

GEOMETRIC ENUMERATION PROBLEMS FOR LATTICES AND EMBEDDED \mathbb{Z} -MODULES

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ABSTRACT. In this review, we count and classify certain sublattices of a given lattice, as motivated by crystallography. We use methods from algebra and algebraic number theory to find and enumerate the sublattices according to their index. In addition, we use tools from analytic number theory to determine the asymptotic behaviour of the corresponding counting functions. Our main focus lies on similar sublattices and coincidence site lattices, the latter playing an important role in crystallography. As many results are algebraic in nature, we also generalise them to \mathbb{Z} -modules embedded in \mathbb{R}^d .

1. INTRODUCTION

Lattices in \mathbb{R}^3 have been used for more than a century in crystallography, as they describe the translational symmetries of idealised, infinitely extended (periodic) crystals. As such, they have been studied intensively, together with space groups, which are finite extensions of lattices (viewed as Abelian groups) and describe the full symmetry of the crystals; compare the Epilogue to this volume. Group-subgroup relations have been applied to analyse various aspects such as phase transitions in crystals.

A special case of the latter is the question of certain kinds of sublattices of a given lattice. Ideal crystals do not exist in nature, and the result of crystallisation is very often not a single crystal, but a mixture of differently orientated crystals of the same kind. The latter are called *grains*, and an important question in crystallography is their mutual orientation and the border between two neighbouring grains, called a *grain boundary*.

To study the latter, one assigns, to each of the two grains, its corresponding lattice, say Γ and Γ' , and computes their intersection $\Gamma \cap \Gamma'$. If the two grains are of the same kind, the two lattices are related by an orthogonal transformation R , which means that we have $\Gamma' = R\Gamma$ for a suitable isometry $R \in O(3, \mathbb{R})$. The corresponding sublattice $\Gamma \cap R\Gamma$ is called a *coincidence site lattice* (CSL).

It was Friedel in 1911 who first recognised the usefulness of CSLs in describing and classifying grain boundaries of crystals [38]. Analogous ideas were later used by Kronberg and Wilson [62]. But it still took some time before their ideas became popular. In fact, the widespread use of CSLs was only triggered by a paper of Ranganathan [75] in 1966. Many important papers were published in the following years. In particular, we mention contributions by Grimmer [46, 47, 48, 50, 51, 49] and Bollmann [20, 21].

The discovery of quasicrystals sparked new interest in CSLs, and a systematic mathematical study started. In particular, the concept of CSLs was generalised to \mathbb{Z} -modules embedded in \mathbb{R}^d , which led to the notion of coincidence site modules (CSMs). They are used to describe grain boundaries in quasicrystals; compare [15, 72, 88] and references therein.

This new development also triggered a more detailed study of lattices in dimensions $d > 3$, as they are used to generate aperiodic point sets by the now common cut and project technique; compare [9, Ch. 7]. In particular, lattices in dimension $d = 4$ such as the hypercubic lattices [4, 94] and the A_4 -lattice [11, 56] were studied.

Further applications of CSLs can be found in coding theory in connection with so-called lattice quantisers, where lattices in large dimensions and with high packing densities are important; compare [34, 85] for general background, as well as [1] for concrete applications of the A_4 -lattice and [2] for the hexagonal lattice. However, not much is known about lattices in dimensions $d > 5$, although there are some partial results for rational lattices [99, 100, 57].

The original concept of CSLs has been generalised in several ways. In particular, one may study the intersection of several rotated copies of a lattice, which are known as multiple CSLs; compare [8, 95, 18]. They have applications to so-called multiple junctions [40, 41, 42], which are multiple crystal grains meeting at some common manifold. Whereas classical CSLs involve only linear isometries, one may consider affine isometries as well, which is directly related to the question of coincidences of crystallographic point packings; compare [64, 66, 63]. The latter are connected to the problem of coincidences of coloured lattices and colour coincidences [65, 63, 67].

The planar case is certainly the best studied. Here, also a connection between CSLs and well-rounded sublattices has been established [17]. Moreover, even some results for the hyperbolic plane [78] have been found.

Naturally, CSLs are not the only sublattices that are of interest in crystallography and coding theory. Classifying sublattices with certain symmetry constraints has a long tradition in mathematics and in crystallography; compare [79, 80] and references therein. An interesting question is the number of sublattices that are *similar* to its parent lattice. It has been answered in detail for a considerable collection of lattices [7, 14, 12] in dimensions $d \leq 4$. For higher dimensions, some existence results have been obtained by Conway, Rains and Sloane, who were motivated by problems in coding theory [26].

Actually, some years ago, a close connection between *similar sublattices* (SSLs) and CSLs has been established [45], which was later generalised to \mathbb{Z} -modules embedded in \mathbb{R}^d [44, 97]. This provides the link for our two main topics, namely the enumeration of coincidence site lattices and similar sublattices, and its generalisation to embedded \mathbb{Z} -modules.

Let us give an outline of this chapter. Our main focus is on lattices and certain \mathbb{Z} -modules, the latter viewed as embedded in some Euclidean space. This point of view is unusual from an algebraic point of view, but motivated by the crystallographic applications to (quasi-)crystals. Therefore, all lattices are regarded as special cases of embedded \mathbb{Z} -modules, and one could

develop the theory for embedded modules right from the beginning. However, the lattice case is without doubt such an important problem in itself that we prefer to first present the theory for lattices, and generalise later. In fact, our text is written in such a way that readers primarily interested in the lattice case can simply skip the discussions of the more general modules.

The chapter is organised as follows. We start with some basic notions and facts about lattices in Section 2. As a motivation and an introduction to the general theory, we consider a variety of counting problems of the square lattice in Section 3. This not only serves to illustrate the special enumeration problems of SSLs and CSLs we are after, but also puts them in a broader range of problems to emphasise the connections to other combinatorial questions. Section 4 provides some useful tools from algebra and analysis.

In Section 5, we discuss SSLs. After the general theory in Section 5.1, we consider several examples, including planar lattices (Section 5.2) and rational lattices in dimensions $d \geq 4$ (Section 5.3), with a detailed presentation of the lattice A_4 in Section 5.4 and the hypercubic lattices in Section 5.5. The results for lattices are finally generalised for embedded \mathbb{Z} -modules in Section 6, which also includes the icosian ring as an example (Section 6.1). In addition, some examples for planar modules can already be found in Section 5.2.

From Section 7 onwards, we deal with CSLs and coincidence site modules. Section 7 presents the general theory, both for simple and multiple CSLs. It includes a section on some connections with monotiles (Section 7.3). In Section 7.5, we generalise our results to embedded \mathbb{Z} -modules and, finally, we investigate the interrelations between coincidence site modules and similar submodules in Section 7.6. This is followed by a series of examples. In Section 8, we deal with planar \mathbb{Z} -modules. After discussing the cubic lattices in Section 9, we move on to the four-dimensional hypercubic lattices in Section 10 and to the lattice A_4 in Section 11, which also covers the icosian ring as an example of a \mathbb{Z} -module embedded in \mathbb{R}^4 . Section 12 is devoted to the multiple CSLs of the cubic lattices. Finally, we present some (rudimentary) results for dimensions $d \geq 5$ in Section 13.

Throughout this chapter, ideals play an important role. In almost all of our examples, we are dealing with principal ideals, which have a single generating element that is unique up to units. Although it is usually more elegant to formulate results in terms of ideals instead of generating elements, we will frequently prefer to deal with generating elements. The main reason is that we usually deal with ideals in algebraic number fields or quaternion algebras, and their elements can be used to parametrise rotations in dimensions $d \leq 4$. However, rotations are parametrised by concrete complex numbers or quaternions, respectively, and not by ideals. As we want to emphasise the direct connection to the rotations and use geometric intuition, we accept the fact that some equations are more cumbersome when formulated with quaternions and hold only up to units. For those who are more interested in an exposition using ideals, we mention [15, Sec. 5], which shows how to formulate matters in ideal-theoretic way in the context of quaternion algebras.

As we proceed, we shall prove many of the structural properties and results — in particular, when they are not trivial or not easily available in the literature. Otherwise, we state concrete results without proof, but with proper (and precise) references.

2. PRELIMINARIES ON LATTICES

Let us begin with some definitions for lattices in \mathbb{R}^d (which are co-compact discrete subgroups of \mathbb{R}^d), where we start from the notions introduced in [9, Ch. 3] and refer to [24, 54] for further background. In particular, a lattice $\Gamma \subset \mathbb{R}^d$ always has full rank d (as a \mathbb{Z} -module), and any lattice basis can also serve as a basis for \mathbb{R}^d .

Definition 2.1. Two lattices $\Gamma_1, \Gamma_2 \subset \mathbb{R}^d$ are called *commensurate*, denoted by $\Gamma_1 \sim \Gamma_2$, if $\Gamma_1 \cap \Gamma_2$ has finite index in both Γ_1 and Γ_2 .

In our terminology, commensurateness means that $\Gamma_1 \cap \Gamma_2$ is a sublattice (of full rank) of both Γ_1 and Γ_2 . Actually, there are several ways to characterise commensurateness [98].

Lemma 2.2. *Let Γ_1 and Γ_2 be lattices in \mathbb{R}^d . Then, the following statements are equivalent.*

- (1) Γ_1 and Γ_2 are commensurate.
- (2) $\Gamma_1 \cap \Gamma_2$ has finite index in both Γ_1 and Γ_2 .
- (3) $\Gamma_1 \cap \Gamma_2$ has finite index in Γ_1 or in Γ_2 .
- (4) There exist (positive) integers m_1 and m_2 such that $m_1\Gamma_1 \subseteq \Gamma_2$ and $m_2\Gamma_2 \subseteq \Gamma_1$.
- (5) There exists an integer $m \neq 0$ such that $m\Gamma_1 \subseteq \Gamma_2$ or $m\Gamma_2 \subseteq \Gamma_1$.
- (6) $\Gamma_1 \cap \Gamma_2$ is a lattice (of full rank d) in \mathbb{R}^d . □

As an immediate consequence, for instance via applying property (4) several times, one obtains that commensurateness is an equivalence relation.

An example of commensurate lattices is provided by similar sublattices. In fact, similarity of lattices is an important concept to us. Recall that an invertible linear map $f: \mathbb{R}^d \rightarrow \mathbb{R}^d$ is called a *similarity transformation* if it is of the form $f = \alpha R$, where R is a (linear) isometry and $0 \neq \alpha \in \mathbb{R}$. Two lattices Γ and Γ' are called *similar*, in symbols $\Gamma \stackrel{s}{\sim} \Gamma'$, if there exists a similarity transformation from one to the other. Clearly, similarity of lattices is an equivalence relation.

Definition 2.3. A similarity transformation that maps a lattice $\Gamma \in \mathbb{R}^d$ onto a sublattice of Γ is called a *similarity transformation of Γ* . A sublattice $\Gamma' \subseteq \Gamma$ is called a *similar sublattice* (SSL) of Γ if Γ' is similar to Γ .

Trivial examples of SSLs are the sublattices $m\Gamma$, with $m \in \mathbb{N}$. Similarly, given an SSL $\Gamma' \subseteq \Gamma$, also $m\Gamma'$ is an SSL. In order to exclude these cases, we introduce the notion of a primitive SSL.

Definition 2.4. An SSL $\Gamma' \subseteq \Gamma$ is called *primitive* if $\frac{1}{n}\Gamma' \subseteq \Gamma$ with $n \in \mathbb{N}$ implies that $n = 1$.

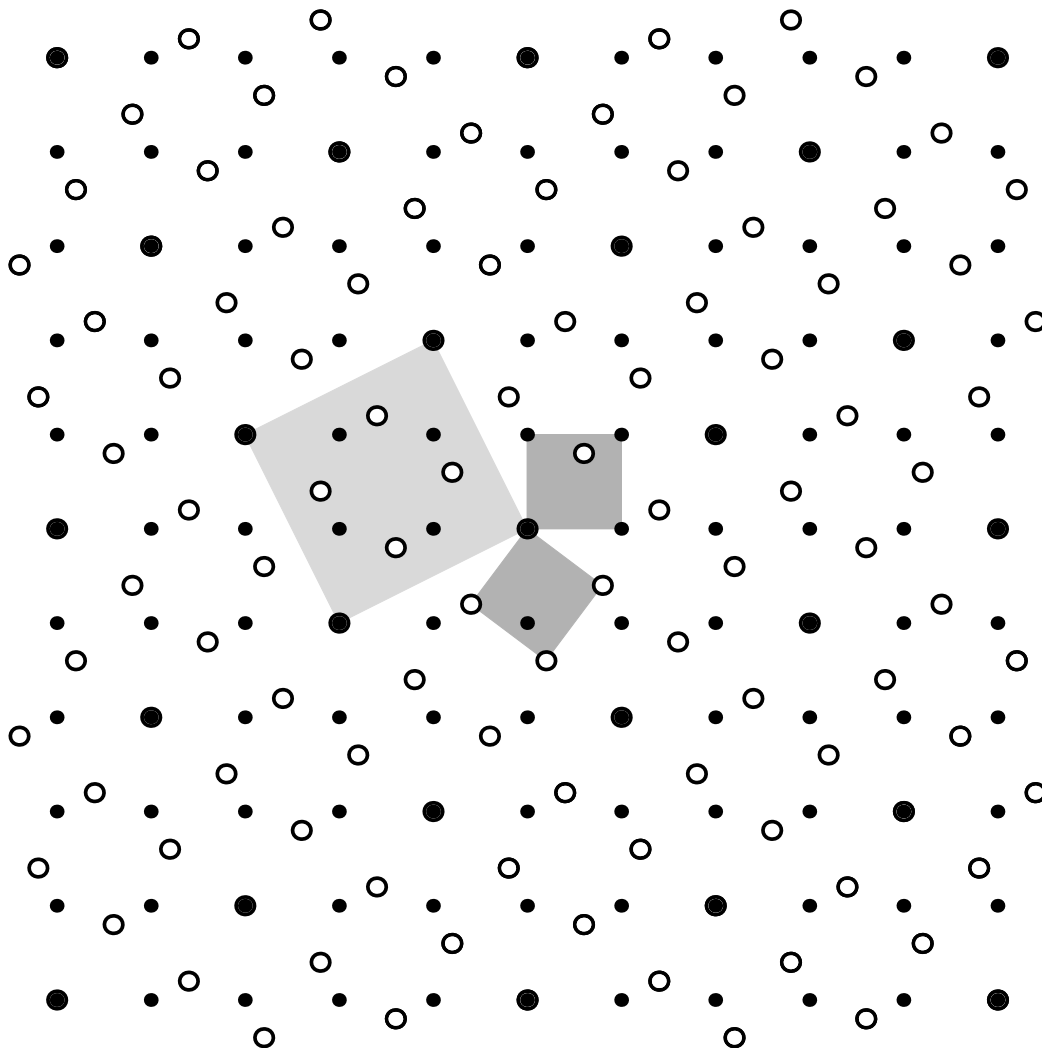


FIGURE 1. A square lattice (all black points) and a rotated copy of it (open circles together with large black points), with relative rotation angle $\alpha = \arctan(\frac{4}{3}) \approx 53.13^\circ$. The large black points mark the intersection of the two lattices, which is the CSL and again a square lattice. The shaded squares show fundamental domains of the three lattices. The larger square is a fundamental domain of the CSL.

In crystallography, the intersection $\Gamma \cap R\Gamma$ plays an important role in describing grain boundaries. If $\Gamma \cap R\Gamma$ is a lattice (of full rank), it is called a *coincidence site lattice* (CSL). A planar example is shown in Figure 1. As we have seen, the intersection $\Gamma \cap R\Gamma$ is a lattice if and only if Γ and $R\Gamma$ are commensurate. This motivates the following definition.

Definition 2.5. Let Γ be a lattice in \mathbb{R}^d , and let $R \in O(d, \mathbb{R})$. If Γ and $R\Gamma$ are commensurate, $\Gamma(R) := \Gamma \cap R\Gamma$ is called a *coincidence site lattice* (CSL). In this case, R is called a *coincidence isometry*. The corresponding index, $\Sigma_\Gamma(R) := [\Gamma : \Gamma(R)]$, is called its *coincidence index*.

Before we embark on a systematic review of CSLs and their properties, let us embed the study of such lattices, in an illustrative fashion, into a wider context that is motivated by geometry and combinatorics.

3. A HIERARCHY OF PLANAR LATTICE ENUMERATION PROBLEMS

It is the intention of this section to shed some more light on the coincidence problem and how it relates to various types of index-oriented sublattice enumerations with geometric constraints. Let us explain this for the square lattice in \mathbb{R}^2 in an informal manner. The results will be given in closed form in terms of zeta functions, and explicitly (for small indices) in Table 1 on page 8.

To this end, let us start with the question of how many sublattices of \mathbb{Z}^2 have index m , without any further restriction. Let us call this number a_m . Clearly, $a_1 = 1$ (only \mathbb{Z}^2 itself is a sublattice of index 1) and $a_2 = 3$ (counting two different rectangular sublattices and one square sublattice). In general, one has $a_{mn} = a_m a_n$ when $m, n \in \mathbb{N}$ are coprime, and one can derive, either from [4, Appendix] or from [83, Lemma 2 on p. 99], the general result that

$$a_m = \sigma_1(m) = \sum_{d|m} d,$$

where σ_1 is a divisor function, whose Dirichlet series generating function reads

$$(3.1) \quad F(s) = \sum_{m=1}^{\infty} \frac{a_m}{m^s} = \zeta(s) \zeta(s-1).$$

Here, $\zeta(s) = \sum_{m=1}^{\infty} m^{-s}$ is Riemann's zeta function [3]. From this, it can be shown that the number of sublattices of index $\leq x$, which is the summatory¹ function $\sum_{k \leq x} a_k$, grows quadratically as $x^2 \pi^2 / 12$; compare [55, Thm. 324]. More precisely, we have

$$\sum_{m \leq x} a_m = \frac{\pi^2}{12} x^2 + \mathcal{O}(x \log(x)) \quad \text{as } x \rightarrow \infty.$$

This counting result is, of course, *algebraic* in nature and thus applies to any planar lattice, and to the free Abelian group of rank 2 in particular (where a_m is the number of distinct subgroups of index m).

As a first geometric refinement step, let us consider those sublattices of \mathbb{Z}^2 which are *well-rounded*, which means that the shortest non-zero lattice vectors span the plane. Here, the

¹As is well known from number theory, arithmetic functions such as $m \mapsto a_m$ are prone to strong fluctuations. The corresponding summatory functions are usually more regular, and show a well-defined asymptotic behaviour; see [3] for background.

result is considerably more difficult (and the most difficult one for this informal discussion), and one finds [17] that the counts $a_{\square}^{\text{wr}}(m)$ lead to the Dirichlet series

$$(3.2) \quad \Phi_{\square}^{\text{wr}}(s) = \Phi_{\square}^{\text{pr}}(s)(1 + \phi_0(s) + \phi_1(s)),$$

where $\Phi_{\square}^{\text{pr}}(s)$ is the generating function for all primitive square sublattices given below in Eq. (3.4), together with

$$\begin{aligned} \phi_0(s) &= \frac{2}{2^s} \sum_{p \in \mathbb{N}} \sum_{p < q < \sqrt{3}p} \frac{1}{p^s q^s}, \\ \phi_1(s) &= \frac{2}{1 + 2^{-s}} \sum_{k \in \mathbb{N}} \sum_{k < \ell < \sqrt{3}k + \frac{\sqrt{3}-1}{2}} \frac{1}{(2k+1)^s (2\ell+1)^s}. \end{aligned}$$

Although no simpler closed expressions for these functions are known, they can be approximated by explicit formulas involving Riemann's zeta function and a certain L -series [17]; see also below (Section 5.2) for further details. This enables us to determine the asymptotic growth rate explicitly, including an error term. As there are considerably fewer well-rounded sublattices than sublattices in total, it is not surprising that the growth rate is smaller, namely $\frac{\log(3)}{2\pi} x \log(x)$ as $x \rightarrow \infty$; see [17]. There exists a linear correction term, and the asymptotic behaviour reads in detail

$$\begin{aligned} \sum_{n \leq x} a_{\square}^{\text{wr}}(n) &= \frac{\log(3)}{3} \frac{L(1, \chi_{-4})}{\zeta(2)} x (\log(x) - 1) + c_{\square} x + \mathcal{O}(x^{3/4} \log(x)) \\ &= \frac{\log(3)}{2\pi} x \log(x) + \left(c_{\square} - \frac{\log(3)}{2\pi} \right) x + \mathcal{O}(x^{3/4} \log(x)), \end{aligned}$$

where, with $\gamma \approx 0.5772157$ denoting the Euler–Mascheroni constant,

$$\begin{aligned} c_{\square} &:= \frac{L(1, \chi_{-4})}{\zeta(2)} \left(\frac{\log(3)}{3} \left(\frac{L'(1, \chi_{-4})}{L(1, \chi_{-4})} + 3\gamma - 2 \frac{\zeta'(2)}{\zeta(2)} - \frac{\log(3)}{4} - \frac{\log(2)}{6} \right) \right. \\ &\quad \left. + \zeta(2) - \sum_{p=1}^{\infty} \frac{1}{p} \left(\frac{\log(3)}{2} - \sum_{p < q < p\sqrt{3}} \frac{1}{q} \right) \right. \\ &\quad \left. - \frac{4}{3} \sum_{k=0}^{\infty} \frac{1}{2k+1} \left(\frac{1}{4} \log(3) - \sum_{k < \ell < k\sqrt{3} + \frac{\sqrt{3}-1}{2}} \frac{1}{2\ell+1} \right) \right) \\ &\approx 0.6272237. \end{aligned}$$

Note that the error term $\mathcal{O}(x^{3/4} \log(x))$ is certainly not optimal; see [17] for more. Here, the numerical values are rounded to the last digit displayed, so that the error is less than 1 in the last digit. The same rule implicitly applies to any numerical values that we will give in the following.

