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Coincidences in 4 dimensions

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The coincidence site lattices (CSLs) of prominent 4-dimensional lattices are considered. CSLs in 3 dimensions have been used for decades to describe grain boundaries in crystals. Quasicrystals suggest to also look at CSLs in dimensions $d > 3$. Here, we discuss the CSLs of the A_4-lattice and the hypercubic lattices, which are of particular interest both from the mathematical and the crystallographic viewpoint. Quaternion algebras are used to derive their coincidence rotations and the CSLs. We make use of the fact that the CSLs can be directly linked to certain ideals and compute their indices, their multiplicities and encapsulate all this in generating functions in terms of Dirichlet series. In addition, we sketch how these results can be generalized for 4–dimensional $\mathbb{Z}$–modules by discussing the icosian ring.

1 Introduction

1.1 *Coincidence site lattices and modules*

Let $\varGamma \subseteq \mathbb{R}^d$ be a d-dimensional lattice and $R \in \mathrm{O}(d)$ an isometry. Then, R is called a *coincidence isometry* if $\varGamma(R) := \varGamma \cap R\varGamma$ is a lattice of finite index in $\varGamma$, and $\varGamma(R)$ is called an (ordinary or simple) *coincidence site lattice (CSL)* (for an introduction, see [1]). The group of all coincidence isometries of $\varGamma$ is called $OC(\varGamma)$, whereas the subgroup of all orientation preserving isometries is called the group of coincidence rotations and referred to as $SOC(\varGamma)$. The *coincidence index* $\Sigma(R)$ is defined as the index of $\varGamma(R)$ in $\varGamma$, and $\sigma = \{\Sigma(R) \mid R \in OC(\varGamma)\}$ denotes the (ordinary or simple) coincidence spectrum. These definitions can be generalized to include the possibility of multiple CSLs, see [2–4].

All these concepts also extend to $\mathbb{Z}$–modules [1,5]. By a $\mathbb{Z}$–module of dimension d and rank k, we mean the $\mathbb{Z}$–span of k rationally independent vectors in $\mathbb{R}^d$.

1.2 *Quaternions and rotations*

Rotations in $\mathbb{R}^4$ can be parameterized by a pair of quaternions [6–8]. Recall that the quaternion algebra $\mathbb{H}(\mathbb{R})$ is the vector space $\mathbb{R}^4$ equipped with a special (associative but non–commutative) product. In standard notation, where $1, i, j, k$ form an orthogonal basis of $\mathbb{R}^4$, the product satisfies the defining relations $i^2 = j^2 = k^2 = -1$ and $ijk = -ijk = -1$. This definition is extended to all quaternions by linearity. All non–zero quaternions $q = (a, b, c, d) = a + bi + cj + dk$ have an inverse $q^{-1} = \frac{1}{|q|^2}\bar{q}$, where $\bar{q} = (a, -b, -c, -d)$ is the conjugate of q and $|q|^2 = a^2 + b^2 + c^2 + d^2$ is its (reduced) norm. With this notation at hand, we can write any rotation in $\mathbb{R}^4$ as

$$Rx = R(q, p)x = \frac{1}{|qp|} qx\bar{p}. \tag{1}$$

Reflections and, more generally, all orientation reversing isometries may be parameterized by a pair of quaternions as well, but a conjugation is required in addition. For our purposes, it is suffient to focus the discussion to (proper) rotations. This is no restriction, since all the lattices and modules we discuss have a reflection as a symmetry operation and thus every coincidence isometry can be written as the product of this reflection and a coincidence rotation with the same index. All CSLs are already obtained by (proper)

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coincidence rotations and the spectrum does not change either. There are exactly as many coincidence rotations as orientation reversing isometries and the total number of coincidence isometries is just twice the number of coincidence rotations.

