a, b, c, d) = a + ib + jc + kd$ , this means  $\bar{q} = (a, -b, -c, -d)$ .

The reduced norm and trace in  $\mathbb{H}(K)$  are defined as usual [27, 21, 22] by

$$(5) \quad \text{nr}(q) = q\bar{q} = |q|^2 \quad \text{and} \quad \text{tr}(q) = q + \bar{q},$$

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  $\text{nr}(q)$  in parallel. An element  $q \in \mathbb{H}(K)$  is called *integral* when both  $\text{nr}(q)$  and  $\text{tr}(q)$  are elements of  $\mathfrak{o} := \mathbb{Z}[\tau]$ , which is the ring of integers of the quadratic field  $K$ , where  $\tau = (1 + \sqrt{5})/2$  is the golden ratio.

In this setting, we use the lattice

$$(6) \quad L = \langle (1, 0, 0, 0), \frac{1}{2}(-1, 1, 1, 1), (0, -1, 0, 0), \frac{1}{2}(0, 1, \tau - 1, -\tau) \rangle_{\mathbb{Z}},$$

which is the root lattice  $A_4$  relative to the inner product  $\text{tr}(x\bar{y}) = 2\langle x|y \rangle$ , where  $\langle x|y \rangle$  denotes the standard Euclidean inner product, see [12, 6] for details. This way,  $L$  is located within the icosian ring  $\mathbb{I}$ ,

$$(7) \quad \mathbb{I} = \langle (1, 0, 0, 0), (0, 1, 0, 0), \frac{1}{2}(1, 1, 1, 1), \frac{1}{2}(1 - \tau, \tau, 0, 1) \rangle_{\mathfrak{o}},$$

which is a maximal order in  $\mathbb{H}(K)$ , compare [19, 21] and references given there. In particular, all elements of  $\mathbb{I}$  (and hence also those of  $L$ ) are integral in  $\mathbb{H}(K)$ . In fact, one can use the quadratic form defined by  $\text{tr}(x\bar{y})$  to define the *dual* of a full  $\mathfrak{o}$ -module  $\Lambda \subset \mathbb{H}(K)$  as

$$(8) \quad \Lambda^* = \{x \in \mathbb{H}(K) \mid \text{tr}(x\bar{y}) \in \mathfrak{o} \text{ for all } y \in \Lambda\}.$$

With this definition, one has the following important property of the icosian ring, compare [24, 19, 12] for details.

**Fact 2.** *The icosian ring is self-dual, i.e., one has  $\mathbb{I}^* = \mathbb{I}$ .* □

Since  $\mathbb{H}(K)$  has class number 1, compare [24, 27], all ideals of  $\mathbb{I}$  are principal. The detailed arithmetic structure of  $\mathbb{I}$  was the key to solving the related sublattice problem [6] for  $L$ . What is more, one significantly profits from another map, called *twist map* in [6], which is an involution of the second kind for  $\mathbb{H}(K)$ . If  $q = (a, b, c, d)$ , it is defined by the mapping  $q \mapsto \tilde{q}$ ,

$$(9) \quad \tilde{q} = (a', b', d', c'),$$

where  $'$  denotes algebraic conjugation in  $K$ , as defined by the mapping  $\sqrt{5} \mapsto -\sqrt{5}$ . Note the unusual combination of algebraic conjugation of all coordinates with a permutation of the last two – which also explains the choice of the term ‘twist map’. The algebraic conjugation in  $K$  is also needed to define the absolute norm on  $K$ , via

$$N(\alpha) = |\alpha\alpha'|.$$

For the various properties of the twist map, we refer the reader to [6] and references therein. The most important one in our present context is the relation between  $L$  and  $\mathbb{I}$ .

**Fact 3.** *Within  $\mathbb{H}(K)$ , one has  $\tilde{\mathbb{I}} = \mathbb{I}$  and  $L = \{x \in \mathbb{I} \mid \tilde{x} = x\}$ .* □

Another useful characterization is possible via the  $\mathbb{Q}$ -linear mappings  $\phi_{\pm}: \mathbb{H}(K) \longrightarrow \mathbb{H}(K)$ , defined by  $\phi_{\pm}(x) = x \pm \tilde{x}$ , which are connected via the relation

$$\phi_{\pm}(\sqrt{5}x) = \sqrt{5}\phi_{\mp}(x)$$

and the obvious property  $\ker(\phi_{\pm}) = \text{im}(\phi_{\mp})$ .