Let us next ask how many of the sublattices of \mathbb{Z}^2 of index m are actually *square* lattices; see [7, 13, 14] for various generalisations of this question. This number can be obtained by

TABLE 1. Some counts of the enumeration problems for \mathbb{Z}^2 . For indices $n \leq 60$, the number of multiple CSLs is the same as for CSLs, except for $n = 25$, where we have 3 multiple CSLs instead of 2 simple ones.

index m	1	2	3	4	5	6	7	8	9	10
sublattices	1	3	4	7	6	12	8	15	13	18
well-rounded	1	1	0	1	2	0	0	1	1	2
square	1	1	0	1	2	0	0	1	1	2
prim. square	1	1	0	0	2	0	0	0	0	2
coincidence	1	0	0	0	2	0	0	0	0	0
index m	11	12	13	14	15	16	17	18	19	20
sublattices	12	28	14	24	24	31	18	39	20	42
well-rounded	0	2	2	0	2	1	2	1	0	2
square	0	0	2	0	0	1	2	1	0	2
prim. square	0	0	2	0	0	0	2	0	0	0
coincidence	0	0	2	0	0	0	2	0	0	0
index m	21	22	23	24	25	26	27	28	29	30
sublattices	32	36	24	60	31	42	40	56	30	72
well-rounded	0	0	0	4	3	2	0	0	2	2
square	0	0	0	0	3	2	0	0	2	0
prim. square	0	0	0	0	2	2	0	0	2	0
coincidence	0	0	0	0	2	0	0	0	2	0
index m	31	32	33	34	35	36	37	38	39	40
sublattices	32	63	48	54	48	91	38	60	56	90
well-rounded	0	1	0	2	2	1	2	0	0	4
square	0	1	0	2	0	1	2	0	0	2
prim. square	0	0	0	2	0	0	2	0	0	0
coincidence	0	0	0	0	0	0	2	0	0	0
index m	41	42	43	44	45	46	47	48	49	50
sublattices	42	96	44	84	78	72	48	124	57	93
well-rounded	2	0	0	0	2	0	0	4	1	3
square	2	0	0	0	2	0	0	0	1	3
prim. square	2	0	0	0	0	0	0	0	0	2
coincidence	2	0	0	0	0	0	0	0	0	0
index m	51	52	53	54	55	56	57	58	59	60
sublattices	72	98	54	120	72	120	80	90	60	168
well-rounded	0	2	2	0	0	0	0	2	0	6
square	0	2	2	0	0	0	0	2	0	0
prim. square	0	0	2	0	0	0	0	2	0	0
coincidence	0	0	2	0	0	0	0	0	0	0

counting the lattice points on circles of radius \sqrt{m} (hence counting solutions of the Diophantine equation $x^2 + y^2 = m$) and afterwards dividing by 4 (the order of C_4 , the rotation part of the point symmetry group of \mathbb{Z}^2). The result is given in [55, Chs. 16.9, 16.10 and 17.9] and leads to the Dirichlet series generating function

$$(3.3) \quad \Phi_{\square}(s) = \zeta_K(s) = \frac{1}{1-2^{-s}} \prod_{p \equiv 1(4)} \left(\frac{1}{1-p^{-s}} \right)^2 \prod_{p \equiv 3(4)} \frac{1}{1-p^{-2s}},$$

where here and in what follows $\zeta_K(s) = \zeta(s)L(s, \chi_{-4})$ is the Dedekind zeta function of the quadratic field $K = \mathbb{Q}(i)$; compare [91, §11]. Recall that

$$L(s, \chi_{-4}) = \sum_{n=1}^{\infty} \frac{\chi_{-4}(n)}{n^s}$$

is the L -series for the Dirichlet character

$$\chi_{-4}(n) = \begin{cases} 0, & \text{if } n \text{ is even,} \\ 1, & \text{if } n \equiv 1 \pmod{4}, \\ -1, & \text{if } n \equiv 3 \pmod{4}. \end{cases}$$

The meaning of Eq. (3.3) becomes clear if one realises that the square sublattices of \mathbb{Z}^2 are precisely the non-trivial ideals of $\mathbb{Z}[i]$, the ring of Gaussian integers within the quadratic field $\mathbb{Q}(i)$; see also [9, Ex. 2.15].

The growth rate of the number of similar sublattices of index $\leq x$ is linear, namely $\frac{\pi}{4}x$, which follows either from the asymptotic properties of $\zeta_K(s)$ near its rightmost pole (at $s = 1$) or just from counting one quarter of the lattice points inside the circle of radius \sqrt{x} , which is $\frac{\pi}{4}x$ to leading order in x . More precisely, one has

$$\sum_{m \leq x} a_{\square}(m) = \frac{\pi}{4}x + \mathcal{O}(\sqrt{x});$$

see [17, Appendix] for details.

In the last case, some of the square lattices fail to be *primitive* (such as $3\mathbb{Z}^2$ etc.), which happens whenever the sublattice is an integer multiple of \mathbb{Z}^2 or of one of its primitive sublattices. If we exclude those, primes $p \equiv 3(4)$ are impossible as divisors of the index m , and some solutions of $p \equiv 1(4)$ also drop out (whenever the index is divisible by a square). Now, the generating function reads

$$(3.4) \quad \Phi_{\square}^{\text{pr}}(s) = (1 + 2^{-s}) \prod_{p \equiv 1(4)} \frac{1 + p^{-s}}{1 - p^{-s}} = \frac{\zeta_K(s)}{\zeta(2s)},$$

and the asymptotic growth rate of the number of primitive square sublattices of index $\leq x$ is again linear, this time with

$$\sum_{m \leq x} a_{\square}^{\text{pr}}(m) = \frac{3}{2\pi}x + \mathcal{O}(\sqrt{x} \log(x)).$$

The leading term can be determined by counting one quarter of the visible points [3] in the circle of radius \sqrt{x} , which is $\frac{1}{4}(\pi x \frac{6}{\pi^2})$; see [17, Appendix] for the error term.

Finally, let us see how the CSLs fit into this picture. As $\text{SO}(2, \mathbb{R})$ is Abelian, the symmetry group of any CSL of \mathbb{Z}^2 must contain a fourfold rotation, which in turn implies that the CSL must be a square lattice. Hence, any CSL is a similar sublattice. Note that this is a rather exceptional feature of the square lattice, which it shares, to our knowledge, only with the planar hexagonal lattice and some embedded modules in the plane. Nevertheless, there is a general connection between SSLs and CSLs, as we shall see in Section 7.6 below. Note, however, that not all square sublattices are CSLs — they only are if they are primitive and if their index is *odd*. This finally results in the generating function of the coincidence problem described above, namely

$$(3.5) \quad \Psi_{\square}(s) = \sum_{m=1}^{\infty} \frac{a_{\square}^{\text{CSL}}(m)}{m^s} = \prod_{p \equiv 1(4)} \frac{1+p^{-s}}{1-p^{-s}} = (1+2^{-s})^{-1} \frac{\zeta_K(s)}{\zeta(2s)}.$$

As $\Psi_{\square}(s)$ differs from $\Phi_{\square}^{\text{pr}}(s)$ only by the factor $(1+2^{-s})^{-1}$, the asymptotic behaviour

$$\sum_{m \leq x} a_{\square}^{\text{CSL}}(m) = \frac{1}{\pi} x + \mathcal{O}(\sqrt{x} \log(x))$$

is similar to the previous case, with the growth rate being lower by a factor of $(1+2^{-1})^{-1} = \frac{2}{3}$. As before, this equation expresses the Dirichlet series generating function in terms of zeta functions; see Table 1 for the first few terms of the corresponding Dirichlet series. Similar formulas will also appear in many of our later examples.

Now, we may even go a step further and ask for *multiple* coincidences, i.e., intersections of any finite number of CSLs. As we shall discuss later (see Section 8 and, in particular, Example 8.5), the set of indices stays the same, but some additional lattices emerge, which are still similar sublattices, but not primitive any more.

We hope that this short digression has put the enumeration problem in a broader perspective, and also in contact with some elementary questions from analytic number theory. Of course, we are also interested in results in higher dimensions, where the picture changes significantly because $\text{O}(d, \mathbb{R})$ is no longer Abelian for $d > 2$. Before we can proceed, we first need to introduce various methods and tools.

4. ALGEBRAIC AND ANALYTIC TOOLS

In writing the square lattice as $\mathbb{Z}^2 = \mathbb{Z}[i]$, we can profit from the algebraic structure of $\mathbb{Z}[i]$, which is a ring that is a *principal ideal domain* (PID). In fact, it is the ring of integers of the imaginary quadratic field $\mathbb{Q}(i)$, and as such the maximal order of the field. Here, the term ‘order’ means that we are dealing with a finitely generated \mathbb{Z} -module whose \mathbb{Q} -span is the entire field. $\mathbb{Z}[i]$ is maximal for this property in the obvious sense, and unique as such.

Note that $\mathbb{Q}(i)$ can also be viewed as a cyclotomic field, which will later be used for an extension to analyse similar submodules and coincidence site modules of the rings $\mathbb{Z}[\xi_n]$ of integers in the cyclotomic field $\mathbb{Q}(\xi_n)$, where ξ_n is a primitive n -th root of unity. We refer to [9, Sec. 2.5] and to [89] for general background in this context.

As we shall see, this number-theoretic approach is truly powerful for planar structures. Consequently, one would like to have related methods also for higher-dimensional problems. This leads to a non-commutative generalisation in the form of certain quaternion algebras and their maximal orders.

4.1. Quaternions. As quaternions are pivotal in what follows, we briefly recall their most important properties. For details, we refer to [9, Sec. 2.5.4], [15, Secs. 3 and 4] and to the general literature [61, 28, 59, 55].

Let $\{e, i, j, k\}$ be the standard basis of \mathbb{R}^4 , where

$$e = (1, 0, 0, 0), \quad i = (0, 1, 0, 0), \quad j = (0, 0, 1, 0), \quad k = (0, 0, 0, 1).$$

The *quaternion algebra* over \mathbb{R} is the associative division algebra

$$\mathbb{H} := \mathbb{H}(\mathbb{R}) = \mathbb{R}e + \mathbb{R}i + \mathbb{R}j + \mathbb{R}k \simeq \mathbb{R}^4,$$

where multiplication is induced by Hamilton's relations

$$i^2 = j^2 = k^2 = ijk = -e.$$

Elements of \mathbb{H} are called quaternions, and an arbitrary quaternion q is written as either $q = q_0e + q_1i + q_2j + q_3k$ or $q = (q_0, q_1, q_2, q_3)$. Given two quaternions q and p , their *inner product* is defined by the standard scalar product of q and p as vectors² in \mathbb{R}^4 .

The *conjugate* of $q = (q_0, q_1, q_2, q_3)$ is $\bar{q} = (q_0, -q_1, -q_2, -q_3)$, and its *norm* is $\text{nr}(q) = |q|^2 = q\bar{q} = q_0^2 + q_1^2 + q_2^2 + q_3^2 \in \mathbb{R}$. One has $\overline{qp} = \bar{p}\bar{q}$ and $|qp|^2 = |q|^2|p|^2$ for any $q, p \in \mathbb{H}$. Given a quaternion $q = (q_0, q_1, q_2, q_3)$, its *real* and *imaginary parts* are defined as $\text{Re}(q) = q_0$ and $\text{Im}(q) = q_1i + q_2j + q_3k$, respectively. It is easy to verify that $\text{Re}(\mathbb{H})$ is the centre of \mathbb{H} , wherefore we can identify e with 1 from now on. The *imaginary space* of \mathbb{H} is the three-dimensional subspace $\text{Im}(\mathbb{H}) = \{\text{Im}(q) \mid q \in \mathbb{H}\} \simeq \mathbb{R}^3$ of \mathbb{H} . For ease of notation, we will identify $\text{Im}(\mathbb{H})$ and \mathbb{R}^3 and, in addition, also the elements $(q_1, q_2, q_3) \in \text{Im}(\mathbb{H})$ with the elements $(0, q_1, q_2, q_3) \in \mathbb{H}$.

Another convenient feature of the quaternions is that they can be used to parametrise rotations in 3 and 4 dimensions; compare [61] and [15]. In \mathbb{R}^3 , any rotation can be parametrised

²We usually identify a quaternion $q = (q_0, q_1, q_2, q_3)$ with the corresponding row vector (q_0, q_1, q_2, q_3) . However, when we use Cayley's parametrisation for rotations (see below), we will identify q with the corresponding column vector $(q_0, q_1, q_2, q_3)^T$.

by a single quaternion $0 \neq q \in \mathbb{H}$ with $q = (\kappa, \lambda, \mu, \nu)$ via

$$(4.1) \quad R(q) = \frac{1}{|q|^2} \begin{pmatrix} \kappa^2 + \lambda^2 - \mu^2 - \nu^2 & -2\kappa\nu + 2\lambda\mu & 2\kappa\mu + 2\lambda\nu \\ 2\kappa\nu + 2\lambda\mu & \kappa^2 - \lambda^2 + \mu^2 - \nu^2 & -2\kappa\lambda + 2\mu\nu \\ -2\kappa\mu + 2\lambda\nu & 2\kappa\lambda + 2\mu\nu & \kappa^2 - \lambda^2 - \mu^2 + \nu^2 \end{pmatrix},$$

where elements of \mathbb{R}^3 are written as column vectors. In particular, we have

$$R(q)x = R(q) \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \frac{qx\bar{q}}{|q|^2}$$

for any $x \in \mathbb{R}^3$, where we have again identified x with $(0, x_1, x_2, x_3)$. Note that the parametrisation of Eq. (4.1), which is known as *Cayley's parametrisation*, is only unique up to a scaling factor, meaning $R(\alpha q) = R(q)$ for $\alpha \neq 0$.

As we are usually interested in specific subgroups of $\text{SO}(3, \mathbb{R})$, let us mention that such subgroups often can be related to suitable subrings of \mathbb{H} ; compare [15, Prop. 1]. In particular, the rotations of $\text{SO}(3, \mathbb{Q})$ can be parametrised by integer quaternions as explained below.

In \mathbb{R}^4 , a pair of quaternions is needed to parametrise a rotation [61, 36]. These quaternions are unique up to positive scaling factors and a common sign change. In particular,

$$(4.2) \quad R(p, q): \mathbb{R}^4 \longrightarrow \mathbb{R}^4, \quad x \longmapsto R(p, q)x = \frac{px\bar{q}}{|pq|}$$

defines a rotation in \mathbb{R}^4 , whose matrix representation—in abuse of notation also written as $R(p, q) = \frac{1}{|pq|}M(p, q)$ —is explicitly given by

$$M(p, q) = \begin{pmatrix} \langle p|q \rangle & \langle p|i|q \rangle & \langle p|j|q \rangle & \langle p|k|q \rangle \\ \langle p|i|q \rangle & \langle p|i|i|q \rangle & \langle p|j|i|q \rangle & \langle p|k|i|q \rangle \\ \langle p|j|q \rangle & \langle p|i|j|q \rangle & \langle p|j|j|q \rangle & \langle p|k|j|q \rangle \\ \langle p|k|q \rangle & \langle p|i|k|q \rangle & \langle p|j|k|q \rangle & \langle p|k|k|q \rangle \end{pmatrix} \\ = \begin{pmatrix} ak + b\ell + cm + dn & -a\ell + bk + cn - dm & -am - bn + ck + dl & -an + bm - cl + dk \\ a\ell - bk + cn - dm & ak + b\ell - cm - dn & -an + bm + cl - dk & am + bn + ck + dl \\ am - bn - ck + dl & an + bm + cl + dk & ak - b\ell + cm - dn & -a\ell - bk + cn + dm \\ an + bm - cl - dk & -am + bn - ck + dl & a\ell + bk + cn + dm & ak - b\ell - cm + dn \end{pmatrix},$$

where $p = (k, \ell, m, n)$ and $q = (a, b, c, d)$. Here, $\langle \cdot | \cdot \rangle$ denotes the standard (Euclidean) inner product in \mathbb{R}^4 .

A quaternion all of whose components are integers is called a *Lipschitz quaternion*. The set \mathbb{L} of Lipschitz quaternions is thus defined as

$$(4.3) \quad \mathbb{L} := \{(q_0, q_1, q_2, q_3) \in \mathbb{H} \mid q_0, q_1, q_2, q_3 \in \mathbb{Z}\}.$$

The Lipschitz quaternions form an order in the quaternion algebra $\mathbb{H}(\mathbb{Q})$, but not a maximal one. A *primitive Lipschitz quaternion* q is a quaternion in \mathbb{L} whose components are relatively prime. Furthermore, a *Hurwitz quaternion* is a quaternion whose components are all integers or all half-integers. The ring \mathbb{J} of Hurwitz quaternions [59] is a maximal order in the quaternion

algebra $\mathbb{H}(\mathbb{Q})$, as is any of its conjugates (which means that one only has uniqueness up to conjugacy here). \mathbb{J} is given by

$$(4.4) \quad \begin{aligned} \mathbb{J} &:= \{(q_0, q_1, q_2, q_3) \in \mathbb{H} \mid \text{all } q_i \in \mathbb{Z} \text{ or all } q_i \in \frac{1}{2} + \mathbb{Z}\} \\ &= \mathbb{L} \cup \left(\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right) + \mathbb{L} \right); \end{aligned}$$

compare [9, Ex. 2.18]. We call a Hurwitz quaternion $q \in \mathbb{J}$ *primitive* if $\frac{1}{n}q \in \mathbb{J}$ with $n \in \mathbb{N}$ implies $n = 1$. The norm $|q|^2$ of any Hurwitz quaternion is an integer. As quaternions of norm $|q|^2 = 2$ play a special role in \mathbb{J} , we distinguish between *odd* and *even* quaternions, where $q \in \mathbb{J}$ is called even or odd depending on whether $|q|^2$ is even or odd. Any quaternion of norm $|q|^2 = 2$ can be represented as $q = (1, 1, 0, 0)u = u'(1, 1, 0, 0)$, where u, u' are unit quaternions. As the group \mathbb{J}^\times of unit quaternions has order 24 and consists of the quaternions

$$(\pm 1, 0, 0, 0), (0, \pm 1, 0, 0), (0, 0, \pm 1, 0), (0, 0, 0, \pm 1) \text{ and } (\pm 1, \pm 1, \pm 1, \pm 1),$$

there are also 24 quaternions of norm $|q|^2 = 2$. The latter, normalised as $\frac{q}{\sqrt{2}}$, together with the units $u \in \mathbb{J}^\times$ form a group of order 48, which is the standard double cover of the octahedral group O .

Recall from [59] and [9, Sec. 2.5.4] that \mathbb{J} is a principal ideal ring, which here means that all right (left) ideals are principal right (left) ideals, and \mathbb{J} is also a maximal order. Thus, for any two right ideals $a\mathbb{J}$ and $b\mathbb{J}$, there exist quaternions g and m such that $g\mathbb{J} = a\mathbb{J} + b\mathbb{J}$ and $m\mathbb{J} = a\mathbb{J} \cap b\mathbb{J}$. These two quaternions g and m are unique up to multiplication by a unit quaternion from the right. We call g a *greatest common left divisor* of a and b , and m a *least common right multiple* of a and b , in symbols $g = \text{gcd}(a, b)$ and $m = \text{lcrm}(a, b)$. As g and m are unique only up to a unit, these equations only make sense as a shorthand notation for the corresponding equation of ideals $g\mathbb{J} = \text{gcd}(a, b)\mathbb{J}$ or as equations of quaternions that hold up to a multiplication by a unit quaternion from the right. In some cases, we may choose a particular g or m . In these cases, the equations involving them are considered to hold exactly. Similarly, we define the *greatest common right divisor* grcd and the *least common left multiple* lclm .

Similarly, the icosian ring \mathbb{I} is a maximal order in $\mathbb{H}(\mathbb{Q}(\sqrt{5}))$; we refer to [9, Ex. 2.19] for the definition. The above notions can thus analogously be defined for \mathbb{I} . One important difference will emerge from the existence of another maximal order, \mathbb{I}' , which is obtained from \mathbb{I} by algebraic conjugation in $\mathbb{Q}(\sqrt{5})$, though it is not of the form $q\mathbb{I}q^{-1}$. Here, the group of units \mathbb{I}^\times is infinite and isomorphic to $\mathbb{Z}[\tau]^\times \times \Delta_{H_4}$, where Δ_{H_4} is a group of order 120; see [9, Ex. 2.19] for details.

For further properties of maximal orders in quaternion algebras, we refer to [77, 87]; see also [15, Sec. 4], where the case of $\mathbb{H}(K)$ with K a real algebraic number field is considered in more detail.

4.2. Tools from analysis. In our enumeration problems, we naturally deal with arithmetic functions $a(m)$, which are functions defined on \mathbb{N} . In many examples, these functions are

multiplicative, which means that $a(mn) = a(m)a(n)$ whenever m and n are coprime. Note that, unless $a \equiv 0$, this implies $a(1) = 1$, and a is then completely determined by its values for p^n with p prime and $n \geq 1$.

In addition, we are often interested in the *summatory function*

$$A(x) = \sum_{m \leq x} a(m)$$

and its behaviour for large x , as this function behaves more regularly than $a(m)$ itself. This suggests to use generating functions and to analyse their analytic properties. In the context of multiplicative functions (although not restricted to those), a natural choice for the generating function is a *Dirichlet series* of the form $F(s) = \sum_{m=1}^{\infty} a(m)m^{-s}$. Let us recall one classic result for the case that $a(m)$ is real and non-negative, which relates $F(s)$ with the asymptotic behaviour of $A(x)$.

Theorem 4.1. *Let $F(s)$ be a Dirichlet series with non-negative coefficients which converges for $\operatorname{Re}(s) > \alpha > 0$. Suppose that $F(s)$ is holomorphic at all points of the line $\{\operatorname{Re}(s) = \alpha\}$ except at $s = \alpha$. Here, when approaching α from the half-plane to the right of it, we assume $F(s)$ to have a singularity of the form $F(s) = h(s)/(s - \alpha)^{n+1}$ where n is a non-negative integer, and $h(s)$ is holomorphic at $s = \alpha$. Then, as $x \rightarrow \infty$, we have*

$$A(x) := \sum_{m \leq x} a(m) \sim \frac{h(\alpha)}{\alpha \cdot n!} x^\alpha (\log(x))^n. \quad \square$$

The proof follows easily from Delange's theorem, for instance by taking $q = 0$ and $\omega = n$ in Tenenbaum's formulation; see [86, Ch. II.7, Thm. 15] and references given there.

5. SIMILAR SUBLATTICES

5.1. General results. Let us now have a more detailed look at similar sublattices. A similarity transformation consists of two ingredients, an isometry and a scaling factor. It thus makes sense to analyse these two parts independently and to introduce the following notions. We call

$$(5.1) \quad \operatorname{OS}(\Gamma) := \{R \in \operatorname{O}(d, \mathbb{R}) \mid \exists \alpha \in \mathbb{R}_+ \text{ such that } \alpha R\Gamma \subseteq \Gamma\}$$

the set of all *similarity isometries* of Γ . Likewise, we define

$$(5.2) \quad \operatorname{SOS}(\Gamma) := \operatorname{OS}(\Gamma) \cap \operatorname{SO}(d, \mathbb{R})$$

to be its orientation-preserving part. The following result is immediate.