1.3 *Equivalent rotations and CSLs*

Two coincidence rotations R and R' are called *symmetrically equivalent* if there is an element Q in the point group $P(\Gamma)$ such that $R' = RQ$. Note that $R\Gamma = R'\Gamma$ holds if and only if R and R' are symmetrically equivalent. In particular, symmetrically equivalent rotations R and R' generate the same CSL, so that $\Gamma(R) = \Gamma(R')$. However, the converse statement is not true in general, i.e., two rotations generating the same CSL need *not* be symmetrically equivalent. In particular, in all the examples presented below there are additional rotations that generate the same CSL.

2 Hypercubic lattices

The hypercubic lattices have been discussed in detail in [1, 9]. Here, we just review the most important facts, reformulate some of them and add some new details, in particular an explicit expression for the number of CSLs.

2.1 *Centred hypercubic lattice*

The centered hypercubic lattice D_4^*, which is the dual lattice of the root lattice D_4, which in turn is a similar sublattice of D_4^*, can be identified with the Hurwitz ring $\mathbb{J}$ of integer quaternions. This is the $\mathbb{Z}$–span (i.e. the set of all integral linear combinations) of the quaternions $(1,0,0,0), (0,1,0,0), (0,0,1,0), \frac{1}{2}(1,1,1,1)$. Any coincidence rotation can be parameterized by a pair of integer quaternions. More generally, a rotation is a coincidence rotation of D_4^* if and only if it can be parameterized by an admissible pair of quaternions [1,9]. Here, we call a quaternion $q \in \mathbb{J}$ primitive if $\frac{1}{n}q \in \mathbb{J}$ with $n \in \mathbb{N}$ implies $n = 1$. A primitive pair (q, p) is called *admissible* if $|qp| \in \mathbb{Z}$. In addition, we call a primitive quaternion $q \in \mathbb{J}$ *reduced* if $|q|^2$ is odd (for a more general discussion of reduced quaternions, see [10]). Due to the unique (left or right) prime decomposition in $\mathbb{J}$, we can decompose any primitive quaternion $q \in \mathbb{J}$ as $q_r s$, where q_r is reduced and $|s|^2$ is a power of 2. Note that q_r is unique up to right multiplication by a unit from $\mathbb{J}$.

For any admissible pair (q, p), we can define the factors

$$\alpha_q := \sqrt{\frac{|p_r|^2}{\gcd(|q_r|^2, |p_r|^2)}}, \qquad \alpha_p := \sqrt{\frac{|q_r|^2}{\gcd(|q_r|^2, |p_r|^2)}}.$$

The pair $(q_\alpha, p_\alpha) := (\alpha_q q_r, \alpha_p p_r)$ is called the *reduced extension* of the pair (q, p). Note that two admissible pairs are symmetrically equivallent if and only if their reduced extension pairs are equal (up to units). The coincidence index of a rotation $R(q, p)$ can now be written [1, 9] as

$$\Sigma_{D_4}(R(q,p)) = \mathrm{lcm}(|q_r|^2, |p_r|^2) = |q_\alpha|^2 = |p_\alpha|^2. \tag{2}$$

Since any (positive) integer can be written as a sum of four squares, this implies that the spectrum σ is the set of all odd natural numbers.

The CSLs can be calculated explicitly [11]. They read

$$\mathbb{J} \cap \frac{q\mathbb{J}\bar{p}}{|qp|} = q_\alpha \mathbb{J} + \mathbb{J}\bar{p}_\alpha. \tag{3}$$

Since the point group of D_4 contains 576 rotations, the number of coincidence rotations of a given index

n can be written as $576 f^{rot}_{D_4}(n)$. This gives a multiplicative arithmetic function, i.e.

$$f^{rot}_{D_4}(mn) = f^{rot}_{D_4}(m) f^{rot}_{D_4}(n) \qquad \text{if } m, n \text{ are coprime,} \tag{4}$$

which is completely determined by $f^{rot}_{D_4}(1) = 1$, $f^{rot}_{D_4}(2^r) = 0$ for $r \geq 1$ and

$$f^{rot}_{D_4}(p^r) = \frac{p+1}{p-1} p^{r-1}(p^{r+1} + p^{r-1} - 2) \quad \text{if } p \text{ is an odd prime, } r \geq 1. \tag{5}$$

The multiplicativity of $f^{rot}_{D_4}(n)$ suggests the use of a Dirichlet series as a generating function for it.