**Lemma 4.** *The lattice  $L$  from (6) satisfies  $L = \{x + \tilde{x} \mid x \in \mathbb{I}\} = \phi_{+}(\mathbb{I})$ .*

*Proof.* For any  $x \in \mathbb{I}$ , we clearly have  $x + \tilde{x} \in L$  by Fact 3. On the other hand, observing  $\tau' = 1 - \tau$ , any  $x \in L$  permits the decomposition

$$x = (\tau + \tau')x = \tau x + \tau' \tilde{x} = \tau x + \tilde{\tau x}.$$

Since  $x \in \mathbb{I}$  and  $\mathbb{I}$  is an  $\mathfrak{o}$ -module, we still have  $\tau x \in \mathbb{I}$ , and the claim follows.  $\square$

**Remark 1.** For  $0 \neq q \in \mathbb{I}$ , one has  $\text{nr}(q) \in \mathfrak{o}$  and  $\text{nr}(q) = q\bar{q} > 0$ . As also  $\tilde{q} \in \mathbb{I}$ , one finds  $\text{nr}(\tilde{q}) \in \mathfrak{o}$  with  $\text{nr}(\tilde{q}) > 0$  and  $\text{nr}(\tilde{q}) = \text{nr}(q)'$ , so that  $\text{nr}(q)$  is always a totally positive element of  $\mathfrak{o}$ .

### 3. COINCIDENCE SITE LATTICES VIA QUATERNIONS

It is clear that we can restrict ourselves to the investigation of rotations only, because  $\bar{L} = L$ , so any orientation reversing operation can be obtained from an orientation preserving one after applying conjugation first.

Let us start by recalling a fundamental result from [6].

**Fact 4.** *If  $q \in \mathbb{I}$ , one has  $qL\tilde{q} \subset L$ . Moreover, all similar sublattices of  $L$  are of the form  $qL\tilde{q}$  with  $q \in \mathbb{I}$ .*  $\square$

For a given SSL of  $L$ , now written as  $qL\tilde{q}$ , the corresponding rotation is then given by the mapping  $x \mapsto \frac{1}{|q\tilde{q}|}qx\tilde{q}$ . It is clear that many different  $q$  result in the same rotation. In fact, we can restrict  $q$  to suitable subsets of icosians without missing any rotation, which we shall do later on.

Below, we need a refinement of Fact 4. Recall that a sublattice  $\Lambda$  of  $L$  is called  *$L$ -primitive* when  $\alpha\Lambda \subset L$ , with  $\alpha \in \mathbb{Q}$ , implies  $\alpha \in \mathbb{N}$ . Similarly, an element  $p \in \mathbb{I}$  is called  *$\mathbb{I}$ -primitive* when  $\alpha p \in \mathbb{I}$ , this time with  $\alpha \in K$ , is only possible with  $\alpha \in \mathfrak{o}$ , see [6] for details, and for a proof of the following result. For brevity, we simply use the term “primitive” in both cases, as the meaning is clear from the context.

**Proposition 1.** *A similar sublattice of  $L$  is primitive if and only if it is of the form  $qL\tilde{q}$  with  $q$  a primitive element of  $\mathbb{I}$ .*  $\square$

By Lemmas 1 and 2, we know how  $\text{SOC}(L)$  and  $\text{SOS}(L)$  are related in general. Here, Fact 4 tells us that any similarity rotation of  $L$  is of the form  $x \mapsto \frac{1}{|q\tilde{q}|}qx\tilde{q}$  with  $q \in \mathbb{I}$ . Among these, we have to identify the  $\text{SOC}(L)$  elements, which is possible as follows.

**Corollary 1.** *Let  $0 \neq q \in \mathbb{I}$  be an arbitrary icosian. The lattice  $\frac{1}{|q\tilde{q}|}qL\tilde{q}$  is commensurate with  $L$  if and only if  $|q\tilde{q}| \in \mathbb{N}$ .*

*Proof.* When  $q = \alpha r$  with  $0 \neq \alpha \in \mathfrak{o}$ , one has  $|q\tilde{q}| = N(\alpha)|r\tilde{r}|$  with  $N(\alpha) \in \mathbb{N}$ . If  $q$  is primitive, the claim is clear by Lemma 2 because  $|q\tilde{q}|$  is then the denominator of the rotation  $x \mapsto \frac{1}{|q\tilde{q}|} qx\tilde{q}$ . Otherwise,  $q$  is an  $\mathfrak{o}$ -multiple of a primitive icosian,  $r$  say, and the claim follows from the initial remark.  $\square$

Let us call an icosian  $q \in \mathbb{I}$  *admissible* when  $|q\tilde{q}| \in \mathbb{N}$ . As  $\text{nr}(\tilde{q}) = \text{nr}(q)'$ , the admissibility of  $q$  implies that  $N(\text{nr}(q))$  is a square in  $\mathbb{N}$ .