Fact 5.1. *$\operatorname{OS}(\Gamma)$ and $\operatorname{SOS}(\Gamma)$ are subgroups of $\operatorname{O}(d, \mathbb{R})$.* □

One would expect that similar lattices should have related OS-groups, which is indeed true.

Lemma 5.2. *Let Γ and Γ' be similar lattices with $\Gamma' = \alpha R\Gamma$. Then,*

$$\operatorname{OS}(\Gamma') = R \operatorname{OS}(\Gamma) R^{-1}.$$

Proof. If $\alpha \neq 0$, the relation $\text{OS}(\Gamma) = \text{OS}(\alpha\Gamma)$ is trivial. The general case follows from the fact that $\beta S\Gamma \subseteq \Gamma$ holds if and only if $\beta RSR^{-1}\Gamma' \subseteq \Gamma'$. \square

Next, we aim to gain some insight into the scaling factors. Let us define

$$(5.3) \quad \begin{aligned} \text{Scal}_\Gamma(R) &:= \{\alpha \in \mathbb{R} \mid \alpha R\Gamma \subseteq \Gamma\} \quad \text{and} \\ \text{scal}_\Gamma(R) &:= \{\alpha \in \mathbb{R} \mid \alpha R\Gamma \sim \Gamma\}. \end{aligned}$$

Note that we have allowed negative values for the scaling factors here. For an arbitrary but fixed $R \in \text{O}(d, \mathbb{R})$, this ensures that $\text{Scal}_\Gamma(R)$ is a \mathbb{Z} -module and that $\text{scal}_\Gamma(R) \cup \{0\}$ is a vector space over the field \mathbb{Q} . As we shall see shortly, this vector space is one-dimensional if $R \in \text{OS}(\Gamma)$, and $\text{Scal}_\Gamma(R)$ is then a one-dimensional lattice.

We defined $\text{Scal}_\Gamma(R)$ and $\text{scal}_\Gamma(R)$ for arbitrary $R \in \text{O}(d, \mathbb{R})$. However, we are really only interested in the non-trivial case where $R \in \text{OS}(\Gamma)$. Clearly, the scaling factor 0 is always contained in $\text{Scal}_\Gamma(R)$, so $\text{Scal}_\Gamma(R)$ is always non-empty. By definition, $R \in \text{OS}(\Gamma)$ if and only if there exists an $\alpha \in \mathbb{R}_+$ such that $\alpha R\Gamma \subseteq \Gamma$. Hence, we have the following elementary result.

Fact 5.3 ([45, Sec. 4]). *Let Γ be a lattice in \mathbb{R}^d and $R \in \text{O}(d, \mathbb{R})$. Then, the following assertions are equivalent.*

- (1) $\text{Scal}_\Gamma(R) \neq \{0\}$;
- (2) $\text{scal}_\Gamma(R) \neq \emptyset$;
- (3) $R \in \text{OS}(\Gamma)$. \square

One expects that two similar lattices should display the same sets of scaling factors. Indeed, one has the following result.

Lemma 5.4. *Let Γ and Γ' be similar lattices, with $\Gamma' = \alpha R\Gamma$. Then,*

$$\text{Scal}_{\Gamma'}(S) = \text{Scal}_\Gamma(R^{-1}SR) \quad \text{and} \quad \text{scal}_{\Gamma'}(S) = \text{scal}_\Gamma(R^{-1}SR).$$

Proof. Let $\beta \in \text{Scal}_{\Gamma'}(S)$, so that $\beta S\Gamma' \subseteq \Gamma' = \alpha R\Gamma$. This is equivalent to $\beta R^{-1}SR\Gamma \subseteq \Gamma$, from which we infer the first identity. The second one follows similarly. \square

For a fixed lattice $\Gamma \subset \mathbb{R}^d$, let us have a closer look at the elements of $\text{Scal}_\Gamma(R)$. By basic facts from linear algebra, we have

$$[\Gamma : \alpha R\Gamma] = |\det(\alpha R)| = \alpha^d |\det(R)| = \alpha^d,$$

whenever αR is a similarity transformation of Γ . Hence, α^d must be an integer for all $\alpha \in \text{Scal}_\Gamma(R)$. More generally, if $\alpha R\Gamma \sim \Gamma$, there exists an integer m such that $m\alpha R\Gamma$ is a similar sublattice of Γ . Consequently, we have $\alpha^d \in \mathbb{Q}$ whenever $\alpha \in \text{scal}_\Gamma(R)$. We have thus proved the following.

Lemma 5.5. *Let $\Gamma \subset \mathbb{R}^d$ be a lattice. For any $\alpha \in \text{Scal}_\Gamma(R)$, we have $\alpha^d \in \mathbb{Z}$. Moreover, for any $\alpha \in \text{scal}_\Gamma(R)$, we have $\alpha^d \in \mathbb{Q}$. \square*

As a consequence, for any fixed lattice Γ , $\text{Scal}_\Gamma(R)$ is a discrete and closed set, or in other words, a locally finite set. Hence, there exists a smallest positive element in $\text{Scal}_\Gamma(R)$. This deserves a name.

Definition 5.6. For any isometry $R \in \text{OS}(\Gamma)$, the smallest positive element in $\text{Scal}_\Gamma(R)$ is called the *denominator* of R , written as $\text{den}_\Gamma(R)$.

Clearly, one has $(\text{den}_\Gamma(R))^d \in \mathbb{N}$. Moreover, $\text{den}_\Gamma(R) = 1$ is equivalent to $R\Gamma = \Gamma$, that is, $\text{den}_\Gamma(R) = 1$ if and only if R is a symmetry operation of the lattice Γ . In particular, $\text{den}_\Gamma(\mathbb{1}) = 1$.

As $\text{Scal}_\Gamma(R)$ is a \mathbb{Z} -module, each integer multiple of $\text{den}_\Gamma(R)$ is again an element of $\text{Scal}_\Gamma(R)$. On the other hand, each $\alpha \in \text{Scal}_\Gamma(R)$ must be a multiple of $\text{den}_\Gamma(R)$, since otherwise we could find a scaling factor α with $0 < \alpha < \text{den}_\Gamma(R)$. This leads to the following result.

Lemma 5.7. *Let $\Gamma \subset \mathbb{R}^d$ be a lattice. For any isometry $R \in \text{OS}(\Gamma)$, we have the relations $\text{Scal}_\Gamma(R) = \text{den}_\Gamma(R)\mathbb{Z}$ and $\text{scal}_\Gamma(R) = \text{den}_\Gamma(R)\mathbb{Q}^\times$.*

Proof. It remains to prove the statement about $\text{scal}_\Gamma(R)$. By definition, $\alpha \in \text{scal}_\Gamma(R)$ means $\alpha R\Gamma \sim \Gamma$. By Lemma 2.2, there exists an $m \in \mathbb{N}$ such that $m\alpha R\Gamma \subseteq \Gamma$, whence $m\alpha \in \text{Scal}_\Gamma(R) = \text{den}_\Gamma(R)\mathbb{Z}$ and thus also $\text{scal}_\Gamma(R) \subseteq \text{den}_\Gamma(R)\mathbb{Q}^\times$. On the other hand, $\text{den}_\Gamma(R)R\Gamma \sim \Gamma$ and $q\Gamma \sim \Gamma$ for all $q \in \mathbb{Q}$ imply that $\alpha R\Gamma \sim \Gamma$ for all $\alpha \in \text{den}_\Gamma(R)\mathbb{Q}^\times$, which shows that $\text{scal}_\Gamma(R) \supseteq \text{den}_\Gamma(R)\mathbb{Q}^\times$ as well. \square

More generally, we have $\text{scal}_\Gamma(R) = \alpha\mathbb{Q}^\times$ for any $\alpha \in \text{scal}_\Gamma(R)$. Note that $\text{scal}_\Gamma(\mathbb{1}) = \mathbb{Q}^\times$ and $\text{Scal}_\Gamma(\mathbb{1}) = \mathbb{Z}$.

Although we are ultimately more interested in the sets $\text{Scal}_\Gamma(R)$, it is worthwhile to discuss $\text{scal}_\Gamma(R)$ as these sets are easier to handle. In particular, we have a natural group structure on $\{\text{scal}_\Gamma(R) \mid R \in \text{OS}(\Gamma)\}$, with the product of two sets A and B defined in the obvious way as $AB := \{\alpha\beta \mid \alpha \in A, \beta \in B\}$, and the inverse of A given by $A^{-1} = \{\alpha^{-1} \mid \alpha \in A\}$. The latter is well defined as $0 \notin A$ whenever $A = \text{scal}_\Gamma(R)$.

Lemma 5.8. *Let $\Gamma \subset \mathbb{R}^d$ be a lattice. For any $R, S \in \text{OS}(\Gamma)$, we have*

$$\text{scal}_\Gamma(R) \text{scal}_\Gamma(S) = \text{scal}_\Gamma(RS) \quad \text{and} \quad \text{scal}_\Gamma(R^{-1}) = (\text{scal}_\Gamma(R))^{-1}.$$

Proof. The group structure is a consequence of the fact that commensurateness is an equivalence relation. Alternatively, this property also follows from Lemma 5.7, which suggests the definition of a natural mapping from the set $\{\text{scal}_\Gamma(R) \mid R \in \text{OS}(\Gamma)\}$ into the multiplicative group $\mathbb{R}_+/\mathbb{Q}_+$, which becomes a group homomorphism with the multiplication as defined in this lemma. \square

Actually, it is the homomorphism mentioned in the previous proof that will establish a general connection between SSLs and CSLs, as we shall discuss in Section 7.6.

Note that $\{\text{scal}_\Gamma(R) \mid R \in \text{OS}(\Gamma)\}$ is an Abelian group, although $\text{OS}(\Gamma)$ is not Abelian in general. In particular, one has $\text{scal}_\Gamma(RS) = \text{scal}_\Gamma(SR)$ even when $RS \neq SR$.

The situation is more involved for the sets $\text{Scal}_\Gamma(R)$. They do not form a group, nor even a semigroup, as $\text{Scal}_\Gamma(R) \text{Scal}_\Gamma(S) \subseteq \text{Scal}_\Gamma(RS)$ is usually a proper inclusion. Nevertheless, we can still extract some information on the denominator from this inclusion; compare [97, 98]. As $\text{den}_\Gamma(R) \text{den}_\Gamma(S)$ must be in $\text{scal}_\Gamma(RS)$, it is an integer multiple of $\text{den}_\Gamma(RS)$, that is,

$$(5.4) \quad \frac{\text{den}_\Gamma(R) \text{den}_\Gamma(S)}{\text{den}_\Gamma(RS)} \in \mathbb{N}.$$

An immediate consequence is that $\text{den}_\Gamma(R) \text{den}_\Gamma(R^{-1})$ is an integer. As $[\Gamma : \text{den}_\Gamma(R)R\Gamma] = (\text{den}_\Gamma(R))^d$ for an isometry $R \in \text{OS}(\Gamma)$, we also have $(\text{den}_\Gamma(R))^d \Gamma \subseteq \text{den}_\Gamma(R)R\Gamma$, from which we infer $(\text{den}_\Gamma(R))^{d-1} R^{-1} \Gamma \subseteq \Gamma$. This proves

$$(5.5) \quad \frac{(\text{den}_\Gamma(R))^{d-1}}{\text{den}_\Gamma(R^{-1})} \in \mathbb{N}.$$

Remark 5.9. Formula (5.5) implies $\text{den}_\Gamma(R^{-1}) \leq (\text{den}_\Gamma(R))^{d-1}$. In fact, this upper bound is sharp. As an example, we consider the \mathbb{Z} -span of the vectors $\xi^{i-1}e_i$, where ξ is the (positive) d -th root of a positive integer and $\{e_1, \dots, e_d\}$ is an orthonormal basis of \mathbb{R}^d . Let R be the rotation that maps e_i onto e_{i+1} for $1 \leq i \leq d-1$ and e_d onto e_1 . Then, $\text{den}_\Gamma(R) = \xi$ and $\text{den}_\Gamma(R^{-1}) = \xi^{d-1}$. \diamond

The example in Remark 5.9 also shows that $\text{den}_\Gamma(R)$ and $\text{den}_\Gamma(R^{-1})$ generally differ if $d \geq 3$. However, in two dimensions, they always agree.

Corollary 5.10. *For any planar lattice Γ , one has $\text{den}_\Gamma(R^{-1}) = \text{den}_\Gamma(R)$.*

Proof. From Eq. (5.5), we infer

$$\frac{\text{den}_\Gamma(R)}{\text{den}_\Gamma(R^{-1})} \in \mathbb{N} \quad \text{as well as} \quad \frac{\text{den}_\Gamma(R^{-1})}{\text{den}_\Gamma(R)} \in \mathbb{N},$$

the latter by symmetry. Together, they imply $\text{den}_\Gamma(R^{-1}) = \text{den}_\Gamma(R)$. \square

It is quite useful to understand the relationship between commensurate lattices in more detail. Using the fact that commensurateness is an equivalence relation, we can prove the following result.

Lemma 5.11. *If Γ and Γ' are two commensurate lattices in \mathbb{R}^d , one has $\text{OS}(\Gamma) = \text{OS}(\Gamma')$ as well as $\text{scal}_\Gamma(R) = \text{scal}_{\Gamma'}(R)$.*

Proof. By Fact 5.3, $R \in \text{OS}(\Gamma)$ if and only if there exists an $\alpha \neq 0$ such that $\alpha R\Gamma \subseteq \Gamma$. Commensurateness guarantees that there are $m, n \in \mathbb{N}$ such that $m\Gamma \subseteq \Gamma'$ and $n\Gamma' \subseteq \Gamma$. Thus, $\alpha R\Gamma \subseteq \Gamma$ implies

$$(5.6) \quad mn\alpha R\Gamma' \subseteq m\alpha R\Gamma \subseteq m\Gamma \subseteq \Gamma',$$

which gives $\text{OS}(\Gamma) \subseteq \text{OS}(\Gamma')$. By symmetry, we conclude $\text{OS}(\Gamma) = \text{OS}(\Gamma')$. Moreover, Eq. (5.6) shows that $\text{den}_\Gamma(R)$ and $\text{den}_{\Gamma'}(R)$ differ only by a factor $q \in \mathbb{Q}$, whence one has $\text{scal}_\Gamma(R) = \text{scal}_{\Gamma'}(R)$ by Lemma 5.7. \square

Of course, we cannot expect the sets $\text{Scal}_\Gamma(R)$ and $\text{Scal}_{\Gamma'}(R)$ to be equal. However, as we can sandwich Γ' between appropriately scaled copies of Γ , we can derive lower and upper bounds as follows.

Proposition 5.12. *Let Γ' be a sublattice of Γ of index m . Then,*

$$m \text{Scal}_\Gamma(R) \subseteq \text{Scal}_{\Gamma'}(R) \subseteq \frac{1}{m} \text{Scal}_\Gamma(R).$$

Moreover, one has

$$\frac{m \text{den}_\Gamma(R)}{\text{den}_{\Gamma'}(R)} \in \mathbb{N} \quad \text{and} \quad \frac{m \text{den}_{\Gamma'}(R)}{\text{den}_\Gamma(R)} \in \mathbb{N}.$$

Proof. If $\alpha \in \text{Scal}_\Gamma(R)$, then

$$\alpha R \Gamma' \subseteq \alpha R \Gamma \subseteq \Gamma \subseteq \frac{1}{m} \Gamma'$$

shows that $m\alpha \in \text{Scal}_{\Gamma'}(R)$. Similarly, $\alpha \in \text{Scal}_{\Gamma'}(R)$ implies

$$\alpha R m \Gamma \subseteq \alpha R \Gamma' \subseteq \Gamma' \subseteq \Gamma,$$

which proves $\text{Scal}_{\Gamma'}(R) \subseteq \frac{1}{m} \text{Scal}_\Gamma(R)$. The statement about the denominators now follows from the explicit expressions for $\text{Scal}_\Gamma(R)$ from Lemma 5.7, or by choosing α to be the denominator in the equations above. \square

Let us add that, more generally, one can show that

$$m_1 m_2 \text{Scal}_\Gamma(R) \subseteq \text{Scal}_{\Gamma'}(R) \subseteq \frac{1}{m_1 m_2} \text{Scal}_\Gamma(R)$$

whenever $m_1 \Gamma \subseteq \Gamma'$ and $m_2 \Gamma' \subseteq \Gamma$.

Let us conclude these general considerations with a remark on the dual lattice, defined as $\Gamma^* = \{x \in \mathbb{R}^d \mid \langle x|y \rangle \in \mathbb{Z} \text{ for all } y \in \Gamma\}$; compare [9, Sec. 3.1].

Lemma 5.13. *If Γ^* is the dual lattice of Γ , one has $\text{OS}(\Gamma) = \text{OS}(\Gamma^*)$ together with*

$$\text{Scal}_{\Gamma^*}(R) = \text{Scal}_\Gamma(R^{-1}).$$

In particular, $\text{den}_{\Gamma^}(R) = \text{den}_\Gamma(R^{-1})$.*

Proof. As $\text{OS}(\Gamma)$ is a group, $R \in \text{OS}(\Gamma)$ if and only if $R^{-1} \in \text{OS}(\Gamma)$. The latter holds if and only if there is an $\alpha \in \mathbb{R}_+$ such that $\alpha R^{-1} \Gamma \subseteq \Gamma$. By the definition of the dual lattice, this is equivalent to $\alpha \langle x|R^{-1}y \rangle \in \mathbb{Z}$ for all $x \in \Gamma^*$ and $y \in \Gamma$.

Now, $\alpha \langle Rx|y \rangle = \alpha \langle x|R^{-1}y \rangle$ shows that $\alpha R \Gamma^* \subseteq \Gamma^*$ holds if and only if $\alpha R^{-1} \Gamma \subseteq \Gamma$, which proves $\text{OS}(\Gamma) = \text{OS}(\Gamma^*)$. On the other hand, this equation shows that $\alpha \in \text{Scal}_{\Gamma^*}(R)$ if and only if $\alpha \in \text{Scal}_\Gamma(R^{-1})$, which completes the proof. \square

5.2. Two dimensions. Let us consider some concrete examples. We start in two dimensions, where we can make use of the field of complex numbers to characterise $\text{SOS}(\Gamma)$ completely. Here, any orientation-preserving similarity transformation can be represented by complex multiplication, and it turns out that the semigroup of similarity transformations then forms a ring, which we call the *multiplier ring*. The latter is denoted by $\text{MR}(\Gamma)$. Actually, there are only two cases. Either $\text{SOS}(\Gamma) = \{\pm 1\}$, or equivalently $\text{MR}(\Gamma) = \mathbb{Z}$, in which case we call Γ *generic*, or $\text{MR}(\Gamma) = \mathcal{O}$ is an order³ in an imaginary quadratic number field; compare [16] and [55, 22, 30] for general background.

For a more precise formulation, we employ the *similarity class* of a given lattice Γ , denoted by $\text{sim}(\Gamma)$, which consists of all lattices $\Gamma' \sim \Gamma$.

Theorem 5.14 ([16, Prop. 2.3 and Thm. 2.6]). *If $\Gamma \subset \mathbb{R}^2$ is a non-generic lattice, its multiplier ring $\text{MR}(\Gamma)$ is an order in an imaginary quadratic field. Explicitly, if $\Gamma \in \text{sim}(\langle 1, \tau \rangle_{\mathbb{Z}})$ with $\tau \in \mathbb{C} \setminus \mathbb{R}$ is a non-generic lattice, the number τ is algebraic of degree 2 over \mathbb{Q} , and one has*

$$\text{MR}(\Gamma) = \langle 1, s\tau \rangle_{\mathbb{Z}}$$

for some non-zero integer s .

Moreover, if K is the field of fractions of $\mathcal{O} := \text{MR}(\Gamma)$, one has $\text{MR}(\Gamma) = \mathcal{O} = \text{MR}(\mathcal{O})$. In particular,

$$\begin{aligned} \text{SOS}(\Gamma) &= \text{SOS}(\mathcal{O}) = \text{SOS}(\mathcal{O}_K) \\ &= \left\{ \frac{w}{|w|} \mid 0 \neq w \in \mathcal{O} \right\} = \left\{ \frac{w}{|w|} \mid 0 \neq w \in \mathcal{O}_K \right\}, \end{aligned}$$

where \mathcal{O}_K is the maximal order of K and thus contains \mathcal{O} . □

Note that the group $\text{SOS}(\Gamma)$ is the same for all lattices in $\text{sim}(\Gamma)$, which follows via Lemma 5.2 from the fact that the group $\text{SO}(2)$ is Abelian. Actually, it is the same for all lattices whose multiplier ring has the same field of fractions, although the corresponding multiplier rings usually differ.

Example 5.15. For the square lattice, which we write as $\mathbb{Z}^2 = \mathbb{Z}[i]$, we have $\text{MR}(\mathbb{Z}[i]) = \mathbb{Z}[i]$. This implies

$$\text{SOS}(\mathbb{Z}[i]) = \left\{ \frac{z}{|z|} \mid 0 \neq z \in \mathbb{Z}[i] \right\} \simeq C_8 \times \mathbb{Z}^{(\mathbb{N}_0)},$$

where $\mathbb{Z}^{(\mathbb{N}_0)}$ denotes the countably infinite sum of infinite cyclic groups (in contrast to the infinite product). Here, the group C_8 is generated by $\frac{1+i}{\sqrt{2}}$ and contains all units of $\mathbb{Z}[i]$, whereas a full set of generators of $\mathbb{Z}^{(\mathbb{N}_0)}$ is the set $\left\{ \frac{\pi_p}{\sqrt{p}} \mid p \equiv 1 \pmod{4} \right\}$, where π_p is a Gaussian

³Note that the symbol \mathcal{O} occurs with two different meanings in this chapter, namely for asymptotic estimates and for orders (in the algebraic sense introduced earlier). Since the meaning will always be clear from the context, we stick to this widely used notation.