$$\begin{aligned} \Phi^{rot}_{D_4}(s) &= \sum_{n=1}^{\infty} \frac{f^{rot}_{D_4}(n)}{n^s} = \prod_{p \neq 2} \frac{(1+p^{-s})(1+p^{1-s})}{(1-p^{1-s})(1-p^{2-s})} \\ &= 1 + \frac{16}{3^s} + \frac{36}{5^s} + \frac{64}{7^s} + \frac{168}{9^s} + \frac{144}{11^s} + \frac{196}{13} + \frac{576}{15} + \frac{324}{17} + \cdots . \end{aligned} \tag{6}$$

Similarly, one can calculate the number $f_{D_4}(n)$ of different CSLs of a given index n. Clearly, $f_{D_4}(n) \leq f^{rot}_{D_4}(n)$, and we do not have equality in general, since two CLSs that are not symmetrically equivalent may generate the same CSL. In fact, we have the following theorem which tells us when two CSLs are equal [11].

Theorem 2.1 Let (q_1, p_1) and (q_2, p_2) be two primitive reduced admissible pairs. Then,

$$\mathbb{J} \cap \frac{q_1 \mathbb{J} p_1}{|q_1 p_1|} = \mathbb{J} \cap \frac{q_2 \mathbb{J} p_2}{|q_2 p_2|} \tag{7}$$

holds if and only if $|q_1 p_1| = |q_2 p_2|$, $\mathrm{lcm}(|q_1|^2, |p_1|^2) = \mathrm{lcm}(|q_2|^2, |p_2|^2)$, $\mathrm{glcd}(q_1, |p_1 q_1|) = \mathrm{glcd}(q_2, |p_2 q_2|)$ and $\mathrm{grcd}(p_1, |p_1 q_1|) = \mathrm{grcd}(p_2, |p_2 q_2|)$ hold.

Here, glcd and grcd denote the greatest left and right common divisors in $\mathbb{J}$, which are defined up to units. We find that $f_{D_4}(n)$ is multiplicative, too, and is determined by $f_{D_4}(1) = 1$, $f_{D_4}(2^r) = 0$ for $r \geq 1$ and

$$f_{D_4}(p^r) = \begin{cases} \frac{(p+1)^2}{p^3-1} \left(p^{2r+1} + p^{2r-2} - 2p^{(r-1)/2}\right), & \text{if } r \geq 1 \text{ is odd,} \\ \frac{(p+1)^2}{p^3-1} (p^{2r+1} + p^{2r-2} - 2p^{r/2-1} \frac{1+p^2}{1+p}), & \text{if } r \geq 2 \text{ is even,} \end{cases} \tag{8}$$

for odd primes p. The corresponding Dirichlet series reads

$$\begin{aligned} \Phi_{D_4}(s) &= \sum_{n=1}^{\infty} \frac{f_{D_4}(n)}{n^s} = \prod_{p \neq 2} \frac{1 + p^{-s} + 2p^{1-s} + 2p^{-2s} + p^{1-2s} + p^{1-3s}}{(1-p^{2-s})(1-p^{1-2s})} \\ &= 1 + \frac{16}{3^s} + \frac{36}{5^s} + \frac{64}{7^s} + \frac{152}{9^s} + \frac{144}{11^s} + \frac{196}{13} + \frac{576}{15} + \frac{324}{17} + \cdots . \end{aligned}$$

Differences to Eq. (6) occur for all integers that are divisible by the square of an odd prime.