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

*Proof.* All CSLs can be obtained from a rotation, as  $L$  is invariant under the conjugation  $x \mapsto \bar{x}$ . By Lemma 1, we need only consider rotations from  $\text{OS}(L)$ , which, by Fact 4, are all of the form  $x \mapsto \frac{1}{|y\tilde{y}|} yx\tilde{y}$  with  $y \in \mathbb{I}$ . If  $y$  is not primitive, we can write it as  $y = \alpha q$  with  $\alpha \in \mathfrak{o}$  and  $q \in \mathbb{I}$  primitive. Since  $\alpha$  is a central element,  $y$  and  $q$  define the same rotation. An application of Corollary 1 now gives the claim.  $\square$

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

**Lemma 5.** *Let  $r, s \in \mathbb{I}$  be primitive and admissible quaternions, with  $r\mathbb{I} = s\mathbb{I}$ . Then, one has  $L \cap \frac{rL\tilde{r}}{|r\tilde{r}|} = L \cap \frac{sL\tilde{s}}{|s\tilde{s}|}$ .*

*Proof.* When  $r\mathbb{I} = s\mathbb{I}$ , one has  $s = r\varepsilon$  for some  $\varepsilon \in \mathbb{I}^\times$ , where  $\mathbb{I}^\times$  denotes the unit group of  $\mathbb{I}$ , see [21] for its structure. Since, by [6, Lemma 4], we then know that  $\varepsilon L\tilde{\varepsilon} = L$ , one has  $rL\tilde{r} = sL\tilde{s}$  in this case. As  $\text{nr}(\varepsilon\tilde{\varepsilon}) = N(\text{nr}(\varepsilon)) = 1$ , one also finds  $|s\tilde{s}| = |r\tilde{r}|$ . Consequently,  $\frac{rL\tilde{r}}{|r\tilde{r}|} = \frac{sL\tilde{s}}{|s\tilde{s}|}$ , and the CSLs of  $L$  defined by  $r$  and  $s$  are equal.  $\square$

**Remark 2.** The converse statement to Lemma 5 is not true, as the equality of two CSLs does *not* imply the corresponding rotations to be symmetry related. 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  $\{(1, 2, 0, 0), (2, -1, 0, 0), (\frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}), (-1, \frac{1}{2}, \frac{\tau-1}{2}, -\frac{\tau}{2})\}$ . However, when two primitive quaternions  $r, s \in \mathbb{I}$  define rotations that are related by a rotation symmetry of  $A_4$ , one has  $r\mathbb{I} = s\mathbb{I}$  as a direct consequence of [6, Lemma 4].

Although the primitive elements of  $\mathbb{I}$  are important in this context, we need a variant for our further discussion. Let  $q \in \mathbb{I}$  be primitive and admissible. Since  $\mathfrak{o}$  is Dedekind, one has the relation  $(x\mathfrak{o})^{-1} = \frac{1}{x}\mathfrak{o}$  for any principal fractional ideal with nonzero  $x \in K$ , see [17, Ch. I.4] for details. Then, the fractional ideal

$$(\text{nr}(q)\mathfrak{o} \cap \text{nr}(\tilde{q})\mathfrak{o})^2 (|q\tilde{q}|^2\mathfrak{o})^{-1} = \frac{(\text{lcm}(\text{nr}(q), \text{nr}(\tilde{q})))^2}{|q\tilde{q}|^2} \mathfrak{o} = \beta_q\mathfrak{o} \beta_{\tilde{q}}\mathfrak{o}$$

is a square as well, where  $\beta_q := \text{lcm}(\text{nr}(q), \text{nr}(\tilde{q}))/\text{nr}(q) \in \mathfrak{o}$  is well-defined up to units of  $\mathfrak{o}$ , as  $\mathfrak{o}$  is a principal ideal domain. Clearly,  $\beta_q\mathfrak{o}$  and  $\beta_{\tilde{q}}\mathfrak{o}$  are coprime by construction. Since their

product is a square in  $\mathfrak{o}$  (up to units), we have  $\beta_q \mathfrak{o} = (\alpha_q \mathfrak{o})^2$  for some  $\alpha_q \in \mathfrak{o}$ . Explicitly, we may choose

$$(10) \quad \alpha_q = \sqrt{\frac{\text{lcm}(\text{nr}(q), \text{nr}(\tilde{q}))}{\text{nr}(q)}} = \sqrt{\frac{\text{lcm}(\text{nr}(q), \text{nr}(q'))}{\text{nr}(q)}} \in \mathfrak{o},$$

where we assume a suitable standardisation for the lcm of two elements of  $\mathfrak{o}$ . Again,  $\alpha_q$  is only defined up to units of  $\mathfrak{o}$ , which is tantamount to saying that we implicitly work with the principal ideal  $\alpha_q \mathfrak{o}$  here. Moreover, we have the relation  $\alpha_{\tilde{q}} = \widetilde{\alpha_q} = \alpha_q'$ .