TABLE 2. Norm forms for the nine maximal orders \mathcal{O}_K of class number 1 in imaginary quadratic number fields, labelled with the field discriminant d_K ; see Lemma 5.16 and Remark 5.17 for details.

d_K	norm form	d_K	norm form	d_K	norm form
-3	$x^2 + xy + y^2$	-8	$x^2 + 2y^2$	-43	$x^2 + xy + 11y^2$
-4	$x^2 + y^2$	-11	$x^2 + xy + 3y^2$	-67	$x^2 + xy + 17y^2$
-7	$x^2 + xy + 2y^2$	-19	$x^2 + xy + 5y^2$	-163	$x^2 + xy + 41y^2$

prime such that $\pi_p \overline{\pi_p} = p$. Note that for any p only one prime of the pair $\pi_p, \overline{\pi_p}$ is needed, as we have $(\frac{\pi_p}{\sqrt{p}})^{-1} = \frac{\overline{\pi_p}}{\sqrt{p}}$. \diamond

The situation is particularly nice if the multiplier ring is a PID. In this case, all ideals are similar sublattices and the situation is completely analogous to that of the square lattice example in Section 3, so we can write down the generating function explicitly. This happens for a finite number of cases only; compare Table 2.

Lemma 5.16 ([30, Thm. 7.30]). *There are precisely nine imaginary quadratic fields with class number 1, meaning their maximal orders being PIDs. These are the fields $K = \mathbb{Q}(\omega_0)$ for*

$$\omega_0 \in \left\{ \frac{1+i\sqrt{3}}{2}, i, \frac{1+i\sqrt{7}}{2}, i\sqrt{2}, \frac{1+i\sqrt{11}}{2}, \frac{1+i\sqrt{19}}{2}, \frac{1+i\sqrt{43}}{2}, \frac{1+i\sqrt{67}}{2}, \frac{1+i\sqrt{163}}{2} \right\},$$

which are fields of discriminant

$$d_K \in \{-3, -4, -7, -8, -11, -19, -43, -67, -163\}.$$

Here, the maximal order of K is $\mathcal{O}_K = \mathbb{Z}[\omega_0]$, while one has $\mathbb{Q}(\omega_0) = \mathbb{Q}(\sqrt{d_K})$. \square

Remark 5.17. In the nine cases of Lemma 5.16, the possible indices of the similar sublattices of \mathcal{O}_K are precisely those positive integers that can be represented by the corresponding norm forms listed in Table 2. As a consequence, the Dirichlet series generating function for the number of SSLs of a given index is the zeta function of \mathcal{O}_K , which is the Dedekind zeta function ζ_K of the quadratic field K . \diamond

Let us recall some properties of the Dedekind zeta function ζ_K . The latter is known [91] to factorise as

$$(5.7) \quad \zeta_K(s) = \zeta(s) L(s, \chi),$$

where $L(s, \chi)$ is the L -series of the non-trivial character $\chi = \chi_{d_K}$ of the quadratic field K . The latter is a totally multiplicative arithmetic function and thus given by $\chi_{d_K}(1) = 1$ together

with its values at the rational primes (that is, primes in $\mathbb{Z} \subset \mathbb{Q}$),

$$\chi_{d_K}(p) = \begin{cases} 0, & p \mid d_K, \\ \left(\frac{d_K}{p}\right), & 2 \neq p \nmid d_K, \\ \left(\frac{d_K}{2}\right), & p = 2 \nmid d_K. \end{cases}$$

Here, $\left(\frac{m}{p}\right)$ and $\left(\frac{m}{2}\right)$ denote the Legendre and the Kronecker symbol, respectively, the latter defined as

$$\left(\frac{m}{2}\right) = \begin{cases} 1, & m \equiv \pm 1 \pmod{8}, \\ -1, & m \equiv \pm 3 \pmod{8}, \\ 0, & m \equiv 0 \pmod{2}. \end{cases}$$

This permits a direct calculation of the zeta function via its Euler product, as the character $\chi(p)$ takes only the values 0, -1 , or 1, depending on whether the rational prime p ramifies, is inert, or splits in the extension from \mathbb{Q} to K . The general formula reads

$$\begin{aligned} \zeta_K(s) &= \prod_{p \in \mathbb{P}} \frac{1}{(1 - p^{-s})(1 - \chi(p)p^{-s})} \\ (5.8) \quad &= \prod_{\substack{p \in \mathbb{P} \\ \chi(p)=0}} \frac{1}{1 - p^{-s}} \prod_{\substack{p \in \mathbb{P} \\ \chi(p)=-1}} \frac{1}{1 - p^{-2s}} \prod_{\substack{p \in \mathbb{P} \\ \chi(p)=1}} \frac{1}{(1 - p^{-s})^2}, \end{aligned}$$

where \mathbb{P} denotes the set of rational primes.

The result on the generating functions now reads as follows.

Theorem 5.18 ([16, Prop. 5.2]). *Let K be any of the nine imaginary quadratic number fields of Lemma 5.16, with p_{ram} its ramified prime, which is the unique rational prime that divides d_K . The Dirichlet series generating function for the number of SSLs of \mathcal{O}_K of a given index is $D_{\mathcal{O}_K}(s) = \zeta_K(s)$ with the Dedekind zeta function of K according to Eq. (5.8).*

Moreover, the generating function for the primitive SSLs of \mathcal{O}_K is

$$D_{\mathcal{O}_K}^{\text{pr}}(s) = \frac{D_{\mathcal{O}_K}(s)}{\zeta(2s)} = (1 + p_{\text{ram}}^{-s}) \prod_{p \text{ splits}} \frac{1 + p^{-s}}{1 - p^{-s}},$$

where the product runs over all rational primes p that split in the extension to K . The same generating function also applies to any other planar lattice $\Gamma \in \text{sim}(\mathcal{O}_K)$. \square

In addition to the PIDs mentioned above, there are four additional (non-maximal) orders with class number 1, which we have summarised in Table 3. Their ideals are closely related to the ideals of their corresponding maximal orders. As a consequence, the generating functions $D_{\mathcal{O}}(s)$ and $D_{\mathcal{O}}^{\text{pr}}(s)$ possess an Euler product. Their Euler factors are the same as those of the corresponding maximal order, except for the Euler factors corresponding to the primes that divide the conductor $f := [\mathcal{O}_K : \mathcal{O}]$. These special Euler factors can be calculated explicitly.

TABLE 3. Basic data for the four non-maximal orders of class number 1 in imaginary quadratic number fields, labelled with their discriminant D ; see Theorem 5.19 for details.

D	K	\mathcal{O}	norm form	$p D$	conductor
-12	$\mathbb{Q}(i\sqrt{3})$	$\mathbb{Z}[i\sqrt{3}]$	$x^2 + 3y^2$	2, 3	2
-16	$\mathbb{Q}(i)$	$\mathbb{Z}[2i]$	$x^2 + 4y^2$	2	2
-27	$\mathbb{Q}(i\sqrt{3})$	$\mathbb{Z}[\frac{1}{2}(1 + i3\sqrt{3})]$	$x^2 + xy + 7y^2$	3	3
-28	$\mathbb{Q}(i\sqrt{7})$	$\mathbb{Z}[i\sqrt{7}]$	$x^2 + 7y^2$	2, 7	2

Theorem 5.19 ([16, Sec. 5.2]). *Let \mathcal{O} be one of the four non-maximal orders of class number 1 in imaginary quadratic number fields as given in Table 3. The sublattice counting functions are multiplicative, which implies that their generating functions $D_{\mathcal{O}}(s)$ and $D_{\mathcal{O}}^{\text{pr}}(s)$ have an Euler product expansion. In particular,*

$$\begin{aligned}
 D_{\mathbb{Z}[i\sqrt{3}]}^{\text{pr}}(s) &= \left(1 + \frac{2}{4^s}\right) \left(1 + \frac{1}{3^s}\right) \prod_{p \equiv 1(3)} \frac{1 + p^{-s}}{1 - p^{-s}}, \\
 D_{\mathbb{Z}[2i]}^{\text{pr}}(s) &= \left(1 + \frac{1}{4^s} + \frac{2}{8^s}\right) \prod_{p \equiv 1(4)} \frac{1 + p^{-s}}{1 - p^{-s}}, \\
 D_{\mathbb{Z}[\frac{1}{2}(1+i3\sqrt{3})]}^{\text{pr}}(s) &= \left(1 + \frac{2}{9^s} + \frac{3}{27^s}\right) \prod_{p \equiv 1(3)} \frac{1 + p^{-s}}{1 - p^{-s}}, \\
 D_{\mathbb{Z}[i\sqrt{7}]}^{\text{pr}}(s) &= \left(1 - \frac{2}{2^s} + \frac{2}{4^s}\right) \left(1 + \frac{1}{7^s}\right) \prod_{p \equiv 1,2,4(7)} \frac{1 + p^{-s}}{1 - p^{-s}}.
 \end{aligned}$$

Again, the possible indices of the SSLs are precisely those positive integers that can be represented by the corresponding norm forms, which we have listed in Table 3. \square

The situation is more involved for class numbers greater than 1, where the existence of non-principal ideals complicates the treatment. In general, the counting functions are no longer multiplicative, because a product of non-principal ideals may be principal. As a consequence, not much is known in these cases. However, there is still one situation that allows further treatment, namely when the discriminant D is one of Euler's *convenient numbers*, in which case the ideal class group is an Abelian 2-group. The latter implies that we have a natural binary grading on the ideals, depending on whether they are principal or not. If the order under investigation is still principal, one can derive the generating function from the zeta function; compare [16].

Example 5.20. Let us consider $\mathcal{O} = \mathbb{Z}[i\sqrt{6}]$, where

$$D_{\mathbb{Z}[i\sqrt{6}]}^{\text{pr}}(s) = \prod_{p \equiv 1,7 \pmod{24}} \frac{1+p^{-s}}{1-p^{-s}} \sum_{m=1}^{\infty} \frac{b(m)}{m^s}$$

with $b(1) = 1$ and $b(m) = 0$ if $p|m$ for some $p \equiv 1, 7, 13, 17, 19, 23 \pmod{24}$. If m is an integer of the form $m = 2^\alpha 3^\beta \prod_{p \equiv 5,11 \pmod{24}} p^{\ell_p}$ with $\alpha, \beta \in \{0, 1\}$ and $\ell_p \in \mathbb{N}_0$, with only finitely many of them $\neq 0$, we have

$$b(m) = (1 + (-1)^{\alpha+\beta+\sum \ell_p})^{\text{card}\{p>3 | \ell_p \neq 0\}}.$$

Obviously, $D_{\mathbb{Z}[i\sqrt{6}]}^{\text{pr}}(s)$ possesses no Euler product representation. \diamond

Example 5.21. As further cases, let us mention the generating functions for the primitive SSLs of $\mathcal{O} = \mathbb{Z}[3i]$,

$$(5.9) \quad D_{\mathbb{Z}[3i]}^{\text{pr}}(s) = \sum_{\substack{m \geq 1 \\ m \equiv 1 \pmod{3}}} (1+9^s) \frac{a_{\square}^{\text{pr}}(m)}{(9m)^s} + \sum_{\substack{m \geq 1 \\ m \equiv 2 \pmod{3}}} \frac{2a_{\square}^{\text{pr}}(m)}{(9m)^s},$$

and of $\mathcal{O} = \mathbb{Z}[5i]$,

$$(5.10) \quad D_{\mathbb{Z}[5i]}^{\text{pr}}(s) = \sum_{\substack{m \geq 1 \\ m \equiv \pm 1 \pmod{5}}} (1+25^s) \frac{a_{\square}^{\text{pr}}(m)}{(25m)^s} + \sum_{\substack{m \geq 1 \\ m \equiv 0, \pm 2 \pmod{5}}} \frac{2a_{\square}^{\text{pr}}(m)}{(25m)^s},$$

where $a_{\square}^{\text{pr}}(m)$ is the number of primitive SSLs of index m of the square lattice; compare Section 3. \diamond

Let us stay in two dimensions a little longer and discuss some \mathbb{Z} -modules with N -fold rotational symmetry. As this works the same way as for lattices, we include their discussion here, but see Section 6 for the general theory behind it. In particular, we consider the ring $\mathbb{Z}[\xi_n]$ of cyclotomic integers, where ξ_n is a primitive n th root of unity. If

$$(5.11) \quad n \in \{3, 4, 5, 7, 8, 9, 11, 12, 13, 15, 16, 17, 19, 20, 21, 24, \\ 25, 27, 28, 32, 33, 35, 36, 40, 44, 45, 48, 60, 84\},$$

the ring $\mathbb{Z}[\xi_n]$ is a PID, which means that the similar submodules are precisely the ideals of $\mathbb{Z}[\xi_n]$; compare [89, 7, 9]. Using the terminology from above, this implies that $\mathbb{Z}[\xi_n]$ is its own multiplier ring. Note that $n = 3$ and $n = 4$ correspond to the hexagonal and the square lattice, respectively; compare [9, Ex. 2.15]. More generally, $\mathbb{Z}[\xi_n]$ is a \mathbb{Z} -module of rank $d = \phi(n)$, which is larger than 2 in the remaining cases; see [9, Rem. 3.7 and Ex. 2.16]. Here, ϕ denotes Euler's totient function. In particular, $\mathbb{Z}[\xi_n]$ has N -fold rotational symmetry, with $N = \text{lcm}(n, 2)$.

As mentioned above, the similar submodules are precisely the non-trivial ideals of $\mathbb{Z}[\xi_n]$, which means that the generating function for the similar submodules of $\mathbb{Z}[\xi_n]$ is given by [7]

$$(5.12) \quad \Phi_{\mathbb{Z}[\xi_n]}(s) = \zeta_{\mathbb{Q}(\xi_n)}(s) := \sum_{\mathfrak{a}} \frac{1}{\text{norm}(\mathfrak{a})^s},$$

where the sum runs over all non-trivial ideals \mathfrak{a} of $\mathbb{Z}[\xi_n]$ and

$$\text{norm}(\mathfrak{a}) := [\mathbb{Z}[\xi_n] : \mathfrak{a}]$$

denotes the norm of \mathfrak{a} . As $\mathbb{Z}[\xi_n]$ is a PID for all n from Eq. (5.11), the counting function for the ideals of fixed index is multiplicative. This, in turn, means that $\Phi_{\mathbb{Z}[\xi_n]}(s)$ has an Euler product expansion [7]

$$(5.13) \quad \Phi_{\mathbb{Z}[\xi_n]}(s) = \prod_{p \in \mathbb{P}} E_n(p^{-s}).$$

The Euler factors $E_n(p^{-s})$ are of the form

$$(5.14) \quad E_n(p^{-s}) = \frac{1}{(1 - p^{-\ell s})^m} = \sum_{j=1}^{\infty} \binom{j+m-1}{m-1} \frac{1}{(p^s)^{\ell j}}$$

where m and ℓ are certain integers that depend on p and n . If p is coprime to n , then ℓ is the residue class degree of p , which is the smallest integer ℓ such that $p^\ell \equiv 1 \pmod{n}$, compare [89, Thm. 2.13] and [7]. The integer m is determined by $m\ell = \phi(n)$. If p divides n (p is a ramified prime in this case), we write $n = rp^t$, where p^t is the maximal power dividing n , so that r is the p -free part of n . The integers ℓ and m are now calculated by replacing n by r in the equations above, where ℓ is the smallest integer such that $p^\ell \equiv 1 \pmod{r}$ and $m\ell = \phi(r)$; compare the remarks after [89, Thm. 2.13] as well as [7]. Explicit values for m and ℓ , for all cases of Eq. (5.11), can be found in [7, Tables 1 and 2].

Example 5.22. Let us take a closer look at $\mathbb{Z}[\xi_5] = \mathbb{Z}[\xi_{10}]$. The only ramified prime is $5 = \varepsilon(1 - \xi_5)^4$, where $\varepsilon = -\xi_5^2/\tau^2$ is a unit in $\mathbb{Z}[\xi_5]$. In terms of ideals, this means $(5) = (1 - \xi_5)^4$. This gives $\ell = m = 1$ for $p = 5$. In addition, we get $\ell = 1$, $m = 4$ for $p \equiv 1 \pmod{5}$, $\ell = 2$, $m = 2$ for $p \equiv -1 \pmod{5}$, and $\ell = 4$, $m = 1$ for $p \equiv \pm 2 \pmod{5}$. Thus, we obtain the generating function

$$\begin{aligned} \Phi_{\mathbb{Z}[\xi_5]}(s) &= \frac{1}{1 - 5^s} \prod_{p \equiv 1(5)} \frac{1}{(1 - p^s)^4} \prod_{p \equiv -1(5)} \frac{1}{(1 - p^{2s})^2} \prod_{p \equiv \pm 2(5)} \frac{1}{1 - p^{4s}} \\ &= 1 + \frac{1}{5^s} + \frac{4}{11^s} + \frac{1}{16^s} + \frac{1}{25^s} + \frac{4}{31^s} + \frac{4}{41^s} + \frac{4}{55^s} + \frac{4}{61^s} \\ &\quad + \frac{4}{71^s} + \frac{1}{80^s} + \frac{1}{81^s} + \frac{4}{101^s} + \frac{10}{121^s} + \frac{1}{125^s} + \frac{4}{131^s} + \dots \end{aligned}$$

for this case. ◇

5.3. Higher dimensions. Let us continue with lattices in higher dimensions. We concentrate on *rational* lattices⁴ here, that is, on lattices Γ for which the inner products satisfy $\langle x|y \rangle \in \mathbb{Q}$ for all $x, y \in \Gamma$. For all scaling factors $\alpha \in \text{Scal}_\Gamma(R)$, one then has $\alpha^2 \in \mathbb{Q}$. By an application of Lemma 5.5, we may conclude that $\alpha^2 \in \mathbb{Z}$. Moreover, one obtains the stronger condition $\alpha \in \mathbb{Z}$ in odd dimensions, again by Lemma 5.5. This gives the following result.

Fact 5.23. *For a rational lattice $\Gamma \subset \mathbb{R}^d$ with d odd, the possible indices of SSLs are exactly the integers of the form n^d with $n \in \mathbb{N}$.* \square

Thus, the question for the possible indices is answered in this case, and we may proceed with lattices in even dimension, say $d = 2k$. As $\alpha^2 \in \mathbb{Z}$, the possible indices of SSLs are all of the form c^k with $c \in \mathbb{N}$. For an important class of $2k$ -dimensional lattices, an answer was given by Conway, Rains and Sloane in [26]. Let \mathbb{Z}_p denote the p -adic integers [9, Ex. 2.10] and define the Hilbert symbol $(a, b)_p$ as

$$(a, b)_p = \begin{cases} 1, & \text{if } z^2 = ax^2 + by^2 \text{ has a non-zero solution in } \mathbb{Z}_p, \\ -1, & \text{otherwise.} \end{cases}$$

Their result can now be formulated as follows.⁵

Theorem 5.24 ([26, Thm. 1]). *Let $\Gamma \subset \mathbb{R}^{2k}$ be a rational lattice. An SSL of index c^k can only exist if the condition*

$$\left(c, (-1)^k \det(\Gamma) \right)_p = 1$$

is satisfied for all primes p that divide $2c \det(\Gamma)$. If Γ is unigeneric and (r) -maximal for some $r \in \mathbb{Q}$, then this condition is also sufficient. \square

Here, (r) -maximal means that Γ is maximal with respect to the property that $\langle x|x \rangle \in r\mathbb{Z}$ for all $x \in \Gamma$. It is *unigeneric* if it is unique in its genus. Recall that the genus of a rational quadratic form is the set of quadratic forms that are \mathbb{R} -equivalent and \mathbb{Z}_p -equivalent for any prime p ; compare [25]. In other words, a rational quadratic form Q is unigeneric if and only if any other quadratic form Q' that is \mathbb{Z}_p -equivalent to Q for any prime p as well as \mathbb{R} -equivalent to Q then also is \mathbb{Z} -equivalent to Q . The correspondence between lattices and quadratic forms then transfers these notions to lattices.

Example 5.25. Theorem 5.24 can now be applied to several lattices [26], which are all unigeneric and (1)- or (2)-maximal.

⁴More generally, one calls a lattice Γ rational if there exists an $\alpha > 0$ such that $\langle x|y \rangle \in \mathbb{Q}$ for all $x, y \in \alpha\Gamma$. In this section, we only use the more restrictive definition.

⁵The authors formulate their results on sublattices in terms of the norm $c = \alpha^2$ of a similarity $\sigma = \alpha R$. We prefer to employ the index $n = [\Gamma : \alpha R\Gamma] = \alpha^d = c^{d/2}$ instead. The use of the norm c is natural for rational lattices, as it is always an integer in these cases. However, it is less meaningful for general lattices, where the natural quantity is the index n . To keep our notation consistent, we stick to the formulation in terms of the index here, which explains the additional exponent $\frac{d}{2}$ in our formulation.

- (1) The root lattice A_4 has SSLs of index c^2 for $c = \text{nr}(z) = zz'$ only, where $z \in \mathbb{Z}[\tau]$ with $\tau = (1 + \sqrt{5})/2$ and z' is the algebraic conjugate of z . Consequently, rational primes $p \equiv \pm 2 \pmod{5}$ appear to even powers in c .
- (2) The hypercubic lattice \mathbb{Z}^6 has SSLs of index c^3 for $c = \text{nr}(z) = |z|^2$ only, where $z \in \mathbb{Z}[i]$. Here, rational primes $p \equiv 3 \pmod{4}$ appear to even powers in c .
- (3) The exceptional root lattice E_6 has SSLs of index c^3 for $c = \text{nr}(z) = |z|^2$ only, where $z \in \mathbb{Z}[(1 + i\sqrt{3})/2]$. Rational primes $p \equiv 2 \pmod{3}$ appear to even powers in c . \diamond

Further details for the root lattice A_4 will be discussed below. Another interesting consequence of Theorem 5.24 is the following result, where the notation for the lattices is taken from [27, Ch. 4].

Corollary 5.26 ([26, Thm. 3]). *The lattices \mathbb{Z}^{4m} , D_{4m} and D_{4m}^+ possess SSLs of index c^{2m} for all $c \in \mathbb{N}$. Similarly, the lattices E_8 , K_{12} , the Barnes–Wall lattice BW_{16} and the Leech lattice Λ_{24} possess SSLs of index c^4 , c^6 , c^8 and c^{12} , respectively, for all $c \in \mathbb{N}$. \square*

5.4. The root lattice A_4 . For the lattice A_4 , we can go further and count the SSLs of a given index explicitly. Usually, A_4 is embedded in \mathbb{R}^5 as a lattice plane, but this is inconvenient for our purposes and we prefer to look at it in \mathbb{R}^4 , since we want to exploit a useful parametrisation by quaternions.