2.2 *Primitive hypercubic lattice*

It is well known that the primitive hypercubic lattice $\mathbb{Z}^4$, which is a sublattice of D_4^* of index 2, has a smaller point group than D_4^*, containing only 192 rotations. As a consequence, every class of symmetrically equivalent rotations splits into three classes, one of which has the same coincidence index as before $\Sigma_{\mathbb{Z}^4}(R) = \Sigma_{D_4}(R)$, while the other two classes have index $2\Sigma_{D_4}(R)$. The number of coincidence rotations

is thus given by $192 f_{\mathbb{Z}^4}(n)$, where $f_{\mathbb{Z}^4}(n)$ is again multiplicative, but slightly more complicated than $f^{rot}_{D_4}(n)$ (see [1,9]) and has the generating function

$$\Phi^{rot}_{\mathbb{Z}^4}(s) = \sum_{n=1}^{\infty} \frac{f^{rot}_{\mathbb{Z}^4}(n)}{n^s} = (1+2^{1-s})\Phi^{rot}_{D_4}(s) = (1+2^{1-s}) \prod_{p\neq 2} \frac{(1+p^{-s})(1+p^{1-s})}{(1-p^{1-s})(1-p^{2-s})}$$
$$= 1 + \frac{2}{2^s} + \frac{16}{3^s} + \frac{36}{5^s} + \frac{32}{6^s} + \frac{64}{7^s} + \frac{168}{9^s} + \frac{72}{10^s} + \frac{144}{11^s} + \frac{196}{13} + \frac{128}{14^s} + \frac{576}{15} + \frac{324}{17} + \cdots . \quad (9)$$

The CSLs split into two classes only, one of which has odd and the other even index. Hence, the generating function for the number of CSLs reads

$$\Phi_{\mathbb{Z}^4}(s) = (1+2^{-s})\Phi_{D_4}(s) = (1+2^{-s}) \prod_{p\neq 2} \frac{1+p^{-s}+2p^{1-s}+2p^{-2s}+p^{1-2s}+p^{1-3s}}{(1-p^{2-s})(1-p^{1-2s})}$$
$$= 1 + \frac{1}{2^s} + \frac{16}{3^s} + \frac{36}{5^s} + \frac{16}{6^s} + \frac{64}{7^s} + \frac{152}{9^s} + \frac{36}{10^s} + \frac{144}{11^s} + \frac{196}{13} + \frac{576}{15} + \frac{324}{17} + \cdots .$$

Differences to Eq. (9) occur for all even integers and all integers that are divisible by the square of an odd prime.

3 A_4 lattice

Usually, the A_4 lattice — we will denote it by L in the following — is embedded in $\mathbb{R}^5$ as a lattice plane. However, this is inconvenient for our purposes and we prefer to look at it in $\mathbb{R}^4$, since we want to exploit the useful parameterization by quaternions which we do not have at hand in 5 dimensions. A possible choice of basis vectors for L is

$$(1,0,0,0), \frac{1}{2}(-1,1,1,1), (0,-1,0,0), \frac{1}{2}(0,1,\tau-1,-\tau), \quad (10)$$

where $\tau = \frac{1+\sqrt{5}}{2}$ is the golden mean and $\tau' = -\frac{1}{\tau}$ is its algebraic conjugate. L cannot be identified with a ring of quaternions. However, if we interpret the basis vectors as quaternions, they relate to the icosian ring $\mathbb{I}$, which is the $\mathbb{Z}[\tau]$–span of the quaternions

$$(1,0,0,0), (0,1,0,0), \frac{1}{2}(1,1,1,1), \frac{1}{2}(1-\tau,\tau,0,1). \quad (11)$$

L has the following remarkable representation:

$$L = \{x \in L | x = \tilde{x}\} = \{x + \tilde{x} | x \in \mathbb{I}\}. \quad (12)$$

Here, $\tilde{x} := (x'_0, x'_1, x'_3, x'_2)$ is an involution of the second kind, i.e. a special kind of antiautomorphism which was called twist map in [12,13]. Note that it is an algebraic conjugation followed by a permutation of the last two components. None of these maps alone is an (anti-)automorphism of L or $\mathbb{I}$.

Any coincidence rotation (and only those) can be parameterized by a single primitive admissible quaternion $q \in \mathbb{I}$ by means of $R(q) = \frac{1}{|q\tilde{q}|} q x \tilde{q}$ (see [13]). Here, admissible means that $|q\tilde{q}| \in \mathbb{N}$.