Let us call the icosian  $\alpha_q q$  the *extension* of the primitive admissible element  $q \in \mathbb{I}$ , and  $(\alpha_q q, \alpha_q' \tilde{q})$  the corresponding *extension pair*. In view of the form of the rotation  $x \mapsto \frac{1}{|q\tilde{q}|} qx\tilde{q}$ , it is actually rather natural to replace  $q$  and  $\tilde{q}$  by certain  $\mathfrak{o}$ -multiples,  $q_\alpha := \alpha_q q$  and  $\tilde{q}_\alpha = \alpha_q' \tilde{q}$ , such that  $\text{nr}(q_\alpha)$  and  $\text{nr}(\tilde{q}_\alpha)$  have the same prime divisors in  $\mathfrak{o}$ . The introduction of the extension pair restores some kind of symmetry of the expressions in relation to the two quaternions involved, which will become evident in the general treatment of 4-space [10].

Clearly, since the extra factors are central, this modification does not change the rotation, so that

$$(11) \quad \frac{qx\tilde{q}}{|q\tilde{q}|} = \frac{q_\alpha x \tilde{q}_\alpha}{|q_\alpha \tilde{q}_\alpha|}$$

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

$$(12) \quad \text{nr}(q_\alpha) = \text{lcm}(\text{nr}(q), \text{nr}(\tilde{q})) = \text{nr}(\tilde{q}_\alpha) = |q_\alpha \tilde{q}_\alpha| \in \mathbb{N},$$

which will be crucial later on.

**Lemma 6.** *For  $q \in \mathbb{I}$  and  $\gamma \in K$ , one has  $q \in \gamma\mathbb{I}$  if and only if  $\{\text{tr}(q\bar{y}) \mid y \in \mathbb{I}\} \subset \gamma\mathfrak{o}$ .*

*Proof.* The statement is clear for  $\gamma = 0$ , so assume  $\gamma \neq 0$ . When  $q \in \mathbb{I}$ , one has  $\text{tr}(q\bar{y}) \in \mathfrak{o}$  for all  $y \in \mathbb{I}$  (as then  $q\bar{y} \in \mathbb{I}$ ), whence  $q \in \gamma\mathbb{I}$  implies  $\text{tr}(q\bar{y}) \in \gamma\mathfrak{o}$ . Conversely,  $\text{tr}(q\bar{y}) \in \mathfrak{o}$  for all  $y \in \frac{1}{\gamma}\mathbb{I}$  means  $q \in (\frac{1}{\gamma}\mathbb{I})^* = \gamma\mathbb{I}^* = \gamma\mathbb{I}$ , by Fact 2, which implies the claim.  $\square$

**Lemma 7.** *If  $q \in \mathbb{I}$  is primitive, there is a quaternion  $z \in \mathbb{I}$  with  $\text{tr}(q\bar{z}) = 1$ . When, in addition,  $q$  is also admissible, there exists a quaternion  $z \in \mathbb{I}$  such that  $\text{tr}(q_\alpha \bar{z}) + \text{tr}(\tilde{z} \tilde{q}_\alpha) = 1$ , where  $q_\alpha$  denotes the extension of  $q$ .*

*Proof.* When  $q \in \mathbb{I}$ , one has  $\text{gcd}\{\text{tr}(q\bar{x})\mathfrak{o} \mid x \in \mathbb{I}\} = \gamma\mathfrak{o}$  with  $\gamma \in \mathfrak{o}$ . If  $\gamma$  is *not* a unit in  $\mathfrak{o}$ , one has  $q \in \gamma\mathbb{I}$  by Lemma 6, whence  $q$  cannot be primitive in this case. So,  $\gamma$  must be a unit, hence  $\gamma\mathfrak{o} = \mathfrak{o}$ . Then, by standard arguments based on the prime ideals, there are *finitely* many icosians  $x_i \in \mathbb{I}$ , say  $\ell$  of them (in fact,  $\ell \leq 4$  suffices), such that

$$\text{gcd}\{\text{tr}(q\bar{x}_i)\mathfrak{o} \mid 1 \leq i \leq \ell\} = \text{tr}(q\bar{x}_1)\mathfrak{o} + \dots + \text{tr}(q\bar{x}_\ell)\mathfrak{o} = \mathfrak{o}.$$

This implies the existence of numbers  $\beta_i \in \mathfrak{o}$ , with  $1 \leq i \leq \ell$ , such that  $z = \sum_i \beta_i x_i$  satisfies  $\text{tr}(q\bar{z}) = 1$ .