Consider the lattice $L \subset \mathbb{R}^4$ that is spanned by the four vectors

$$(5.15) \quad (1, 0, 0, 0), \frac{1}{2}(-1, 1, 1, 1), (0, -1, 0, 0), \frac{1}{2}(0, 1, \tau - 1, -\tau),$$

with $\tau = (1 + \sqrt{5})/2$ as before. Then, L is similar to A_4 , with the scale reduced by a factor $\sqrt{2}$; compare [9, Ex. 3.3] or [12]. This way, we have $L \subset \mathbb{I}$, where \mathbb{I} denotes the icosian ring; see [9, Ex. 2.19] and references therein.

Let us begin by recalling some properties of L . Both L and \mathbb{I} are invariant under quaternionic conjugation, so $L = \overline{L}$ and $\mathbb{I} = \overline{\mathbb{I}}$, but neither of them is invariant under algebraic conjugation $\tau \mapsto \tau'$. Combining the algebraic conjugation with a permutation of the last two (quaternionic) components yields another involution, $x \mapsto \tilde{x} := (x'_0, x'_1, x'_3, x'_2)$, which is an involution of the second kind in the terminology of [60] and was called the *twist map* in [12, 11]. Note that $L = \tilde{L}$ is invariant under the twist map, which, in addition, is an anti-automorphism of \mathbb{I} . In other words, the twist map has the following properties.

Fact 5.27 ([12, Lemma 1]). *For any $x, y \in \mathbb{I}$ and $\alpha \in \mathbb{Q}(\tau)$, one has*

- (1) $\widetilde{x + y} = \tilde{x} + \tilde{y}$ and $\widetilde{\alpha x} = \alpha' \tilde{x}$;
- (2) $\widetilde{xy} = \tilde{y} \tilde{x}$ and $\tilde{\tilde{x}} = x$;
- (3) $\widetilde{\tilde{x}} = \overline{\tilde{x}}$ and, for $x \neq 0$, $(\tilde{x})^{-1} = \widetilde{x^{-1}}$. \square

The twist map is the key to our analysis as it gives us a convenient parametrisation of the similarity rotations—and later also the coincidence rotations. Furthermore, it provides us

with the following characterisation [12, Prop. 1] of the lattice L as a subset of \mathbb{I} ,

$$(5.16) \quad L = \{x \in \mathbb{I} \mid x = \tilde{x}\}.$$

By Cayley's parametrisation (4.2), we know that any rotation in \mathbb{R}^4 can be written as $R(p, q)x = \frac{1}{|pq|}px\bar{q}$. Using the properties of the twist map and the characterisation of L from above, we immediately see that $qL\tilde{q} \subseteq L$ is a similar sublattice of L for any $q \in \mathbb{I}$. In fact, any SSL of L is of the form $\alpha qL\tilde{q} \subseteq L$, with $q \in \mathbb{I}$ and $\alpha \in \mathbb{Q}(\tau)$; see [12, Cor. 1].

In order to classify the SSLs, it is convenient to introduce a suitable primitivity notion on \mathbb{I} . A quaternion $q \in \mathbb{I}$ is called \mathbb{I} -*primitive* (or primitive for short) if $\alpha q \in \mathbb{I}$ with $\alpha \in \mathbb{Q}(\tau)$ implies $\alpha \in \mathbb{Z}[\tau]$. Equivalently, $q \in \mathbb{I}$ is \mathbb{I} -primitive if the \mathbb{I} -content of q ,

$$\text{cont}_{\mathbb{I}}(q) := \text{lcm}\{\alpha \in \mathbb{Z}[\tau] \setminus \{0\} \mid q \in \alpha\mathbb{I}\},$$

is a unit in $\mathbb{Z}[\tau]$. Note that the notion of an lcm makes sense because $\mathbb{Z}[\tau]$ is a Euclidean domain. Of course, $\text{cont}_{\mathbb{I}}(q)$ is defined only up to a unit in $\mathbb{Z}[\tau]$. We can now fully characterise the SSLs as follows.

Lemma 5.28 ([12, Cor. 2]). *The primitive SSLs of L are precisely the sublattices of the form $qL\tilde{q}$, where $q \in \mathbb{I}$ is \mathbb{I} -primitive. Consequently, the SSLs of L are precisely the sublattices of the form $nqL\tilde{q}$ with $n \in \mathbb{N}$ and $q \in \mathbb{I}$ primitive. \square*

As we also want to determine the number of distinct SSLs of a given index, we need to ensure that we do not count the same SSL twice. In general, different quaternions may generate the same SSL, so we need a criterion to determine whether two SSLs $qL\tilde{q}$ and $pL\tilde{p}$ are equal. One first observes that $L = qL\tilde{q}$ holds for an \mathbb{I} -primitive quaternion q if and only if $q \in \mathbb{I}^\times$, where \mathbb{I}^\times is the unit group in \mathbb{I} ; see [9, Ex. 2.19] for an explicit description and [70, 71] for further background. From here, one can infer the following result.

Fact 5.29 ([12, Lemma 5]). *For \mathbb{I} -primitive quaternions $p, q \in \mathbb{I}$, one has $pL\tilde{p} = qL\tilde{q}$ if and only if $p\mathbb{I} = q\mathbb{I}$. \square*

This fact reduces the problem of counting SSLs of L to the problem of counting primitive right ideals of \mathbb{I} . Here, we call a right ideal $q\mathbb{I}$ primitive if q is \mathbb{I} -primitive.

The index of a primitive SSL can be determined by an explicit calculation. We mention that $|\tilde{q}|^2 = (|q|^2)'$ holds for any $q \in \mathbb{I}$. Recall from [9, Ex. 2.14] that the *norm* of an element $\alpha \in \mathbb{Q}(\tau)$ is defined as

$$\text{nr}(\alpha) = \alpha\alpha'.$$

The index of a primitive SSL $qL\tilde{q}$ then satisfies $[L : qL\tilde{q}] = \text{nr}(|q|^4)$. As $q\mathbb{I}$ has index $\text{nr}(|q|^4)$ in \mathbb{I} as well, we get the following result.

Lemma 5.30 ([12, Prop. 4]). *There is a bijective correspondence between the primitive right ideals of \mathbb{I} and the primitive SSLs of L , given by $q\mathbb{I} \leftrightarrow qL\tilde{q}$. Moreover, one has*

$$[\mathbb{I} : q\mathbb{I}] = \text{nr}(|q|^4) = [L : qL\tilde{q}],$$

which means that the bijection preserves the index. \square

As a consequence, all possible indices are squares of integers of the form $k^2 + k\ell - \ell^2 = \text{nr}(k + \ell\tau)$. In fact, all these indices are realised [12, 26]. As the number of right ideals of \mathbb{I} of a given index is well known, we can deduce the numbers $b_{A_4}(m)$ and $b_{A_4}^{\text{pr}}(m)$ of SSLs and primitive SSLs of index m , respectively. This can efficiently be done by employing the corresponding Dirichlet series generating functions. To do so, we first recall the Dirichlet character

$$\chi_5(n) = \begin{cases} 0, & \text{if } n \equiv 0 \pmod{5}, \\ 1, & \text{if } n \equiv \pm 1 \pmod{5}, \\ -1, & \text{if } n \equiv \pm 2 \pmod{5}. \end{cases}$$

Its corresponding L -series, $L(s, \chi_5) = \sum_{n=1}^{\infty} \chi_5(n)n^{-s}$, defines (via analytic continuation) an entire function on the complex plane. The Dedekind zeta function of $K = \mathbb{Q}(\tau)$ is given by $\zeta_K(s) = \zeta(s)L(s, \chi_5)$, which is a meromorphic function. Likewise, the zeta function $\zeta_{\mathbb{I}}$ of the icosian ring [87, 14], which counts the right (or left) ideals of \mathbb{I} , is meromorphic in the entire complex plane and reads

$$(5.17) \quad \zeta_{\mathbb{I}}(s) = \zeta_K(2s)\zeta_K(2s-1).$$

As the Dirichlet series of the two-sided ideals is given by $\zeta_K(4s)$, one obtains the zeta function $\zeta_{\mathbb{I}}^{\text{pr}}$ of the primitive ideals [14] as

$$(5.18) \quad \zeta_{\mathbb{I}}^{\text{pr}}(s) = \frac{\zeta_K(2s)\zeta_K(2s-1)}{\zeta_K(4s)}.$$

This leads to the following result.

Theorem 5.31 ([12, Thm. 1]). *The Dirichlet series generating functions for the numbers $b_{A_4}(n)$ and $b_{A_4}^{\text{pr}}(n)$ of SSLs and primitive SSLs of the root lattice A_4 of a given index are*

$$\Phi_{A_4}(s) = \sum_{n \in \mathbb{N}} \frac{b_{A_4}(n)}{n^s} = \zeta(4s) \frac{\zeta_{\mathbb{I}}(s)}{\zeta_K(4s)} = \frac{\zeta_K(2s)\zeta_K(2s-1)}{L(4s, \chi_5)}$$

and

$$\Phi_{A_4}^{\text{pr}}(s) = \sum_{n \in \mathbb{N}} \frac{b_{A_4}^{\text{pr}}(n)}{n^s} = \zeta_{\mathbb{I}}^{\text{pr}}(s) = \frac{\zeta_K(2s)\zeta_K(2s-1)}{\zeta_K(4s)}. \quad \square$$

Both generating functions from Theorem 5.31 possess Euler products, which read

$$(5.19) \quad \begin{aligned} \Phi_{A_4}(s) &= \frac{1}{(1-5^{-2s})(1-5^{1-2s})} \prod_{p \equiv \pm 1(5)} \frac{1+p^{-2s}}{(1-p^{-2s})(1-p^{1-2s})^2} \\ &\times \prod_{p \equiv \pm 2(5)} \frac{1+p^{-4s}}{(1-p^{-4s})(1-p^{2-4s})} \end{aligned}$$

and

$$(5.20) \quad \Phi_{A_4}^{\text{pr}}(s) = \frac{1 + 5^{-2s}}{1 - 5^{1-2s}} \prod_{p \equiv \pm 1(5)} \frac{(1 + p^{-2s})^2}{(1 - p^{1-2s})^2} \prod_{p \equiv \pm 2(5)} \frac{1 + p^{-4s}}{1 - p^{2-4s}}.$$

From these identities, we can obtain explicit expressions for $b_{A_4}(n)$ and $b_{A_4}^{\text{pr}}(n)$, which are multiplicative arithmetic functions. Thus, they are determined by their values at prime powers. As $b_{A_4}(p^{2r+1}) = b_{A_4}^{\text{pr}}(p^{2r+1}) = 0$, we only need to state their values for primes at even powers ≥ 2 . The result is [12]

$$b_{A_4}(p^{2r}) = \begin{cases} \frac{5^{r+1}-1}{4}, & \text{if } p = 5, \\ \frac{(r+1)(p^2-1)p^{r-2}(p^{r+1}-1)}{(p-1)^2}, & \text{if } p \equiv \pm 1(5), \\ \frac{p^{r+2}+p^r-2}{p^2-1}, & \text{if } p \equiv \pm 2(5) \text{ and } r \text{ even,} \\ 0, & \text{if } p \equiv \pm 2(5) \text{ and } r \text{ odd,} \end{cases}$$

and

$$b_{A_4}^{\text{pr}}(p^{2r}) = \begin{cases} 6 \cdot 5^{r-1}, & \text{if } p = 5, \\ (r+1)p^r + 2rp^{r-1} + (r-1)p^{r-2}, & \text{if } p \equiv \pm 1(5), \\ p^r + p^{r-2}, & \text{if } p \equiv \pm 2(5) \text{ and } r \text{ even,} \\ 0, & \text{if } p \equiv \pm 2(5) \text{ and } r \text{ odd.} \end{cases}$$

It follows from these formulas that all possible indices are not only realised for some SSL, but even realised for some *primitive* SSL. In fact, it will turn out that the majority of SSLs of a given index are primitive. This can be illustrated by comparing the first few terms of Φ_{A_4} and $\Phi_{A_4}^{\text{pr}}$,

$$\begin{aligned} \Phi_{A_4}(s) &= 1 + \frac{6}{4^{2s}} + \frac{6}{5^{2s}} + \frac{11}{9^{2s}} + \frac{24}{11^{2s}} + \frac{26}{16^{2s}} + \frac{40}{19^{2s}} + \frac{36}{20^{2s}} + \frac{31}{25^{2s}} + \cdots, \\ \Phi_{A_4}^{\text{pr}}(s) &= 1 + \frac{5}{4^{2s}} + \frac{6}{5^{2s}} + \frac{10}{9^{2s}} + \frac{24}{11^{2s}} + \frac{20}{16^{2s}} + \frac{40}{19^{2s}} + \frac{30}{20^{2s}} + \frac{30}{25^{2s}} + \cdots. \end{aligned}$$

The explicit form of the generating functions $\Phi_{A_4}(s)$ and $\Phi_{A_4}^{\text{pr}}$ allows us to calculate the asymptotic behaviour of $b_{A_4}(n)$ and $b_{A_4}^{\text{pr}}(n)$. The result reads as follows.

Corollary 5.32 ([12, Sec. 4]). *The asymptotic growth of the summatory function of $b_{A_4}(n)$ is*

$$\sum_{m \leq x} b_{A_4}(m) \sim \frac{\rho}{2}x, \quad \text{as } x \rightarrow \infty,$$

where ρ is given by

$$\rho = \frac{\zeta_K(2)L(1, \chi_5)}{L(4, \chi_5)} = \frac{1}{2}\sqrt{5} \log(\tau) \approx 0.538011.$$

The asymptotic growth for $b_{A_4}^{\text{pr}}(n)$ is also linear, now with

$$\rho^{\text{pr}} = \frac{\zeta_K(2)L(1, \chi_5)}{\zeta(4)L(4, \chi_5)} = \frac{45}{\pi^4} \sqrt{5} \log(\tau) \approx 0.497089. \quad \square$$

Sketch of proof. We apply again Theorem 4.1, this time to the generating functions given in Theorem 5.31. The fact that both Dirichlet series are meromorphic functions, which are analytic in the half-plane $\{\text{Re}(s) > 1\}$ and have the proper behaviour on the line $\{\text{Re}(s) = 1\}$, implies the linear growth. The explicit calculations for the sum $\sum_{m \leq x} b_{A_4}(m)$ are similar⁶ to those from [12, Sec. 4, p. 1402]. The case of the primitive SSLs is analogous, and just gives an additional factor $\frac{1}{\zeta(4)}$. \square

5.5. Hypercubic lattices in \mathbb{R}^4 . There are, up to similarity, two hypercubic lattices in 4 dimensions, namely the primitive hypercubic lattice \mathbb{Z}^4 and the centred hypercubic lattice D_4 ; compare [27] and [9, Ex. 3.2]. The latter is similar to its dual lattice D_4^* , which we identify with the Hurwitz ring \mathbb{J} .

Recall that any rotation in 4 dimensions can be parametrised by a pair of quaternions; compare Section 4.1. It turns out that any similarity rotation of $\Gamma \in \{D_4^*, \mathbb{Z}^4\}$ can be parametrised by a pair (p, q) of Hurwitz quaternions. Moreover, any SSL of Γ is of the form $p\Gamma\bar{q}$, where we can choose p to be odd and primitive; compare [14, Rem. 1 and Lemma 2]. With this convention, in the case of $\Gamma = D_4^* = \mathbb{J}$, p and q are unique up to multiplication by a unit of \mathbb{J} from the right [14, Prop. 3]. Hence, counting SSLs of D_4^* is equivalent to counting right ideals of \mathbb{J} .

The situation is slightly more complicated for \mathbb{Z}^4 , as its symmetry is lower. As a consequence, there may be three distinct (but, of course, congruent) SSLs of \mathbb{Z}^4 that correspond to a single SSL of \mathbb{J} . This only happens if the index of the SSL is even. We thus obtain the following result for the generating functions of the SSLs, where we make use of the zeta function of \mathbb{J} , which reads [14, 87, 77]

$$(5.21) \quad \zeta_{\mathbb{J}}(s) = \sum_{I \subseteq \mathbb{J}} \frac{1}{[\mathbb{J} : I]^s} = (1 - 2^{1-2s}) \zeta(2s) \zeta(2s - 1).$$

Theorem 5.33 ([14, Thm. 2]). *The possible indices of similar sublattices of hypercubic lattices in \mathbb{R}^4 are precisely the squares of rational integers. The number of distinct SSLs of a given index is a multiplicative arithmetic function. For the case of $\mathbb{J} = D_4^*$, the corresponding Dirichlet series generating function $\Phi_{\mathbb{J}}$ reads*

$$\Phi_{\mathbb{J}}(s) = \frac{(\zeta_{\mathbb{J}}(s))^2}{(1 + 4^{-s}) \zeta(4s)} = \frac{(1 - 2^{1-2s})^2 (\zeta(2s) \zeta(2s - 1))^2}{1 + 4^{-s} \zeta(4s)}.$$

⁶Note that a different definition for the counting function was applied in [12]. There, the function $f(m) = b_{A_4}(m^2)$ was discussed, which makes sense as $b_{A_4}(n)$ is non-zero only for squares. Correspondingly, the asymptotics for $f(m)$ are given by $\sum_{m \leq x} f(m) \sim \frac{\rho}{2} x^2$ as $x \rightarrow \infty$.

The same function also applies to the lattice D_4 , while we obtain

$$\Phi_{\mathbb{Z}^4}(s) = \left(1 + \frac{2}{4^s}\right) \Phi_{\mathbb{J}}(s)$$

for the primitive hypercubic lattice \mathbb{Z}^4 . □

From the generating functions of Theorem 5.33, we can extract the corresponding counting functions $b_{\mathbb{J}}(m)$ and $b_{\mathbb{Z}^4}(m)$. We formulate them in terms of the function

$$(5.22) \quad g(n, r) = (r + 1)n^r + 2 \frac{1 - (r + 1)n^r + rn^{r+1}}{(n - 1)^2}$$

for integers $r \geq 0$ and $n > 1$.

Corollary 5.34 ([14, Cor. 1]). *The arithmetic functions $b_{\mathbb{J}}(m)$ and $b_{\mathbb{Z}^4}(m)$ are multiplicative. They are non-zero if and only if m is a square, and are then determined by*

$$b_{\mathbb{J}}(p^{2r}) = \begin{cases} 1, & \text{if } p = 2, \\ g(p, r), & \text{if } p \text{ is an odd prime,} \end{cases}$$

for all $r \geq 0$, and by $b_{\mathbb{Z}^4}(m) = (2 + (-1)^m) b_{\mathbb{J}}(m)$. □

The first few terms of $\Phi_{\mathbb{J}}(s)$ read

$$\begin{aligned} \Phi_{\mathbb{J}}(s) = & 1 + \frac{1}{4^s} + \frac{8}{9^s} + \frac{1}{16^s} + \frac{12}{25^s} + \frac{8}{36^s} + \frac{16}{49^s} + \frac{1}{64^s} + \frac{41}{81^s} + \frac{12}{100^s} \\ & + \frac{24}{121^s} + \frac{8}{144^s} + \frac{28}{169^s} + \frac{16}{196^s} + \frac{96}{225^s} + \frac{1}{256^s} + \frac{36}{289^s} + \dots, \end{aligned}$$

which corresponds to sequence A045771 in [84].

Corollary 5.35 ([14, Cor. 2]). *The asymptotic growth of the summatory arithmetic function $\sum_{m \leq x} b_{\Gamma}(m)$ is given by⁷*

$$\sum_{m \leq x} b_{\Gamma}(m) \sim C_{\Gamma} x \log(x)$$

as $x \rightarrow \infty$, where the constant C_{Γ} is given by

$$C_{\Gamma} = \operatorname{res}_{s=1}((s - 1)\Phi_{\Gamma}(s)) = \begin{cases} \frac{1}{8}, & \text{for } \Gamma = \mathbb{J}, \\ \frac{3}{16}, & \text{for } \Gamma = \mathbb{Z}^4. \end{cases} \quad \square$$

Finally, let us comment on the primitive SSLs. A pair (p, q) of Hurwitz quaternions generates a primitive SSL of \mathbb{J} if and only if both p and q are \mathbb{J} -primitive and at least one of them is odd.

In this case, the denominator of the corresponding rotation is given by

$$(5.23) \quad \operatorname{den}_{\mathbb{J}}(R(p, q)) = |pq|.$$

⁷Note that in [14] the asymptotics of the counting function $f_{\Gamma}(m) = b_{\Gamma}(m^2)$ instead of $b_{\Gamma}(m)$ are discussed; compare Footnote 6. Correspondingly, the asymptotics for $f_{\Gamma}(m)$ are given by $\sum_{m \leq x} f_{\Gamma}(m) \sim 2C_{\Gamma} x^2 \log(x)$ as $x \rightarrow \infty$.

For \mathbb{Z}^4 , a pair of \mathbb{J} -primitive quaternions does not necessarily generate an SSL of \mathbb{Z}^4 . This only works if $pq \in \mathbb{Z}^4$. Consequently, primitive SSLs are either of the form $p\mathbb{Z}^4\bar{q}$ or $2p\mathbb{Z}^4\bar{q}$, depending on whether $pq \in \mathbb{Z}^4$ or not. Correspondingly, the denominator for \mathbb{Z}^4 reads

$$(5.24) \quad \text{den}_{\mathbb{Z}^4}(R(p, q)) = \begin{cases} |pq|, & \text{if } pq \in \mathbb{Z}^4, \\ 2|pq|, & \text{if } pq \notin \mathbb{Z}^4. \end{cases}$$

As a consequence, we have $\Phi_\Gamma^{\text{pr}}(s) = \Phi_\Gamma(s)/\zeta(4s)$ for $\Gamma \in \{\mathbb{J}, \mathbb{Z}^4\}$. Finally, this yields the asymptotic behaviour

$$\sum_{m \leq x} b_\Gamma^{\text{pr}}(m) \sim C_\Gamma^{\text{pr}} x \log(x) \quad \text{with} \quad C_\Gamma^{\text{pr}} = \begin{cases} \frac{45}{4\pi^4}, & \text{for } \Gamma = \mathbb{J}, \\ \frac{135}{8\pi^4}, & \text{for } \Gamma = \mathbb{Z}^4. \end{cases}$$

6. SIMILAR SUBMODULES

Here, we are interested in \mathbb{Z} -modules as generalisations of lattices. As such, they are mainly considered as *geometric* (as opposed to algebraic) objects. Let us thus begin with a definition of the geometric setting.