Admissibility garantuees that one can define the factors

$$\alpha_q := \sqrt{\frac{|\tilde{q}|^2}{\gcd(|q|^2, |\tilde{q}|^2)}}, \qquad \alpha_{\tilde{q}} := \alpha'_q = \sqrt{\frac{|q|^2}{\gcd(|q|^2, |\tilde{q}|^2)}}, \quad (13)$$

which are elements of $\mathbb{Z}[\tau]$. Note, however, that they are only defined up to units of $\mathbb{Z}[\tau]$. In addition, we define the extension of a primitive admissible quaternion by $q_\alpha = \alpha_q q$. The coincidence index now reads [13]

$$\Sigma_{A_4}(R(q) = \frac{|q\tilde{q}|^2}{\gcd(|q|^2, |\tilde{q}|^2)} = |q\tilde{q}|\alpha_q\alpha_{\tilde{q}} = \mathrm{lcm}(|q|^2, |\tilde{q}|^2). \tag{14}$$

Consequently the coincidence spectrum is $\mathbb{N}$. An explicit expression for the CSLs exists, too:

$$L \cap \frac{q_\alpha L \tilde{q}_\alpha}{|q_\alpha \tilde{q}_\alpha|} = \{q_\alpha x + \tilde{x}\tilde{q}_\alpha | x \in \mathbb{I}\} = (q_\alpha \mathbb{I} + \mathbb{I}\tilde{q}_\alpha) \cap L. \tag{15}$$

Along the same lines as for the hypercubic lattices one can calculate the number of coincidence rotations and the number of CSLs of a given index n. The expressions obtained are slightly more complicated, since one has to distinguish between the three cases $p = 5$, $p = \pm 1 \pmod 5$ and $p = \pm 2 \pmod 5$, as these primes behave differently and correspond to the ramifying, splitting and inert primes of $\mathbb{Z}[\tau]$. If $120 f^{rot}_{A_4}(n)$ is the number of coincidence rotations — recall that the point group of L contains 120 elements — its generating Dirichlet series is given by

$$\begin{aligned}\Phi^{rot}_{A_4}(s) &= \frac{1+5^{1-s}}{1-5^{2-s}} \prod_{p\equiv\pm1(5)} \frac{(1+p^{-s})(1+p^{1-s})}{(1-p^{1-s})(1-p^{2-s})} \prod_{p\equiv\pm2(5)} \frac{1+p^{-s}}{1-p^{2-s}} \\ &= 1 + \frac{5}{2^s} + \frac{10}{3^s} + \frac{20}{4^s} + \frac{30}{5^s} + \frac{50}{6^s} + \frac{50}{7^s} + \frac{80}{8^s} + \frac{90}{9^s} + \frac{150}{10^s} + \frac{144}{11^s} + \cdots .\end{aligned}$$

Similarly, we have for the number of CSLs

$$\begin{aligned}\Phi_{A_4}(s) &= \left(1 + 6\frac{5^{-s}}{1-5^{2-s}}\right) \prod_{p\equiv\pm2(5)} \frac{1+p^{-s}}{1-p^{2-s}} \prod_{p\equiv\pm1(5)} \frac{1+p^{-s}+2p^{1-s}+2p^{-2s}+p^{1-2s}+p^{1-3s}}{(1-p^{2-s})(1-p^{1-2s})} \\ &= 1 + \frac{5}{2^s} + \frac{10}{3^s} + \frac{20}{4^s} + \frac{6}{5^s} + \frac{50}{6^s} + \frac{50}{7^s} + \frac{80}{8^s} + \frac{90}{9^s} + \frac{30}{10^s} + \frac{144}{11^s} + \cdots .\end{aligned}$$

Here, a criterion analogous to Theorem 2.1 exists, which will be published elsewhere [11].

4 Icosian Ring

It is also interesting to discuss the coincidences of the icosian ring $\mathbb{I}$ itself. Note that it is no lattice in 4–space but a $\mathbb{Z}$–module of rank 8. However, this does not matter and one can argue similarly to the hypercubic case. The main difference is that one has to work with $\mathbb{Z}[\tau]$ instead of $\mathbb{Z}$, which does not cause any problems. In fact, some steps are even easier since the prime 2 does not play a special role here. So, a primitive quaternion is already reduced and hence the notion of reducibility is not needed here.