For the second claim, assume that  $q$  is also admissible and denote its extension by  $q_\alpha$ . Let  $z \in \mathbb{I}$  be the icosian from the first part of the proof, so that  $\text{tr}(q\bar{z}) = 1$ . Since  $q_\alpha = \alpha_q q$  with



$\alpha_q \in \mathfrak{o}$ , this implies  $\operatorname{tr}(q_\alpha \bar{z}) = \alpha_q$  and thus also

$$\alpha'_q = \tilde{\alpha}_q = (\operatorname{tr}(q_\alpha \bar{z}))^\sim = \operatorname{tr}(\widetilde{q_\alpha \bar{z}}) = \operatorname{tr}(\tilde{z} \tilde{q}_\alpha).$$

Since the ideals  $\alpha_q \mathfrak{o}$  and  $\alpha'_q \mathfrak{o}$  are relatively prime by construction, we have  $\alpha_q \mathfrak{o} + \alpha'_q \mathfrak{o} = \mathfrak{o}$  and thus the existence of  $\beta, \delta \in \mathfrak{o}$  with  $\beta \alpha_q + \delta \alpha'_q = 1$ . The icosians  $x = \beta z$  and  $y = \delta' z$  then satisfy  $\operatorname{tr}(q_\alpha \bar{x}) + \operatorname{tr}(\tilde{y} \tilde{q}_\alpha) = 1$  as well as  $\operatorname{tr}(\tilde{x} \tilde{q}_\alpha) + \operatorname{tr}(q_\alpha \bar{y}) = 1$ , where the second identity follows from the first via  $(\operatorname{tr}(u\bar{v}))^\sim = \operatorname{tr}(\tilde{v} \tilde{u})$ .

Finally, observe that  $\operatorname{tr}(u\bar{v}) \in K$  for all  $u, v \in \mathbb{H}(K)$ , so that one also has the relation  $(\operatorname{tr}(u\bar{v}))' = \operatorname{tr}(\tilde{v} \tilde{u})$ . Consequently, defining  $z = \tau x + (1 - \tau)y$  with the  $x, y$  from above,  $z$  is an icosian that satisfies

$$\operatorname{tr}(q_\alpha \bar{z}) + \operatorname{tr}(\tilde{z} \tilde{q}_\alpha) = \tau (\operatorname{tr}(q_\alpha \bar{x}) + \operatorname{tr}(\tilde{y} \tilde{q}_\alpha)) + (1 - \tau) (\operatorname{tr}(q_\alpha \bar{y}) + \operatorname{tr}(\tilde{x} \tilde{q}_\alpha)) = 1,$$

which establishes the second claim.  $\square$

For our further discussion, it is convenient to define the set

$$(13) \quad L(q) = \{qx + \tilde{x}\tilde{q} \mid x \in \mathbb{I}\} = \phi_+(q\mathbb{I}),$$

which is a sublattice of  $L$ , compare Lemma 4. Note that, due to  $\tilde{\mathbb{I}} = \mathbb{I}$ , one has  $L(q) = \widetilde{L(q)}$ .

**Theorem 2.** *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*

$$L \cap \frac{1}{|q\tilde{q}|} qL\tilde{q} = L(q_\alpha),$$

with  $L(q_\alpha)$  defined as in Eq. (13).

*Proof.* To show the equality claimed, we have to establish two inclusions, where we may use the fact that  $q$  and  $q_\alpha$  define the same rotation in 4-space, see Eq. (11).

First, since  $L(q_\alpha) \subset L$  is clear, we need to show that  $|q_\alpha \tilde{q}_\alpha| L(q_\alpha) \subset q_\alpha L\tilde{q}_\alpha$ . If  $x \in L(q_\alpha)$ , there is some  $y \in \mathbb{I}$  with  $x = q_\alpha y + \tilde{y}\tilde{q}_\alpha$ . Consequently, observing the norm relations from Eq. (12), we find

$$|q_\alpha \tilde{q}_\alpha| x = q_\alpha y \overline{q_\alpha \tilde{q}_\alpha} + q_\alpha \overline{\tilde{y}\tilde{q}_\alpha} = q_\alpha (y \overline{q_\alpha} + \overline{\tilde{y}\tilde{q}_\alpha}) \tilde{q}_\alpha \in q_\alpha L(q_\alpha) \tilde{q}_\alpha \subset q_\alpha L\tilde{q}_\alpha,$$

which gives the first inclusion.