Definition 6.1. A \mathbb{Z} -module M of rank n is called (properly) *embedded* in \mathbb{R}^d when $M \subset \mathbb{R}^d$ and when there is a \mathbb{Z} -basis $\{b_1, \dots, b_n\}$ of M whose \mathbb{R} -span is \mathbb{R}^d .

In particular, this requires that $n \geq d$, where n is the *rank* of M and d may be called its *embedding dimension*. A lattice is an embedded module with $n = d$. An important class of embedded modules is given by what we call \mathcal{S} -lattices.

Definition 6.2. Let $\mathcal{S} \subset \mathbb{R}$ be a ring with identity that is also a finitely generated, free \mathbb{Z} -module. Then, we call an embedded \mathbb{Z} -module $M \subset \mathbb{R}^d$ an \mathcal{S} -*lattice* if there exist d linearly independent vectors $b_i \in \mathbb{R}^d$ such that M is the \mathcal{S} -span of $\{b_1, \dots, b_d\}$, so $M = \langle b_1, \dots, b_d \rangle_{\mathcal{S}}$.

We call a \mathbb{Z} -module $M' \subseteq M$ a (full) *submodule* of M if M' and M have the same rank.⁸ This implies that M' and M also have the same embedding dimension, wherefore the index $[M : M']$ is finite.

Just as for lattices, we define the more general notion of commensurate modules.

Definition 6.3. Two (properly embedded) \mathbb{Z} -modules $M_1, M_2 \subset \mathbb{R}^d$ are called *commensurate*, which is denoted by $M_1 \sim M_2$, if their intersection $M_1 \cap M_2$ has finite index in both modules, M_1 and M_2 .

In our terminology, this means that M_1 and M_2 are commensurate if and only if $M_1 \cap M_2$ is a submodule of both M_1 and M_2 in our above sense. This implies that M_1 and M_2 can only be commensurate if they have the same rank. Once we know that two embedded modules in

⁸More generally, one calls any \mathbb{Z} -module $M' \subseteq M$ a submodule of M regardless of its rank, but we do not need this more general notion in our context.

\mathbb{R}^d have the same rank, the situation becomes easier as we can characterise commensurateness in several ways [98], which we recall here.

Lemma 6.4. *Let $M_1, M_2 \subseteq \mathbb{R}^d$ be two properly embedded \mathbb{Z} -modules of rank k . Then, the following statements are equivalent.*

- (1) M_1 and M_2 are commensurate.
- (2) $M_1 \cap M_2$ has finite index in both M_1 and M_2 .
- (3) $M_1 \cap M_2$ has finite index in M_1 or in M_2 .
- (4) There exist (positive) integers m_1 and m_2 such that $m_1 M_1 \subseteq M_2$ and $m_2 M_2 \subseteq M_1$.
- (5) There exists an integer m such that $m M_1 \subseteq M_2$ or $m M_2 \subseteq M_1$.
- (6) $M_1 \cap M_2$ has rank k . □

To continue, two properly embedded modules M_1 and M_2 are called *similar*, $M_1 \stackrel{\sim}{\simeq} M_2$, if there exists a similarity transformation between them. Clearly, similarity of modules is an equivalence relation.

Definition 6.5. A similarity transformation that maps a module $M \subset \mathbb{R}^d$ onto a submodule of M is called a *similarity transformation of M* . A submodule $M' \subseteq M$ is called a *similar submodule* (SSM) of M if $M' \stackrel{\sim}{\simeq} M$.

We proceed as before and consider coincidence isometries and scaling factors separately. We first define

$$(6.1) \quad \text{OS}(M) := \{R \in \text{O}(d, \mathbb{R}) \mid \exists \alpha \in \mathbb{R}_+ \text{ such that } \alpha R M \subseteq M\}$$

whose elements are called *similarity isometries* of M . Similarly, we use

$$(6.2) \quad \text{SOS}(M) := \text{OS}(M) \cap \text{SO}(d, \mathbb{R})$$

to denote the set of similarity rotations. The following results are immediate generalisations of the corresponding results for lattices in Fact 5.1 and Lemma 5.2.

Fact 6.6. *$\text{OS}(M)$ and $\text{SOS}(M)$ are subgroups of $\text{O}(d, \mathbb{R})$. Further, if M and $M' = \alpha R M$ are similar modules which are both embedded in \mathbb{R}^d , we have*

$$\text{OS}(M') = R \text{OS}(M) R^{-1}. \quad \square$$

Next, we consider the scaling factors. We first define

$$(6.3) \quad \begin{aligned} \text{Scal}_M(R) &:= \{\alpha \in \mathbb{R} \mid \alpha R M \subseteq M\} \quad \text{and} \\ \text{scal}_M(R) &:= \{\alpha \in \mathbb{R} \mid \alpha R M \sim M\}. \end{aligned}$$

Again, we have allowed negative values for the scaling factors here to ensure that $\text{Scal}_M(R)$ is a \mathbb{Z} -module. This creates no problem because $-M = M$. However, the situation is more complicated than in the case of lattices, as there are significantly fewer restrictions on the scaling factors here.

Note that $\text{Scal}_M(R)$ is non-empty for all R as $0 \in \text{Scal}_M(R)$, but it is non-trivial only if $R \in \text{OS}(M)$, as we have the following generalisation of Fact 5.3.

Fact 6.7 ([98, p. 14]). *Let $M \subset \mathbb{R}^d$ be an embedded \mathbb{Z} -module and consider $R \in \text{O}(d, \mathbb{R})$. Then, the following properties are equivalent.*

- (1) $\text{Scal}_M(R) \neq \{0\}$;
- (2) $\text{scal}_M(R) \neq \emptyset$;
- (3) $R \in \text{OS}(M)$. □

As a first consequence, we mention a result on the possible values of $\text{Scal}_M(\mathbb{1})$. Recall that $[x]$ denotes the largest integer $n \leq x$.

Theorem 6.8 ([98, Thm. 2.1.6 and Cor. 2.1.7]). *Let $M \subset \mathbb{R}^d$ be an embedded \mathbb{Z} -module of rank k . Then, $\text{Scal}_M(\mathbb{1})$ is a ring with unit all elements of which are algebraic integers. Moreover, $\text{Scal}_M(\mathbb{1})$ is a finitely generated, free \mathbb{Z} -module, whose rank is a divisor of k and is at most $\lfloor \frac{k}{d} \rfloor$.*

Furthermore, $\text{scal}_M(\mathbb{1}) \cup \{0\}$ is the field of fractions of $\text{Scal}_M(\mathbb{1})$. □

For \mathcal{S} -lattices, we can immediately determine $\text{Scal}_M(\mathbb{1})$ and $\text{scal}_M(\mathbb{1})$.

Fact 6.9. *If M is an \mathcal{S} -lattice, then $\text{Scal}_M(\mathbb{1}) = \mathcal{S}$ and $\text{scal}_M(\mathbb{1}) \cup \{0\}$ is the field of fractions of \mathcal{S} .*

Proof. Since \mathcal{S} is a ring and M is the \mathcal{S} -span of d linearly independent vectors $b_i \in \mathbb{R}^d$, we have $\mathcal{S} \subseteq \text{Scal}_M(\mathbb{1})$. On the other hand, the linear independence of the b_i guarantees $\text{Scal}_M(\mathbb{1})b_1 \subseteq M \cap \mathbb{R}b_1 = \mathcal{S}b_1$, whence we have the reverse inclusion $\text{Scal}_M(\mathbb{1}) \subseteq \mathcal{S}$. The second part now follows immediately from Theorem 6.8; compare also [44, Remark 3.11]. □

For general similarity isometries R , we have the following result.

Theorem 6.10 ([98, Thm. 2.1.9]). *Let $M \subset \mathbb{R}^d$ be an embedded \mathbb{Z} -module. Then, for any isometry $R \in \text{OS}(M)$, $\text{Scal}_M(R)$ is a finitely generated, free \mathbb{Z} -module. Moreover, one has $\beta \text{Scal}_M(R) \subseteq \text{Scal}_M(R)$ for any $\beta \in \text{Scal}_M(\mathbb{1})$, and $\text{Scal}_M(R)$ is thus also a finitely generated $\text{Scal}_M(\mathbb{1})$ -module.* □

Observe that $\text{Scal}_M(R)$ is generally not a free $\text{Scal}_M(\mathbb{1})$ -module, unless $\text{Scal}_M(\mathbb{1})$ is a PID; see [98, p. 15] for an example.

For lattices, Lemma 5.5 asserted that $\alpha^d \in \mathbb{Z}$ for all $\alpha \in \text{Scal}_\Gamma(R)$. The corresponding result for embedded modules reads as follows.

Theorem 6.11 ([98, Thm. 2.1.10]). *As before, let $M \subset \mathbb{R}^d$ be an embedded \mathbb{Z} -module of finite rank. Then, any $\alpha \in \text{Scal}_M(R)$ is an algebraic integer. If M has rank $k = 1$, one always has $\text{Scal}_M(R) = \mathbb{Z}$, so α is a rational integer in this case. If $k \geq 2$, the degree of α is at most $k(k-1)$.* □

The set $\{\text{scal}_M(R) \mid R \in \text{OS}(M)\}$ has again a group structure, under the multiplication defined by

$$\text{scal}_M(R) \text{scal}_M(S) := \{\alpha\beta \mid \alpha \in \text{scal}_M(R), \beta \in \text{scal}_M(S)\}.$$

We have the following generalisation of Lemma 5.8.

Theorem 6.12 ([98, Lemmas 2.1.11 and 2.1.12 and Thm. 2.1.12]). *Let $M \subset \mathbb{R}^d$ be an embedded \mathbb{Z} -module. Then, one has the following properties.*

- (1) *For any $R, S \in \text{OS}(M)$, we have the product relation*

$$\text{scal}_M(R) \text{scal}_M(S) = \text{scal}_M(RS)$$

together with $\text{scal}_M(R^{-1}) \text{scal}_M(R) = \text{scal}_M(\mathbb{1})$.

- (2) *$\{\text{scal}_M(R) \mid R \in \text{OS}(M)\}$ is an Abelian group. Its neutral element is $\text{scal}_M(\mathbb{1})$, and the inverse of $\text{scal}_M(R)$ is $\text{scal}_M(R^{-1})$.*
- (3) *$\{\text{scal}_M(R) \mid R \in \text{OS}(M)\}$ is isomorphic to a multiplicative subgroup of the group $\mathbb{R}_+ / (\text{scal}_M(\mathbb{1}) \cap \mathbb{R}_+)$.*
- (4) *There exists a natural homomorphism*

$$\phi: \text{OS}(M) \longrightarrow \{\text{scal}_M(R) \mid R \in \text{OS}(M)\}$$

via $R \mapsto \text{scal}_M(R)$. □

In fact, this theorem will be the key to establish the connection between CSMs and SSMS in Section 7.6.

As $\text{Scal}_M(R)$ need not be a PID, we cannot characterise it by a denominator as in Section 5. This makes it more difficult to establish a connection between the sets $\text{Scal}_M(R)$ for related modules. Nevertheless, there are some results.

Lemma 6.13 ([98, Lemmas 2.2.1 and 2.2.2]). *If M and N are commensurate modules, one has $\text{OS}(M) = \text{OS}(N)$ and $\text{scal}_N(R) = \text{scal}_M(R)$ for any $R \in \text{OS}(M) = \text{OS}(N)$.* □

For $\text{Scal}_M(R)$, a weaker result applies.

Theorem 6.14 ([98, Thm. 2.2.3]). *Let N be a submodule of M of index m . Then, one has $m \text{Scal}_M(R) \subseteq \text{Scal}_N(R) \subseteq \frac{1}{m} \text{Scal}_M(R)$.* □

Above, we have already considered some examples of planar modules in Section 5.2. We conclude our discussion of SSMS with an important example in \mathbb{R}^4 .

6.1. The icosian ring. We already met the icosian ring \mathbb{I} in connection with the lattice A_4 , where it was used as a tool to determine the SSLs of A_4 . But it is also interesting to classify the SSMS of \mathbb{I} itself.

Actually, the way to determine the SSMS is completely analogous to the case of \mathbb{J} in the previous section, which is related to the fact that both \mathbb{J} and \mathbb{I} are maximal orders in their corresponding quaternion algebras; compare [77]. Although \mathbb{I} is not a lattice but a \mathbb{Z} -module

in \mathbb{R}^4 , all steps can be easily generalised for \mathbb{I} , as the latter can be viewed as a $\mathbb{Z}[\tau]$ -module of rank 4 (or a $\mathbb{Z}[\tau]$ -lattice in our above terminology) that is properly embedded in \mathbb{R}^4 . Moreover, any quaternion in \mathbb{I} has a norm which lies in $\mathbb{Z}[\tau]$. Thus, the zeta function of the number field $K = \mathbb{Q}(\tau)$ comes into play again, and we can express the generating function of the SSMS in terms of $\zeta_{\mathbb{I}}(s)$, which we know from Eq. (5.17).

Theorem 6.15 ([14, Thm. 3]). *The possible indices of similar submodules of the icosian ring are precisely the squares of rational integers that can be represented by the quadratic form $x^2 + xy - y^2$. The number of SSMS of a given index is a multiplicative arithmetic function, whose Dirichlet series generating function $\Phi_{\mathbb{I}}$ reads*

$$\Phi_{\mathbb{I}}(s) = \frac{(\zeta_{\mathbb{I}}(s))^2}{\zeta_K(4s)} = \frac{(\zeta_K(2s)\zeta_K(2s-1))^2}{\zeta_K(4s)}$$

with $K = \mathbb{Q}(\tau)$. □

This theorem allows us to infer the corresponding counting function $b_{\mathbb{I}}(m)$. Using the function $g(n, r)$ defined previously in Eq. (5.22), we obtain the following explicit result.

Corollary 6.16 ([14, Cor. 3]). *The arithmetic function $b_{\mathbb{I}}(m)$ is multiplicative and vanishes unless m is a square. It is completely determined by specifying $b_{\mathbb{I}}(p^{2r})$ for all rational primes p and all $r \geq 0$. With the function g of Eq. (5.22), one has*

$$b_{\mathbb{I}}(p^{2r}) = \begin{cases} g(5, r), & \text{if } p = 5, \\ 0, & \text{if } p \equiv \pm 2 \pmod{5} \text{ and } r \text{ is odd,} \\ g(p^2, \frac{r}{2}), & \text{if } p \equiv \pm 2 \pmod{5} \text{ and } r \text{ is even,} \\ \sum_{\ell=0}^r g(p, \ell)g(p, r-\ell), & \text{if } p \equiv \pm 1 \pmod{5}. \end{cases} \quad \square$$

The first few terms of $\Phi_{\mathbb{I}}(s)$ read

$$\begin{aligned} \Phi_{\mathbb{I}}(s) = & 1 + \frac{10}{4^{2s}} + \frac{12}{5^{2s}} + \frac{20}{9^{2s}} + \frac{48}{11^{2s}} + \frac{66}{16^{2s}} + \frac{80}{19^{2s}} + \frac{120}{20^{2s}} + \frac{97}{25^{2s}} \\ & + \frac{120}{29^{2s}} + \frac{128}{31^{2s}} + \frac{200}{36^{2s}} + \frac{168}{41^{2s}} + \frac{480}{44^{2s}} + \frac{240}{45^{2s}} + \dots \end{aligned}$$

Along the same lines as before, we can evaluate the asymptotic behaviour.

Corollary 6.17 ([14, Cor. 4]). *The asymptotic growth of the summatory arithmetic function $\sum_{m \leq x} b_{\mathbb{I}}(m)$ is given by⁹*

$$\sum_{m \leq x} b_{\mathbb{I}}(m) \sim \frac{3 \log(\tau)^2}{5\sqrt{5}} x \log(x) \approx 0.062135 x \log(x)$$

as $x \rightarrow \infty$. □

⁹Compare Footnotes 6 and 7 on pages 30 and 31, respectively.

Let us now turn our attention to the related problem of coincidence site lattices. It is less common in the mathematical literature, due to its origin in crystallography. As we shall see, it is technically more involved and thus less developed from a structural point of view. Nevertheless, its consideration is completely natural and intrinsically connected with the SSL problem, as we shall see later on.

7. COINCIDENCE SITE LATTICES AND MODULES

7.1. Basic facts. Let us return to the CSLs, which we have introduced in Definition 2.5. To parallel our approach to the SSLs, we introduce the set

$$(7.1) \quad \text{OC}(\Gamma) := \{R \in \text{O}(d, \mathbb{R}) \mid \Gamma \sim R\Gamma\},$$

where $\Gamma \subset \mathbb{R}^d$ is a (given) lattice. Likewise, we use the notation

$$(7.2) \quad \text{SOC}(\Gamma) := \{R \in \text{OC}(\Gamma) \mid \det(R) = 1\}$$

for the set of all orientation-preserving coincidence isometries, which are also known as coincidence rotations. Let us mention that the groups $\text{OC}(\Gamma)$ and $\text{SOC}(\Gamma)$ can be interpreted as *commensurator groups* of the lattice Γ ; compare [15].

Fact 7.1 ([4, Thm. 2.1]). *The sets $\text{OC}(\Gamma)$ and $\text{SOC}(\Gamma)$ are subgroups of $\text{O}(d, \mathbb{R})$.* \square

Note that $\text{OC}(\Gamma)$ contains the symmetry group $\text{O}(\Gamma)$ of Γ as a subgroup. Indeed, $\text{O}(\Gamma)$ is precisely the group of all coincidence isometries of index $\Sigma_\Gamma(R) = [\Gamma : \Gamma(R)] = 1$; compare Definition 2.5.

One certainly expects connections between lattices that are closely related. Here, one has the following elementary result.

Lemma 7.2 ([4, Cor. 2.1 and Lemma 2.6]). *Commensurate lattices have the same OC-groups. In particular, all sublattices of a lattice Γ have the same group of coincidence isometries.* \square

We have seen earlier in Lemma 5.2 that similar lattices have conjugate OS-groups. A corresponding result for coincidence isometries exists as well.

Lemma 7.3 ([4, Lemma 2.5]). *Similar lattices have conjugate OC-groups. In particular, for any $0 \neq \alpha \in \mathbb{R}$ and any $R \in \text{O}(d, \mathbb{R})$, one has*

$$\text{OC}(\alpha R\Gamma) = R \text{OC}(\Gamma) R^{-1},$$

together with $\Sigma_{\alpha R\Gamma}(S) = \Sigma_\Gamma(R^{-1}SR)$. \square

Unsurprisingly, there is also a close connection between a lattice and its dual lattice; compare [4].

Lemma 7.4. *Let Γ^* be the dual lattice of a lattice $\Gamma \subseteq \mathbb{R}^d$. Then, $\text{OC}(\Gamma^*) = \text{OC}(\Gamma)$ and $\Sigma_{\Gamma^*}(R) = \Sigma_\Gamma(R)$ for all $R \in \text{OC}(\Gamma)$.*

Proof. As two lattices are commensurate if and only if their duals are commensurate, we have $\Gamma^* \sim R\Gamma^*$ if and only if $\Gamma \sim R\Gamma$, where one needs the relation $(R\Gamma)^* = R\Gamma^*$. By definition, this implies $\text{OC}(\Gamma^*) = \text{OC}(\Gamma)$. Now,

$$[\Gamma^* : \Gamma^*(R)] = [\Gamma^* : (\Gamma + R\Gamma)^*] = [\Gamma + R\Gamma : \Gamma] = [\Gamma : \Gamma(R)],$$

which proves the claim. \square

An interesting observation is that the coincidence indices of a coincidence isometry and its inverse are the same. This fact can be proved by geometric arguments [4] involving the dual lattice, which we will repeat here.

Lemma 7.5. *Let $\Gamma \subseteq \mathbb{R}^d$ be a lattice. For any $R \in \text{OC}(\Gamma)$, one has*

$$\Sigma_\Gamma(R) = \Sigma_\Gamma(R^{-1}).$$

Proof. The key is the fact that $[\Gamma : \Gamma(R)]$ can be interpreted geometrically: It is the ratio of the volumes of fundamental cells of $\Gamma(R)$ and Γ , which is independent of the particular choice of the latter. As isometries preserve the volume, we have

$$\begin{aligned} \Sigma_\Gamma(R) &= [\Gamma : \Gamma(R)] = [R\Gamma : \Gamma(R)] = [R\Gamma : \Gamma \cap R\Gamma] \\ &= [\Gamma : R^{-1}\Gamma \cap \Gamma] = \Sigma_\Gamma(R^{-1}), \end{aligned}$$

which completes the argument. \square

As $\text{OC}(\Gamma)$ is a group, it is natural to ask whether there is a connection between the indices $\Sigma_\Gamma(R_1)$, $\Sigma_\Gamma(R_2)$ and $\Sigma_\Gamma(R_1R_2)$ for $R_1, R_2 \in \text{OC}(\Gamma)$. Although no general formula exists which expresses one of them in terms of the other two, we have the following results.

Theorem 7.6 ([96], [98, Lemma 3.4.3 and Thm. 3.4.4]). *For any lattice $\Gamma \subset \mathbb{R}^d$ and for any $R_1, R_2 \in \text{OC}(\Gamma)$, one has the following relations.*

- (1) $\Sigma_\Gamma(R_1R_2)$ divides $\Sigma_\Gamma(R_1)\Sigma_\Gamma(R_2)$.
- (2) $\Sigma_\Gamma(R_1R_2) = \Sigma_\Gamma(R_1)\Sigma_\Gamma(R_2)$ whenever $\Sigma_\Gamma(R_1)$ and $\Sigma_\Gamma(R_2)$ are coprime. \square

Remark 7.7. In particular, one has $\Sigma_\Gamma(RS) = \Sigma_\Gamma(R)$ if $\Sigma_\Gamma(S) = 1$, or in other words, if $S \in \text{O}(\Gamma)$, which means that S is a symmetry operation of Γ . Actually, if $S \in \text{O}(\Gamma)$, one even has $\Gamma(RS) = \Gamma(R)$. This motivates us to call two coincidence isometries R and R' *symmetry related* if there exists an $S \in \text{O}(\Gamma)$ such that $R' = RS$. Thus, symmetry-related coincidence isometries generate the same CSL, but the converse is not true in general; see Example 7.16 below for an instance of two coincidence isometries that are not symmetry related but generate the same CSL. \diamond

Remark 7.8. One of the quantities we are after is the set of possible coincidence indices. In line with [15], we call this set,

$$\sigma(\Gamma) = \Sigma(\text{OC}(\Gamma)) = \{\Sigma_\Gamma(R) \mid R \in \text{OC}(\Gamma)\},$$

the *coincidence spectrum* of Γ . Sometimes, we call it the ordinary or simple coincidence spectrum to distinguish it from the multiple coincidence spectrum, which we define later; compare Section 7.2. Likewise, $\Sigma(\text{SOC}(\Gamma)) = \{\Sigma_\Gamma(R) \mid R \in \text{SOC}(\Gamma)\}$ is the subset of indices of the coincidence rotations. Clearly, we have $\Sigma(\text{SOC}(\Gamma)) \subseteq \Sigma(\text{OC}(\Gamma))$ in general, but in many cases we have $\Sigma(\text{SOC}(\Gamma)) = \Sigma(\text{OC}(\Gamma))$. By Remark 7.7, $\Sigma(\text{SOC}(\Gamma)) = \Sigma(\text{OC}(\Gamma))$ whenever an orientation-reversing isometry exists in $\text{O}(\Gamma)$, but this is only a sufficient condition and by no means a necessary one. \diamond

It is not uncommon that one needs to relate the coincidence structure of a lattice to that of various sublattices. Let us consider some consequences on the coincidence indices.