Let us call a pair $(q, p) \in \mathbb{I} \times \mathbb{I}$ *primitive admissible* if q, p are primitive and $|qp| \in \mathbb{Z}[\tau]$. Then, a rotation is a coincidence rotation if and only if it is parameterized by a primitive admissible pair (q, p). For any primitive admissible pair (q, p), we can once more define

$$\alpha_q := \sqrt{\frac{|p|^2}{\gcd(|q|^2, |p|^2)}}, \qquad \alpha_p := \sqrt{\frac{|q|^2}{\gcd(|q|^2, |p|^2)}},$$

which are again elements of $\mathbb{Z}[\tau]$, defined up to units. As before, $(q_\alpha, p_\alpha) := (\alpha_q q, \alpha_p p)$ is the corresponding

extension pair. We get the following expression for the coincidence index [11]:

$$\Sigma_{\mathbb{I}}(R(q,p)) = \mathrm{N}(\mathrm{lcm}(|q|^2, |p|^2)) = \mathrm{N}(|q_\alpha|^2) = \mathrm{N}(|p_\alpha|^2).$$

Here $\mathrm{N}(a) = |aa'|$ is the (number theoretic) norm of $a \in \mathbb{Z}[\tau]$. Thus the coincidence spectrum consists of all integers that do not contain odd powers of prime factors $p = \pm 2 \pmod 5$. The CSMs read explicitly

$$\mathbb{I} \cap \frac{q\mathbb{I}p}{|qp|} = q_\alpha \mathbb{I} + \mathbb{I} p_\alpha .$$

If $7200 f_{\mathbb{I}}^{rot}(n)$ denotes the number of coincidence rotations and $f_{\mathbb{I}}(n)$ the number of CSMs, we get again $f_{\mathbb{I}}^{rot}(n) \geq f_{\mathbb{I}}(n)$. Again, equality fails to hold in general, and a complete analogue of Theorem 2.1 tells us which CSMs are equal [11]. The corresponding Dirichlet series read

$$\begin{aligned}\Phi_{\mathbb{I}}^{rot}(s) &= \frac{(1+5^{-s})(1+5^{1-s})}{(1-5^{1-s})(1-5^{2-s})} \prod_{p\equiv\pm1(5)} \left(\frac{(1+p^{-s})(1+p^{1-s})}{(1-p^{1-s})(1-p^{2-s})} \right)^2 \prod_{p\equiv\pm2(5)} \frac{(1+p^{-2s})(1+p^{2-2s})}{(1-p^{2-2s})(1-p^{4-2s})} \\ &= 1 + \frac{25}{4^s} + \frac{36}{5^s} + \frac{100}{9^s} + \frac{288}{11^s} + \frac{440}{16^s} + \frac{400}{19^s} + \frac{900}{20^s} + \frac{960}{25^s} + \cdots \end{aligned} \tag{16}$$

and

$$\begin{aligned}\Phi_{\mathbb{I}}(s) &= \frac{1+5^{-s}+2\cdot5^{1-s}+2\cdot5^{-2s}+5^{1-2s}+5^{1-3s}}{(1-5^{2-s})(1-5^{1-2s})} \prod_{p\equiv\pm1(5)} \frac{(1+p^{-s}+2p^{1-s}+2p^{-2s}+p^{1-2s}+p^{1-3s})^2}{(1-p^{2-s})(1-p^{1-2s})} \\ &\quad \times \prod_{p\equiv\pm2(5)} \frac{1+p^{-2s}+2p^{2-2s}+2p^{-4s}+p^{2-4s}+p^{2-6s}}{(1-p^{4-2s})(1-p^{2-4s})} \\ &= 1 + \frac{25}{4^s} + \frac{36}{5^s} + \frac{100}{9^s} + \frac{288}{11^s} + \frac{410}{16^s} + \frac{400}{19^s} + \frac{900}{20^s} + \frac{912}{25^s} + \cdots . \end{aligned} \tag{17}$$

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