Conversely, when  $x \in L \cap \frac{1}{|q\tilde{q}|} qL\tilde{q}$ , Lemma 7 tells us that there exists an icosian  $z \in \mathbb{I}$  such that  $\operatorname{tr}(q_\alpha \bar{z}) + \operatorname{tr}(\tilde{z} \tilde{q}_\alpha) = 1$ . At the same time, there is some  $y \in L$  so that  $x = \frac{qy\tilde{q}}{|q\tilde{q}|} = \frac{q_\alpha y \tilde{q}_\alpha}{|q_\alpha \tilde{q}_\alpha|}$ . Observing  $x = \tilde{x}$  and the norm relations in Eq. (12), one finds

$$x = \operatorname{tr}(q_\alpha \bar{z})x + \tilde{x} \operatorname{tr}(\tilde{z} \tilde{q}_\alpha) = (q_\alpha \bar{z} + z \overline{q_\alpha})x + \tilde{x} (\tilde{z} \tilde{q}_\alpha + \overline{\tilde{z} \tilde{q}_\alpha}) = q_\alpha (\bar{z}x + \tilde{y}\tilde{z}) + (\tilde{x}\tilde{z} + zy)\tilde{q}_\alpha,$$

which shows  $x$  to be an element of  $L(q_\alpha)$ .  $\square$

## 4. COINCIDENCE INDICES AND GENERATING FUNCTIONS

With the explicit identification of the CSL that emerges from the rotation defined by an admissible primitive icosian  $q$ , one can then calculate the corresponding index. This is either possible by a more direct (though somewhat tedious) calculation along the lines of reference [8] or by relating  $\Sigma^2$  to the corresponding index of the coincidence site module of  $\mathbb{I}$ , see [10] for details. The result reads as follows.

**Theorem 3.** *If  $q \in \mathbb{I}$  is an admissible primitive icosian, the rotation  $x \mapsto \frac{1}{|q\tilde{q}|}qx\tilde{q}$  is a coincidence isometry of  $L$ . Moreover, the corresponding coincidence index satisfies*

$$(\Sigma(q))^2 = N(\text{lcm}(\text{nr}(q), \text{nr}(q)')) = N(\text{nr}(q_\alpha)),$$

which is a square in  $\mathbb{N}$ . Equivalently, one has the formula

$$\Sigma(q) = \text{nr}(q_\alpha) = \text{lcm}(\text{nr}(q), \text{nr}(q)'),$$

which is then, with our above convention from Eq. (10), always an element of  $\mathbb{N}$ .  $\square$

Due to the subtle aspects of the factorisations of icosians into irreducible elements, we have not yet found a clear and systematic approach to the number  $f(m)$  of CSLs of  $A_4$  of index  $m$ , though we will indicate later what the answer might look like. However, at this point, it is possible to determine the number  $f_{\text{rot}}(m)$  for  $m$  a prime power.

Clearly, we have  $f_{\text{rot}}(1) = 1$ . When  $g(m)$  denotes the number of *primitive* SSLs of  $A_4$  of index  $m^2$ , one can immediately extract some cases from the explicit results in [16, 6]. In particular, one has  $f_{\text{rot}}(p^r) = g(p^{2r})$  both for  $p = 5$  and for all rational primes  $p \equiv \pm 2 \pmod{5}$ . The remaining case with  $p \equiv \pm 1 \pmod{5}$ , where  $p$  splits as  $p = \pi\pi'$  on the level of  $\mathfrak{o}$ , is slightly more difficult, because one has to keep track of how the algebraically conjugate primes of  $\mathfrak{o}$  are distributed between  $\text{nr}(q)$  and  $\text{nr}(\tilde{q})$ . Observe the relation

$$\frac{1 + p^{-2s}}{1 - p^{1-2s}} = 1 + \sum_{\ell \geq 1} (p^\ell + p^{\ell-1})p^{-2\ell s},$$

which, for  $p \equiv \pm 1 \pmod{5}$ , happens to be the generating function for the primitive right ideals  $q\mathbb{I}$  of the icosian ring of  $p$ -power index such that  $\text{nr}(q)$  is a power of  $\pi$  (up to units). Those with  $\text{nr}(q)$  a power of  $\pi'$  produce an Euler factor of the same form. With this, one can explicitly calculate  $f_{\text{rot}}(p^r)$  by collecting all contributions to the index  $\Sigma = p^r$  according to Theorem 3. This turns out to be completely analogous to the calculations for the centred hypercubic lattice in 4-space presented<sup>1</sup> in [1, 28], and the formula for  $f$  reads

$$(14) \quad f_{\text{rot}}(p^r) = \begin{cases} 6 \cdot 5^{2r-1}, & \text{if } p = 5, \\ \frac{p+1}{p-1} p^{r-1} (p^{r+1} + p^{r-1} - 2), & \text{if } p \equiv \pm 1 \pmod{5}, \\ p^{2r} + p^{2r-2}, & \text{if } p \equiv \pm 2 \pmod{5}. \end{cases}$$

<sup>1</sup>Note that the arithmetic functions in [1, 28], in the case of 4 dimensions, also count the coincidence rotations in multiples of the number of rotation symmetries, and *not* the CSLs themselves, hence giving the generating function (4) rather than (3) in this case.