Lemma 7.9. *Let Λ be a sublattice of $\Gamma \subseteq \mathbb{R}^d$ of index m . Then, $\Sigma_\Lambda(R)$ divides $m\Sigma_\Gamma(R)$ and $\Sigma_\Gamma(R)$ divides $m\Sigma_\Lambda(R)$.*

Proof. As $\Lambda(R) \subseteq \Gamma(R) \subseteq \Gamma$, the coincidence index $\Sigma_\Gamma(R)$ divides

$$[\Gamma : \Lambda(R)] = [\Gamma : \Lambda][\Lambda : \Lambda(R)] = m\Sigma_\Lambda(R),$$

which proves the second claim.

The first claim can be proved by applying Lemma 7.4. It is well known that $\Lambda \subseteq \Gamma$ implies $\Gamma^* \subseteq \Lambda^*$. Since $\Sigma_\Gamma(R) = \Sigma_{\Gamma^*}(R)$ by Lemma 7.4, for any lattice Γ , the result now follows immediately from the first part of the proof. \square

Lemma 7.9 provides us with some useful bounds on the coincidence indices of a sublattice. In certain cases, we can even get sharper bounds [65, 98]. As an example, we mention the following result, which is a special case of [98, Thm. 3.1.10] or [65, Thm. 2.2] (with $u = 1$ in the notation used there).

Lemma 7.10. *Let Λ be a sublattice of Γ of index m , and let $R \in \text{OC}(\Gamma)$ be such that $\Lambda \cap R(t + \Lambda) = \emptyset$ for all $t \in \Gamma \setminus \Lambda$. Then, $\Sigma_\Lambda(R)$ divides $\Sigma_\Gamma(R)$.* \square

Note that this result is the basis of the concept of *colour coincidences*; compare [65, 63, 67].

Remark 7.11. Lemma 7.10 is only useful in practice if it is reasonably easy to check the condition $\Lambda \cap R(t + \Lambda) = \emptyset$ for all $t \in \Gamma \setminus \Lambda$. This is possible if the points of Λ and $\Gamma \setminus \Lambda$ lie on different shells, that is, if the sets $\{|x| \mid x \in \Lambda\}$ and $\{|x| \mid x \in \Gamma \setminus \Lambda\}$ are disjoint. This way, one can show that the three classes of cubic lattices have the same coincidence indices, as we shall see later in Section 9. \diamond

Remark 7.12. The shelling structure of lattices is a well-studied problem. It leads to Θ -series, which are nicely summarised in [27, Sec. 2.2.3]. The problem has also been investigated for embedded \mathbb{Z} -modules such as rings of cyclotomic integers in the plane [6], for the icosian ring in 4-space [70], or for \mathbb{Z} -modules in 3-space with icosahedral symmetry [90]. Also, Penrose-type tilings have been considered, where the notion of an *averaged shelling* was introduced [10]. In the latter case, an interpretation of the results in a wider setting is still missing. \diamond

7.2. Multiple coincidences. We can generalise our considerations on CSLs by looking at intersections of more than two commensurate lattices. The analogous step for modules will briefly be discussed in Section 7.5. This problem is interesting for various reasons. On the one hand, these intersections naturally occur in the discussion of the counting functions for CSLs; see Section 7.4 and [96]. On the other hand, they are important in crystallography in connection with multiple junctions [40, 41, 42]. Another interesting application arises in the theory of lattice quantisers where one usually deals with rather complex lattices. There, one hopes to simplify the problem by representing a complex lattice as the intersection of simpler lattices [34, 85].

In fact, intersections of more than two isometric commensurate copies of a lattice have already been discussed in [8, 95, 18, 98]. Let us first recall the corresponding definitions.

Definition 7.13. Let $\Gamma \subseteq \mathbb{R}^d$ be a lattice and assume $R_i \in \text{OC}(\Gamma)$, with $i \in \{1, \dots, m\}$. The lattice

$$\Gamma(R_1, \dots, R_m) := \Gamma \cap R_1\Gamma \cap \dots \cap R_m\Gamma = \Gamma(R_1) \cap \dots \cap \Gamma(R_m)$$

is then called a *multiple* CSL (MCSL) of order m . Its index in Γ is denoted by $\Sigma(R_1, \dots, R_m)$.

In order to distinguish CSLs of the type $\Gamma(R) = \Gamma \cap R\Gamma$ from multiple CSLs, we will occasionally use the term simple or ordinary CSL for $\Gamma(R)$.

Note that $\Sigma(R_1, \dots, R_m)$ is finite since $\Gamma(R_1, \dots, R_m)$ is a finite intersection of mutually commensurate lattices [4]. In particular, an immediate consequence of the second isomorphism theorem for groups is the following result.

Lemma 7.14 ([98, Lemma 3.3.1]). *For $R_1, R_2 \in \text{OC}(\Gamma)$, one has*

$$\Sigma(R_1, R_2) = \frac{\Sigma(R_1) \Sigma(R_2)}{\Sigma_+(R_1, R_2)},$$

where $\Sigma_+(R_1, R_2)$ is the index of the direct sum $\Gamma_+(R_1, R_2) = \Gamma(R_1) + \Gamma(R_2)$ in the original lattice Γ . □

More generally, one has the following relation.

Lemma 7.15 ([98, Lemma 3.3.2]). *For any $R_i \in \text{OC}(\Gamma)$,*

$$\Sigma(R_1, \dots, R_m) = \frac{\Sigma(R_1, \dots, R_{m-1}) \Sigma(R_m)}{\Sigma_+(R_1, \dots, R_{m-1}; R_m)},$$

where $\Sigma_+(R_1, \dots, R_{m-1}; R_m)$ is the index of

$$\Gamma_+(R_1, \dots, R_{m-1}; R_m) = \Gamma(R_1, \dots, R_{m-1}) + \Gamma(R_m)$$

in Γ . In particular, $\Sigma(R_1, \dots, R_m)$ divides $\Sigma(R_1) \cdots \Sigma(R_m)$. □

This result allows us to infer some basic properties of the coincidence spectrum. Recall from Remark 7.8 that the simple coincidence spectrum was defined as $\sigma(\Gamma) = \{\Sigma_{\Gamma}(R) \mid R \in \text{OC}(\Gamma)\}$. Likewise, we introduce the *multiple coincidence spectrum* as the set

$$\sigma_{\infty}(\Gamma) = \{\Sigma(R_1, \dots, R_m) \mid R_i \in \text{OC}(\Gamma), m \in \mathbb{N}\}.$$

Clearly, we have

$$(7.3) \quad \sigma(\Gamma) \subseteq \sigma_{\infty}(\Gamma) \subseteq \widehat{\sigma}(\Gamma),$$

where $\widehat{\sigma}(\Gamma)$ is the set of all positive integers that divide an integer from the (multiplicative) semigroup generated by $\sigma(\Gamma)$. We shall come back to this relation and possible consequences at the end of Section 12.2.

7.3. MCSLs and monotiles. In [9, Sec. 5.7.7], the SCD monotile due to Schmitt, Conway and Danzer for \mathbb{R}^3 is discussed. This convex tile, together with translated and rotated copies (but no reflected copies), allows to form periodic two-dimensional layers L , which can only be stacked vertically by rotating the layers by a fixed irrational rotation R . In particular, any tiling \mathcal{T} of \mathbb{R}^d obtained this way must have the form

$$(7.4) \quad \mathcal{T} = \bigcup_{m \in \mathbb{Z}} (mc + R^m L),$$

where c is a suitable vector orthogonal to the plane of the layer L ; compare [9, Eq. (5.7)] and [33, 5]. As $R^n \neq \mathbb{1}$ for any $n \in \mathbb{Z} \setminus \{0\}$, any resulting tiling of \mathbb{R}^d is aperiodic.

Let us analyse this construction in some more detail, in terms of MCSLs. Let L be one fixed layer of an SCD tiling. If Γ is the group of translations that leaves L invariant, then the stack of $n+1$ layers $\mathcal{T} = \bigcup_{m=0}^n (mc + R^m L)$ is invariant under the MCSL $\Gamma_n := \Gamma \cap R\Gamma \cap \dots \cap R^n \Gamma$, with $\Gamma_0 = \Gamma$. As $\bigcap_{n \in \mathbb{N}_0} \Gamma_n = \{0\}$, the tiling is aperiodic; compare [9, Lemma 5.8 and Rem. 5.12].

If we pursue these ideas further, we see that we can construct monotiles in all odd dimensions $2m+1 \geq 3$. Let us start with a lattice $\Gamma \in \mathbb{R}^d$ for $d = 2m$ and assume that Γ has a coincidence rotation R such that $R^n \neq \mathbb{1}$ for any $n \in \mathbb{Z} \setminus \{0\}$. We choose a unit cell U (possibly convex or a parallelohedron, with suitable markers) of the CSL $\Gamma \cap R\Gamma$ such that no lattice point of Γ or $R\Gamma$ is on the boundary. We can always choose U in such a way that it tiles \mathbb{R}^d only periodically, with Γ as the corresponding lattice of periods. We define a prototile T in \mathbb{R}^{d+1} as $U \times [0, 1]$ and add markings on the bottom and the top of T as follows. On the bottom, we mark each lattice point of Γ that is contained in U (to avoid any complication, we choose some mark without any symmetry) and on top we mark the lattice points of $R\Gamma$ (with the same marks just rotated by R). This guarantees that we can stack these layers of tiles vertically only by rotating them by R . Hence, the only tilings we can get are tilings of the form (7.4), with L replaced by Γ .

As $R^n \neq \mathbb{1}$ for any $n \in \mathbb{Z} \setminus \{0\}$, the tiling is not periodic in the remaining (transversal) direction. To exclude any periodicity in a direction parallel to the layers, we need $\bigcap_{n \in \mathbb{N}_0} \Gamma_n =$

$\{0\}$. Such an R exists for the square lattice. In fact, each coincidence rotation R that is not a symmetry of the square lattice has this property. Likewise, \mathbb{Z}^{2m} has infinitely many coincidence rotations R that satisfy $\bigcap_{n \in \mathbb{N}_0} \Gamma_n = \{0\}$. In particular, we may choose R as the direct product of two-dimensional coincidence rotations, each of which fails to be a symmetry of the square lattice.

However, note that, although all these tilings are aperiodic, they are not *strongly aperiodic*, as there is still a skew rotation symmetry left, which means that the symmetry group contains a subgroup isomorphic to \mathbb{Z} ; compare [9, Def. 5.22]. In this sense, also the original SCD tiling is aperiodic, but not strongly aperiodic. To the best of our knowledge, no strongly aperiodic monotile in 3-space is known.

With this restriction, the above construction establishes the existence of monotiles in odd dimensions. For even dimensions, the analogous construction fails, as the corresponding lattice then has odd dimension and any coincidence rotation of it leaves at least one lattice direction invariant. Whether monotiles exist in even dimensions is still an open problem. Only in dimension $d = 2$, a monotile for the Euclidean plane (with next-to-nearest neighbour local rules) was discovered by Joan Taylor; see [9, Sec. 5.7.6] and references therein for a more detailed account of the tiling, its properties (due to Socolar and Taylor) and predecessors (due to Penrose).

7.4. Counting functions. As sketched in Section 3, we are interested in several enumeration problems. In particular, for a given index, we are after the number of coincidence isometries and the number of CSLs. For a fixed lattice Γ , we shall denote the number of CSLs of a given index n by $c_\Gamma(n)$. As the same CSL can be generated by several coincidence isometries, it is not useful to deal with the total number of coincidence isometries directly, but it is more convenient to use a properly normalised counting function instead.

If S is a symmetry operation of Γ , we have $\Gamma(RS) = \Gamma(R)$ for any coincidence isometry R . This means that the number of coincidence isometries with a given index is a multiple of $\text{card}(\text{O}(\Gamma))$, where $\text{O}(\Gamma)$ is the symmetry group of Γ . Thus, we prefer to deal with the function $c_\Gamma^{\text{iso}}(n)$, which counts the coincidence isometries modulo the symmetry group. Then, the number of coincidence isometries of a given index n is given by $\text{card}(\text{O}(\Gamma))c_\Gamma^{\text{iso}}(n)$. Likewise, we define $c_\Gamma^{\text{rot}}(n)$ for all coincidence rotations, now counted modulo $\text{SO}(\Gamma) = \text{O}(\Gamma) \cap \text{SO}(d)$. This guarantees $c_\Gamma^{\text{iso}}(1) = c_\Gamma^{\text{rot}}(1) = c_\Gamma(1)$.

Let us mention that $c_\Gamma^{\text{rot}}(n) = c_\Gamma^{\text{iso}}(n)$ holds whenever there exists an orientation-reversing symmetry operation. In particular, $c_\Gamma^{\text{rot}}(n) = c_\Gamma^{\text{iso}}(n)$ holds for every lattice Γ in odd dimensions.

Recall from Remark 7.7 that two coincidence isometries R and R' are called *symmetry related*, if there exists a symmetry operation $S \in \text{O}(\Gamma)$ such that $R' = RS$. As symmetry-related coincidence isometries generate the same CSL, it follows that $c_\Gamma^{\text{iso}}(n)$ is an upper bound

for $c_\Gamma(n)$. However, these two numbers differ in general, as non-symmetry-related coincidence isometries may still generate the same CSL.

Example 7.16. As an example for differing counting functions for lattices versus isometries, we consider the rectangular lattice $\Gamma = \mathbb{Z}[i\sqrt{3}] \subset \mathbb{R}^2$, which is a sublattice of the hexagonal lattice $\Lambda = \mathbb{Z}[\omega]$ with $\omega = \frac{1+i\sqrt{3}}{2}$. Then, one has the inclusions $2\Lambda \subset \Gamma \subset \Lambda$ with indices $[\Lambda : \Gamma] = [\Gamma : 2\Lambda] = 2$. As ω^k with $k \not\equiv 0 \pmod{3}$ is a symmetry operation for Λ but not for Γ , we infer $\Sigma_\Gamma(\omega^k) > 1 = \Sigma_\Lambda(\omega^k)$ for $k \in \{1, 2\}$. It follows from Lemma 7.9 that one in fact has $\Sigma_\Gamma(\omega^k) = 2 = [\Gamma : 2\Lambda]$. Together with $\Gamma(\omega^k) \supseteq 2\Lambda$, this gives $\Gamma(\omega^k) = 2\Lambda$ for $k \in \{1, 2\}$. As ω and ω^2 fail to be symmetry related, this implies $c_\Gamma^{\text{iso}}(2) = c_\Gamma^{\text{rot}}(2) > c_\Gamma(2)$. In fact, a more detailed analysis yields $c_\Gamma^{\text{rot}}(2) = 2 > 1 = c_\Gamma(2)$.

This example can easily be generalised as follows. Whenever one has a lattice $\Lambda \subset \Gamma$ such that the index $[\Gamma : \Lambda] = p$ is a prime and such that $\text{O}(\Gamma) \subset \text{O}(\Lambda)$ with $[\text{O}(\Lambda) : \text{O}(\Gamma)] \geq 3$, one can infer $c_\Gamma^{\text{iso}}(p) > c_\Gamma(p)$ by analogous arguments. Moreover, if p is not in the coincidence spectrum of Λ , one can even show that

$$c_\Gamma^{\text{iso}}(p) = [\text{O}(\Lambda) : \text{O}(\Gamma)] - 1 > 1 = c_\Gamma(p).$$

This follows from $\Sigma_\Gamma(R) = p$ together with the observation that $\Gamma(R) = \Lambda$ for any isometry $R \in \text{O}(\Lambda) \setminus \text{O}(\Gamma)$. \diamond

In several important examples, all these counting functions are multiplicative, which suggests the use of generating functions of Dirichlet series type to determine their asymptotic growth rate, as we have done in several examples so far. In general, however, the counting functions fail to be multiplicative, though we have the following weaker result.

Theorem 7.17 ([96, 98]). *The arithmetic function $c_\Gamma^{\text{iso}}(n)$, $c_\Gamma^{\text{rot}}(n)$ and $c_\Gamma(n)$ are supermultiplicative, that is, $c_\Gamma^{\text{iso}}(mn) \geq c_\Gamma^{\text{iso}}(m)c_\Gamma^{\text{iso}}(n)$ holds for coprime integers m and n , and likewise for the other functions. \square*

Given the close relationship of similar sublattices and coincidence site lattices, which we will analyse below, one might be tempted to assume that the counting functions $b_\Gamma^{\text{pr}}(n)$ and $b_\Gamma(n)$ for similar sublattices are multiplicative if and only if the corresponding counting functions $c_\Gamma(n)$ and $c_\Gamma^{\text{iso}}(n)$ are multiplicative. However, this is not true. In fact, SSLs seem to be more prone to violation of multiplicativity than CSLs. For instance, for $\Gamma = \mathbb{Z} \times 5\mathbb{Z}$, multiplicativity is violated for $b_\Gamma^{\text{pr}}(n)$ and $b_\Gamma(n)$, compare [16], while $c_\Gamma(n)$ and $c_\Gamma^{\text{iso}}(n)$ are still multiplicative [37].

We expect that the connection between $c_\Gamma^{\text{iso}}(n)$ and $c_\Gamma(n)$ must be closer, and in fact one has the following result.

Theorem 7.18 ([96, 98]). *If the arithmetic function $c_\Gamma^{\text{iso}}(n)$ is multiplicative, then so is the function $c_\Gamma(n)$. \square*

It is presently unknown whether the converse holds or not. As the counting functions $c_\Gamma(n)$ and $c_\Gamma^{\text{iso}}(n)$ are generally not multiplicative, it is desirable to have some criteria when they are. For $c_\Gamma(n)$, we have the following result.

Theorem 7.19 ([96, 98]). *For a lattice $\Gamma \subset \mathbb{R}^d$, the following statements are equivalent.*

- (1) *The arithmetic function $c_\Gamma(m)$ is multiplicative.*
- (2) *Every simple CSL $\Gamma(R)$ has a representation of the form*

$$\Gamma(R) = \Gamma(R_1) \cap \dots \cap \Gamma(R_n)$$

with all indices $\Sigma_\Gamma(R_i)$ being powers of distinct primes.

- (3) *Every MCSL $\Gamma(R_1, \dots, R_n)$ of order n has a representation of the form*

$$\Gamma(R_1, \dots, R_n) = \Gamma_1 \cap \dots \cap \Gamma_k$$

where the Γ_i are MCSLs of order at most n whose indices Σ_i are powers of distinct primes. \square

Let us mention that the representation $\Gamma(R) = \Gamma(R_1) \cap \dots \cap \Gamma(R_n)$, if it exists, is unique up to the order of the $\Gamma(R_i)$. In fact, if $\Sigma(R) = p_1^{r_1} \cdots p_n^{r_n}$ is the prime factorisation of $\Sigma(R)$ and $m_i := \Sigma(R) p_i^{-r_i}$, then $\Gamma(R_i)$ can be calculated via

$$\Gamma(R_i) = \left(\frac{1}{m_i} \Gamma(R) \right) \cap \Gamma.$$

Note that the right-hand side is always a sublattice of Γ of index $p_i^{r_i}$. The key in proving Theorem 7.19 is to show that it is actually a CSL if $c_\Gamma(m)$ is multiplicative. On the other hand, one can show that $\Gamma(R_1) \cap \dots \cap \Gamma(R_n)$ is always a simple CSL if the indices are coprime, which allows one to count all CSLs that have such a representation. Analogous results hold for MCSLs; compare [96, 98].

A similar criterion exists for $c_\Gamma^{\text{iso}}(n)$. In order to formulate it, we need some terminology. We call a bijection $\pi = \{p_1, p_2, \dots\}$ from the positive integers onto the prime numbers an ordering of the prime numbers. We call a decomposition of a coincidence isometry $R = R_1 \cdots R_n$ a π -decomposition of R if, for any i , $\Sigma_\Gamma(R_i)$ is a power of p_i (we allow $\Sigma_\Gamma(R_i) = p_i^0 = 1$). It is clear that any π -decomposition is unique up to point group elements.

Theorem 7.20 ([96, 98]). *The following statements are equivalent.*

- (1) *The arithmetic function $c_\Gamma^{\text{iso}}(m)$ is multiplicative.*
- (2) *There exists an ordering π of the prime numbers such that any coincidence isometry R has a (unique) π -decomposition.*
- (3) *For any ordering π of the prime numbers, there exists a π -decomposition of every coincidence isometry R . \square*

7.5. Generalisations to \mathbb{Z} -modules. The considerations on CSLs can be generalised to embedded \mathbb{Z} -modules. As most of the definitions and results depend only on the algebraic properties, their generalisation is straightforward. However, some of our previous proofs involved the use of the dual lattice, which has no immediate counterpart for \mathbb{Z} -modules. In these cases, some care and new approaches are needed.

We recall from Definition 6.3 that two embedded \mathbb{Z} -modules M_1 and M_2 are called commensurate, $M_1 \sim M_2$, if their intersection $M_1 \cap M_2$ has finite index in both M_1 and M_2 . The notion of a coincidence site lattice can now easily be transferred to the case of modules as follows.

Definition 7.21. Let $M \subset \mathbb{R}^d$ be a properly embedded \mathbb{Z} -module of finite rank, and consider $R \in O(d, \mathbb{R})$. If $M \sim RM$, then $M(R) := M \cap RM$ is called a *coincidence site module* (CSM). Then, R is called a *coincidence isometry*. The corresponding index $\Sigma_M(R) := [M : M(R)]$ is called its *coincidence index*.