**Theorem 4.** *Let  $120f_{\text{rot}}(m)$  be the number of coincidence rotations of  $A_4$  of index  $m$ . Then,  $f_{\text{rot}}(m)$  is a multiplicative arithmetic function, with Dirichlet series generating function*

$$\begin{aligned}
\Phi_{A_4}^{\text{rot}}(s) &= \sum_{m=1}^{\infty} \frac{f_{\text{rot}}(m)}{m^s} = \frac{\zeta_K(s-1)}{1+5^{-s}} \frac{\zeta(s)\zeta(s-2)}{\zeta(2s)\zeta(2s-2)} \\
(15) \quad &= \frac{1+5^{1-s}}{1-5^{2-s}} \prod_{p \equiv \pm 1 (5)} \frac{(1+p^{-s})(1+p^{1-s})}{(1-p^{1-s})(1-p^{2-s})} \prod_{p \equiv \pm 2 (5)} \frac{1+p^{-s}}{1-p^{2-s}} \\
&= 1 + \frac{5}{2^s} + \frac{10}{3^s} + \frac{20}{4^s} + \frac{30}{5^s} + \frac{50}{6^s} + \frac{50}{7^s} + \frac{80}{8^s} + \frac{90}{9^s} + \frac{150}{10^s} + \frac{144}{11^s} + \dots
\end{aligned}$$

where  $\zeta(s)$  is Riemann's zeta function and  $\zeta_K(s)$  denotes the Dedekind zeta function of the quadratic field  $K = \mathbb{Q}(\sqrt{5})$ .

*Proof.* The multiplicativity of  $f_{\text{rot}}$  is inherited from the unique factorisation in  $\mathbb{I}$  together with the divisor properties of the coincidence index from Lemma 3. Consequently, Eq. (15) fixes  $f_{\text{rot}}(m)$  for all  $m \in \mathbb{N}$  via the identity  $f_{\text{rot}}(mn) = f_{\text{rot}}(m)f_{\text{rot}}(n)$  for integers  $m$  and  $n$  that are relatively prime.

It is a routine exercise to calculate the Euler factors of the corresponding Dirichlet series generating function and to express  $\Phi_{A_4}^{\text{rot}}$  in terms of the two zeta functions mentioned.  $\square$

Note that  $\zeta_K(s) = \zeta(s)L(s, \chi)$ , where  $L(s, \chi)$  is the  $L$ -series of the primitive Dirichlet character  $\chi$  defined by

$$\chi(n) = \begin{cases} 0, & n \equiv 0 (5), \\ 1, & n \equiv \pm 1 (5), \\ -1, & n \equiv \pm 2 (5). \end{cases}$$

Observe next that  $f_{\text{rot}}(m) > 0$  for all  $m \in \mathbb{N}$ , so that also the number  $f(m)$  of CSLs must be positive (though we can still have  $0 < f(m) < f_{\text{rot}}(m)$ ). Moreover, each element of  $\text{OC}(A_4)$  can be written as a product of a rotation with a reflection that maps  $A_4$  onto itself. Consequently, the simple coincidence spectrum  $\Sigma(\text{OC}(A_4))$  is the set of all positive integers. Although multiple coincidences may produce further lattices, compare [4, 29, 9], the total spectrum  $\Sigma_{A_4}$  cannot be larger than the elementary one, so that the following consequence is clear.

**Corollary 2.** *The multiple coincidence spectra of the root lattice  $A_4$  coincide with the elementary one, and one has  $\Sigma_{A_4} = \Sigma(\text{OC}(A_4)) = \Sigma(\text{SOC}(A_4)) = \mathbb{N}$ , which is a monoid.*  $\square$

The Dirichlet series  $\Phi_{A_4}^{\text{rot}}(s)$  is analytic in the open right half-plane  $\{s = \sigma + it \mid \sigma > 3\}$ , and has a simple pole at  $s = 3$ . The corresponding residue is given by

$$(16) \quad \text{res}_{s=3} \Phi_{A_4}^{\text{rot}}(s) = \frac{125}{126} \frac{\zeta_K(2)\zeta(3)}{\zeta(4)\zeta(6)} = \frac{450\sqrt{5}}{\pi^6} \zeta(3) \simeq 1.258124,$$

which is based on the special values

$$\zeta(4) = \frac{\pi^4}{90}, \quad \zeta(6) = \frac{\pi^6}{945}, \quad \zeta_K(2) = \frac{2\pi^4}{75\sqrt{5}},$$

together with  $\zeta(3) \simeq 1.202057$ , compare [7] and references given there. The value of  $\zeta(3)$  is known to be irrational, but has to be calculated numerically.

With this information, we can extract the asymptotic behaviour of the counts  $f_{\text{rot}}(m)$  from the generating function  $\Phi_{A_4}^{\text{rot}}(s)$  by Delange's theorem, see [7, Appendix] for a formulation tailored to this situation. One obtains, as  $x \rightarrow \infty$ ,

$$(17) \quad \sum_{m \leq x} f_{\text{rot}}(m) \sim \text{res}_{s=3} \Phi_{A_4}^{\text{rot}}(s) \frac{x^3}{3} \simeq 0.419375 x^3.$$

Clearly, this is also an upper bound for the asymptotic behaviour of the true CSL counts.

As mentioned earlier, one is primarily interested in the number  $f(m)$  of CSLs of index  $m$ , which satisfies  $0 < f(m) \leq f_{\text{rot}}(m)$  for all  $m \in \mathbb{N}$  in view of Corollary 2. Some preliminary calculations show that also  $f(m)$  is multiplicative. In fact, one has  $f(p^r) = f_{\text{rot}}(p^r)$  for all primes  $p \equiv \pm 2 \pmod{5}$ , and  $f(5^r) = f_{\text{rot}}(5^r)/5$  for  $r \geq 1$ . For the remaining primes  $p \equiv \pm 1 \pmod{5}$ , one has  $f(p) = f_{\text{rot}}(p)$ , but differences occur for all powers  $p^r$  with  $r \geq 2$ . This happens first for  $m = 11^2 = 121$  and is induced by the more complicated factorisation for these primes, compare [3] for a similar phenomenon. Consequently, the modification for the prime 5 is sufficient up to index  $m = 120$ . The Dirichlet series generating function thus starts as

$$\Phi_{A_4}(s) = \sum_{m=1}^{\infty} \frac{f(m)}{m^s} = 1 + \frac{5}{2^s} + \frac{10}{3^s} + \frac{20}{4^s} + \frac{6}{5^s} + \frac{50}{6^s} + \frac{50}{7^s} + \frac{80}{8^s} + \frac{90}{9^s} + \frac{30}{10^s} + \frac{144}{11^s} + \dots$$

At this stage, the general mechanism behind this is not completely unravelled, but we hope to present it in greater generality in [10].

## 5. RELATED RESULTS AND OUTLOOK

In one dimension, the CSL problem becomes trivial, so that  $\Phi(s) \equiv 1$  in this case. In two dimensions, a rather general approach to lattices and modules is possible via classic algebraic number theory, see [23, 4] and references therein, which includes the treatment of multiple coincidences. For the root lattice  $A_2$ , the CSL generating function reads

$$(18) \quad \Phi_{A_2}(s) = \Phi_{A_2}^{\text{rot}}(s) = \prod_{p \equiv 1 \pmod{3}} \frac{1 + p^{-s}}{1 - p^{-s}} = \frac{1}{1 + 3^{-s}} \frac{\zeta_{\mathbb{Q}(\xi_3)}(s)}{\zeta(2s)},$$

where  $\xi_3$  is a primitive cube root of 1. Here, the equality is a consequence of the commutativity of  $\text{SOC}(A_2)$ . The simple coincidence spectrum of this lattice is the multiplicative monoid of integers that is generated by the rational primes  $p \equiv 1 \pmod{3}$ .

In 3-space, various examples are derived in [1] and have recently been proved by quaternionic methods [8] similar to the ones used here. Among these cases is the root lattice  $A_3$ , which happens to be the face centred cubic lattice in 3-space, with generating function

$$(19) \quad \Phi_{A_3}(s) = \Phi_{A_3}^{\text{rot}}(s) = \prod_{p \neq 2} \frac{1 + p^{-s}}{1 - p^{1-s}} = \frac{1 - 2^{1-s}}{1 + 2^{-s}} \frac{\zeta(s) \zeta(s-1)}{\zeta(2s)}.$$

The equality of the two Dirichlet series to the left is non-trivial, and was proved in [8] with an argument involving Eichler orders. The same formula also applies to the other cubic lattices in 3-space [1, 9]. The simple coincidence spectrum is thus the set of odd integers, which is

again a monoid. The multiple analogues have recently been derived in [29, 30], see also [4, 9] for related results.

Several of these results are also included by now in [25]. In 4-space, various other lattices and modules of interest exist, for which some results are given in [1, 28, 30], with more structural proofs and generalisations being in preparation [10]. Beyond dimension 4, very little is known [31, 32], though it should be possible to derive the simple coincidence spectra for certain classes of lattices.

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