Again, we are interested in the sets

$$(7.5) \quad \text{OC}(M) := \{R \in O(d, \mathbb{R}) \mid M \sim RM\}$$

and

$$(7.6) \quad \text{SOC}(M) := \{R \in \text{OC}(M) \mid \det(R) = 1\}.$$

As expected, these sets are indeed groups.

Theorem 7.22. *If $M \subset \mathbb{R}^d$ is a properly embedded \mathbb{Z} -module, the set of all coincidence isometries, $\text{OC}(M)$, forms a subgroup of $O(d, \mathbb{R})$. Likewise, the group $\text{SOC}(M)$ is a subgroup of $\text{SO}(d, \mathbb{R})$. \square*

Lemmas 7.2 and 7.3 immediately generalise as follows.

Lemma 7.23 ([98, Lemmas 3.1.2 and 3.1.3]). *The OC-groups are equal for commensurate modules. Moreover, similar modules have conjugate OC-groups. In particular, one has $\text{OC}(\alpha RM) = R \text{OC}(M) R^{-1}$ and $\Sigma_{\alpha RM}(S) = \Sigma_M(R^{-1}SR)$. \square*

Obviously, there is no analogue of Lemma 7.4. Thus, it is not evident whether an analogue of Lemma 7.5 exists. Fortunately, it does, but its proof requires some results on irreducible polynomials over the ring \mathbb{Z} ; compare [98].

Theorem 7.24 ([98, Thm. 3.1.6]). *Let $M \subseteq \mathbb{R}^d$ be an embedded \mathbb{Z} -module of finite rank. For any $R \in \text{OC}(M)$, we have $\Sigma_M(R) = \Sigma_M(R^{-1})$. \square*

Again, it is interesting to compare the coincidence indices of modules with those of their submodules.

Theorem 7.25 ([98, Thm. 3.1.9]). *Let N be a submodule of M of index m . Then, $\Sigma_M(R)$ divides $m\Sigma_N(R)$ and $\Sigma_N(R)$ divides $m\Sigma_M(R)$. \square*

Whereas the second statement of Lemma 7.9 can be generalised immediately, the first claim of Theorem 7.25 requires a different approach, as we generally lack the notion of a dual module. The proof is algebraic in nature and can be found in [98]; compare also [65], where a similar approach for lattices is described.

7.6. Similar versus coincidence submodules. After we have dealt with similar sublattices and coincidence site lattices and their generalisations, let us return to the connections between them. It is clear that there are substantial connections, as became obvious from the groups we defined along the way. In line with Section 3, let us illustrate this in more detail with the square lattice, the latter once again identified with $\mathbb{Z}[i]$, the ring of Gaussian integers.

Example 7.26. We know from Theorem 5.14 and Example 5.15 that $\text{SOS}(\mathbb{Z}[i])$ is given by

$$\text{SOS}(\mathbb{Z}[i]) = \left\{ \frac{z}{|z|} \mid 0 \neq z \in \mathbb{Z}[i] \right\} \simeq C_8 \times \mathbb{Z}^{(\mathbb{N}_0)}.$$

In comparison, we have

$$\text{SOC}(\mathbb{Z}[i]) = \left\{ \frac{z}{\bar{z}} \mid 0 \neq z \in \mathbb{Z}[i] \right\} = \left\{ \frac{z^2}{|z|^2} \mid 0 \neq z \in \mathbb{Z}[i] \right\} \simeq C_4 \times \mathbb{Z}^{(\mathbb{N}_0)},$$

where C_4 is the groups of units of $\mathbb{Z}[i]$, while a full set of generators of $\mathbb{Z}^{(\mathbb{N}_0)}$ is provided by $\left\{ \frac{\pi_p}{\bar{\pi}_p} = \frac{\pi_p^2}{|\pi_p|^2} \mid p \equiv 1 \pmod{4} \right\}$, where, for each p of this kind, π_p is one of the Gaussian primes with $\pi_p \bar{\pi}_p = p$. Comparing these with the set of generators for $\text{SOS}(\mathbb{Z}[i])$ in Example 5.15, one sees that all generators of $\text{SOC}(\mathbb{Z}[i])$ are squares of generators of $\text{SOS}(\mathbb{Z}[i])$, and we infer that

$$\text{SOS}(\mathbb{Z}[i]) / \text{SOC}(\mathbb{Z}[i]) \simeq C_2^{(\mathbb{N}_0)},$$

which means that the factor group $\text{SOS}(\mathbb{Z}[i]) / \text{SOC}(\mathbb{Z}[i])$ is an infinite Abelian 2-group; compare [45]. \diamond

Let us now see how this observation can be put on a more general basis. We will formulate the main results immediately for modules; compare [97, 98]. For the special cases of lattices, we refer to [45]. The corresponding results for a special class of modules, namely the \mathcal{S} -lattices from Definition 6.2, can be found in [44].

Lemma 7.27 ([98, Lemma 3.2.1]). *Let $M \subseteq \mathbb{R}^d$ be a finitely generated free \mathbb{Z} -module. Then,*

- (1) $R \in \text{OC}(M)$ if and only if $1 \in \text{scal}_M(R)$.
- (2) $R \in \text{O}(M)$ if and only if $1 \in \text{Scal}_M(R)$. \square

Here, $\text{O}(M)$ is the point symmetry group of M . An immediate consequence for lattices is the following result.

Corollary 7.28. *If $\Gamma \subset \mathbb{R}^d$ is a lattice, one has $R \in \text{OC}(\Gamma)$ if and only if $R \in \text{OS}(\Gamma)$ together with $\text{den}_\Gamma(R) \in \mathbb{N}$. \square*

It is often helpful to know some connections between the coincidence indices and the corresponding denominators; compare [97].

Lemma 7.29. *Let Γ be a lattice in \mathbb{R}^d . For any $R \in \text{OC}(\Gamma)$, one has*

- (1) $\text{lcm}(\text{den}_\Gamma(R), \text{den}_\Gamma(R^{-1}))$ divides $\Sigma_\Gamma(R)$;
- (2) $\Sigma_\Gamma(R)$ divides $\text{gcd}(\text{den}_\Gamma(R), \text{den}_\Gamma(R^{-1}))^d$.
- (3) $\Sigma_\Gamma(R)^2$ divides $\text{lcm}(\text{den}_\Gamma(R), \text{den}_\Gamma(R^{-1}))^d$.

Proof. For (1), recall that $\Gamma(R)$ has index $\Sigma(R)$ in Γ , thus

$$\Sigma(R)\Gamma \subseteq \Gamma(R) \subseteq R\Gamma,$$

or, equivalently, $\Sigma(R)R^{-1}\Gamma \subseteq \Gamma$. Consequently, $\Sigma(R)$ is a multiple of $\text{den}(R^{-1})$. By symmetry, $\text{den}(R)$ is a divisor of $\Sigma(R^{-1}) = \Sigma(R)$ as well, and claim (1) follows.

For (2), we exploit that $\text{den}(R)$ is an integer for $R \in \text{OC}(\Gamma)$. Consequently, $\text{den}(R)R\Gamma$ is a sublattice of both Γ and $R\Gamma$, wherefore one has $\text{den}(R)R\Gamma \subseteq \Gamma(R)$. Comparing the indices of $\text{den}(R)R\Gamma$ and $\Gamma(R)$ in Γ shows that $\Sigma(R)$ divides $\text{den}(R)^d$. Using $\Sigma(R^{-1}) = \Sigma(R)$ as above yields (2).

Finally, let $a := \text{lcm}(\text{den}(R), \text{den}(R^{-1}))$. Then, $a\Gamma$ and $aR\Gamma$ are both sublattices of Γ and of $R\Gamma$, hence $a(\Gamma + R\Gamma)$ is a sublattice of $\Gamma \cap R\Gamma$ with index

$$[R \cap R\Gamma : a(\Gamma + R\Gamma)] = \frac{a^d}{\Sigma(R)^2},$$

as $\Sigma(R) = [\Gamma : \Gamma(R)] = [\Gamma + R\Gamma : \Gamma]$. Hence $\Sigma(R)^2$ divides a^d . \square

The situation becomes particularly simple for planar lattices, where we get the following result by recalling $\text{den}_\Gamma(R) = \text{den}_\Gamma(R^{-1})$.

Corollary 7.30 ([97, Cor. 2.6]). *Let Γ be a lattice in \mathbb{R}^2 . Then, for any $R \in \text{OC}(\Gamma)$, one has $\Sigma_\Gamma(R) = \text{den}_\Gamma(R)$. \square*

Our main result follows from Theorem 6.12.

Theorem 7.31 ([98, Thm. 3.2.2]). *Let $M \subset \mathbb{R}^d$ be an embedded \mathbb{Z} -module of finite rank. Then, the kernel of the homomorphism*

$$\begin{aligned} \phi: \text{OS}(M) &\longrightarrow \mathbb{R}_+ / (\text{scal}_M(\mathbb{1}) \cap \mathbb{R}_+), \\ R &\longmapsto \text{scal}_M(R) \cap \mathbb{R}_+, \end{aligned}$$

is the group $\text{OC}(M)$. Thus, $\text{OC}(M)$ is a normal subgroup of $\text{OS}(M)$, and $\text{OS}(M)/\text{OC}(M)$ is Abelian. \square

This result was first proved for lattices in [45] and later generalised to \mathcal{S} -lattices in [44].

If $M \subseteq \mathbb{R}^d$ is a lattice or an \mathcal{S} -lattice, all elements of $\text{OS}(M)/\text{OC}(M)$ have finite order. In particular, their order is a divisor of d ; see [45, 44].

Theorem 7.32. *Let $M \subseteq \mathbb{R}^d$ be a lattice or an \mathcal{S} -lattice. Then, the factor group given by $\text{OS}(M)/\text{OC}(M)$ is the direct sum of cyclic groups of prime power order that divide d . \square*

The close relationship between SSLs and CSLs is also reflected in the following condition for two CSLs to be equal.

Lemma 7.33 ([98, Lemma 3.4.2]). *Let $\Gamma \subset \mathbb{R}^d$ be a lattice. Assume that $R_1, R_2 \in \text{OC}(\Gamma)$ generate the same CSL, so $\Gamma(R_1) = \Gamma(R_2)$. Then, one has $\Sigma(R_1) = \Sigma(R_2)$ together with $\text{den}(R_1^{-1}) = \text{den}(R_2^{-1})$.*

Proof. The statement about Σ is trivial. For the denominator, observe that

$$\text{den}(R_1^{-1})\Gamma \subseteq \Gamma(R_1) = \Gamma(R_2) \subseteq R_2\Gamma.$$

Consequently,

$$\text{den}(R_1^{-1})R_2^{-1}\Gamma \subseteq \Gamma,$$

which shows that $\text{den}(R_1^{-1})$ is a multiple of $\text{den}(R_2^{-1})$. Then, by symmetry, $\text{den}(R_2^{-1})$ is a multiple of $\text{den}(R_1^{-1})$ as well, and the claim follows. \square

This result is particularly useful in the following examples, when we have to characterise those coincidence isometries that generate the same CSL. Let us start our series of illustrations with some examples in the plane.

8. (M)CSMS OF PLANAR MODULES WITH N -FOLD SYMMETRY

We can generalise the results of the square lattice to all rings $\mathbb{Z}[\xi_n]$ of cyclotomic integers which are PIDs; compare [72, 8]. Thus, let n be one of the numbers given in Eq. (5.11). We have seen in Section 5.2 that the similar submodules are then exactly the non-trivial ideals of $\mathbb{Z}[\xi_n]$, and that the similarity rotations are given by $\frac{v}{|v|}$ with $v \in \mathbb{Z}[\xi_n]$.

As any of these 29 modules is also a ring, we have $\text{MR}(\mathbb{Z}[\xi_n]) = \mathbb{Z}[\xi_n]$. This implies that the coincidence rotations are precisely given by $e^{i\varphi} = \frac{v}{|v|}$ for which $|v|^2 = v\bar{v}$ is a square in $\mathbb{Z}[\xi_n]$. In other words, using the unique prime factorisation up to units in $\mathbb{Z}[\xi_n]$, the coincidence rotations are precisely the rotations of the form $\varepsilon \frac{w}{\bar{w}}$ with $0 \neq w \in \mathbb{Z}[\xi_n]$, where ε is a unit in $\mathbb{Z}[\xi_n]$. Here, we may assume that $\frac{w}{\bar{w}}$ is a reduced fraction, which means that w and \bar{w} are coprime. Under this assumption, one finds

$$(8.1) \quad \mathbb{Z}[\xi_n] \cap \varepsilon \frac{w}{\bar{w}} \mathbb{Z}[\xi_n] = w \mathbb{Z}[\xi_n].$$

To find the possible values of w , we mention that a prime $\omega \in \mathbb{Z}[\xi_n]$ can be a factor of w only if $\frac{\omega}{\bar{\omega}}$ is not a unit in $\mathbb{Z}[\xi_n]$. Thus, we only have to consider the so-called *complex splitting primes*. To expand on this, consider the prime factorisation of a rational prime p over the real

subring $\mathcal{o}_n = \mathbb{Z}[\xi_n + \bar{\xi}_n]$, which is the ring of integers of the maximal real subfield $\mathbb{Q}(\xi_n + \bar{\xi}_n)$ of $\mathbb{Q}(\xi_n)$. Let π be a prime in \mathcal{o}_n . Now, the complex splitting primes are those primes π that split as $\pi = \omega_\pi \bar{\omega}_\pi$ over $\mathbb{Z}[\xi_n]$, with ω_π and $\bar{\omega}_\pi$ being non-associated primes in $\mathbb{Z}[\xi_n]$, which means that $\frac{\omega_\pi}{\bar{\omega}_\pi}$ is not a unit. Thus, the possible values of w are of the form

$$(8.2) \quad w = \varepsilon \prod_{\pi} \omega_{\pi}^{t_{\pi}^{+}} \bar{\omega}_{\pi}^{t_{\pi}^{-}},$$

where ε is a unit, $t_{\pi}^{+} t_{\pi}^{-} = 0$, and the product runs over all primes $\pi \in \mathcal{o}_n$ that divide $w \bar{w}$. In other words, any coincidence rotation in $\text{SOC}(\mathbb{Z}[\xi_n])$ can be written as a finite product

$$(8.3) \quad e^{i\varphi} = \varepsilon' \frac{w}{\bar{w}} = \varepsilon' \prod_{\pi} \left(\frac{\omega_{\pi}}{\bar{\omega}_{\pi}} \right)^{t_{\pi}},$$

with $t_{\pi} = t_{\pi}^{+} - t_{\pi}^{-}$, where π runs over the complex splitting primes of \mathcal{o}_n and where ε' is again a unit.

Any complex splitting prime $\pi \in \mathcal{o}_n$ lies over a unique rational prime p , which is the norm of π in \mathcal{o}_n . Then, one also calls p a complex splitting prime of the field extension $\mathbb{Q}(\xi_n)/\mathbb{Q}$. The set of all such rational primes is abbreviated as \mathcal{C}_n and thus consists of all rational primes that split in the final step from $\mathbb{Q}(\xi_n + \bar{\xi}_n)$ to $\mathbb{Q}(\xi_n)$. To expand on the structure of the primes and their splitting, we recall that the index $[\mathbb{Z}[\xi_n] : \omega_{\pi} \mathbb{Z}[\xi_n]] = p^{\ell_p}$ depends only on p , where ℓ_p is an integer which we will specify below. As a result, the CSM $\mathbb{Z}[\xi_n] \cap \varepsilon \frac{w}{\bar{w}} \mathbb{Z}[\xi_n] = w \mathbb{Z}[\xi_n]$ has index

$$(8.4) \quad \Sigma_{\mathbb{Z}[\xi_n]} \left(\varepsilon \frac{w}{\bar{w}} \right) = \prod_{\pi} p^{\ell_p |t_{\pi}|}$$

with t_{π} as introduced above. Thus, the possible coincidence indices are products of the so-called *basic indices* p^{ℓ_p} , and the coincidence spectrum is the (multiplicative) monoid generated by these basic indices. In other words,

$$(8.5) \quad \sigma(\mathbb{Z}[\xi_n]) = \left\{ \prod_{p \in \mathcal{C}_n} p^{\ell_p t_p} \mid t_p \in \mathbb{N}, \text{ only finitely many } t_p \neq 0 \right\},$$

where \mathcal{C}_n is the set of complex splitting primes as introduced above.

As $\mathbb{Z}[\xi_n]$ is a PID for the list of n we consider here, the counting function $c_n(m) = c_{\mathbb{Z}[\xi_n]}(m)$ is multiplicative, wherefore it suffices to determine it for $m = p^{\ell_p}$. This is now a purely combinatorial task, and one finally arrives at the following result.

Theorem 8.1 ([72, Thm. 3] and [8, Thm. 1]). *Let n be one of the 29 numbers from Eq. (5.11). Then, the generating function for the number $c_n(m) = c_{\mathbb{Z}[\xi_n]}(k)$ of CSMs of $\mathbb{Z}[\xi_n]$ of index k is given by*

$$\Psi_{\mathbb{Z}[\xi_n]}(s) = \sum_{k=1}^{\infty} \frac{c_n(k)}{k^s} = \frac{\zeta_{\mathbb{K}_n}(s)}{\zeta_{\mathbb{L}_n}(2s)} \begin{cases} (1 + p^{-s})^{-1}, & \text{if } n = p^r, \\ 1, & \text{otherwise,} \end{cases}$$

where $\zeta_{\mathbb{K}_n}(s)$ and $\zeta_{\mathbb{L}_n}(2s)$ are the Dedekind zeta functions of the number field $\mathbb{K}_n = \mathbb{Q}(\xi_n)$ and its maximal real subfield $\mathbb{L}_n = \mathbb{Q}(\xi_n + \bar{\xi}_n)$, respectively. If \mathcal{C}_n denotes the set of complex splitting primes for the field extension \mathbb{K}_n/\mathbb{Q} , then $\Psi_{\mathbb{Z}[\xi_n]}(s)$ has the Euler product expansion

$$\Psi_{\mathbb{Z}[\xi_n]}(s) = \prod_{p \in \mathcal{C}_n} \left(\frac{1 + p^{-\ell_p s}}{1 - p^{-\ell_p s}} \right)^{\frac{m_p}{2}},$$

with certain integers ℓ_p and m_p as follows. If $p \nmid n$, one has $m_p = \frac{\phi(n)}{\ell_p}$ where ℓ_p is the smallest positive integer such that $p^{\ell_p} \equiv 1 \pmod{n}$. If $p|n$ together with $n = p^t r$, where r and p are coprime, one has $m_p = \frac{\phi(r)}{\ell_p}$ where ℓ_p is the smallest positive integer such that $p^{\ell_p} \equiv 1 \pmod{r}$. \square

For explicit values of ℓ_p and m_p , see [8, Tables 1 and 2]. The first terms of $\Psi_{\mathbb{Z}[\xi_n]}(s)$ for all n from Eq. (5.11) are listed in [8, Table 4].

The explicit expression of $\Psi_{\mathbb{Z}[\xi_n]}(s)$ in terms of zeta functions allows us to determine the asymptotic behaviour of $c_n(k)$. Here, $\Psi_{\mathbb{Z}[\xi_n]}(s)$ is a meromorphic function that is analytic in the half-plane $\{\operatorname{Re}(s) > 1\}$ and has a simple pole at $s = 1$, which results in linear growth for the summatory function of $c_n(k)$. In particular, using Theorem 4.1, we get the following result.

Corollary 8.2 ([8, Cor. 1]). *The asymptotic behaviour of the number $c_n(k)$ of CSMs of $\mathbb{Z}[\xi_n]$ of index k is given by*

$$\sum_{k \leq x} c_n(k) \sim \gamma_n x$$

as $x \rightarrow \infty$, where γ_n is the residue of $\Psi_{\mathbb{Z}[\xi_n]}(s)$ at $s = 1$, which is given by

$$\gamma_n = \frac{\alpha_n}{\zeta_{\mathbb{L}_n}(2)} \begin{cases} p/(p+1), & \text{if } n = p^r, \\ 1, & \text{otherwise,} \end{cases}$$

with $\alpha_n := \operatorname{res}_{s=1}(\zeta_{\mathbb{K}_n}(s))$. \square

Note that the constants α_n and γ_n can be calculated by expressing $\zeta_{\mathbb{K}_n}(s)$ and $\zeta_{\mathbb{L}_n}(s)$ in terms of Riemann's zeta function $\zeta(s)$ and certain L -series; compare [8, Sec. 4]. For some examples including $n \in \{3, 4, 5, 7, 8, 12\}$, we refer to [72, Sec. 4], where the average $\gamma_n = \lim_{x \rightarrow \infty} \frac{1}{x} \sum_{k \leq x} c_n(k)$ has been evaluated explicitly. Numerical values for α_n and γ_n are listed in [8, Table 3].

Let us continue with multiple coincidences. As any MCSM is an intersection of simple CSMs, we see that

$$\begin{aligned} (8.6) \quad & \mathbb{Z}[\xi_n] \cap \varepsilon_1 \frac{w_1}{w_1} \mathbb{Z}[\xi_n] \cap \dots \cap \varepsilon_k \frac{w_k}{w_k} \mathbb{Z}[\xi_n] \\ & = w_1 \mathbb{Z}[\xi_n] \cap \dots \cap w_k \mathbb{Z}[\xi_n] = w \mathbb{Z}[\xi_n] \end{aligned}$$

with $w = \text{lcm}(w_1, \dots, w_k)$. Again, any MCSM is an ideal of $\mathbb{Z}[\xi_n]$, but w is more general now. Nevertheless, w is still of the form of a finite product,

$$(8.7) \quad w = \varepsilon \prod_{\pi} \omega_{\pi}^{t_{\pi}^{+}} \bar{\omega}_{\pi}^{t_{\pi}^{-}},$$

but now without any further restriction on the non-negative integers t_{π}^{+} and t_{π}^{-} . This shows that the coincidence spectrum does not change, so that

$$(8.8) \quad \sigma(\mathbb{Z}[\xi_n]) = \sigma_{\infty}(\mathbb{Z}[\xi_n]);$$

compare [8, Cor. 2].

It follows from Eq. (8.6) that any MCSM can actually be written as the intersection of only two simple CSMS. This allows one to determine the number $c_n^{\infty}(k)$ of MCSMs of $\mathbb{Z}[\xi_n]$ of index k . The result reads as follows.

Theorem 8.3 ([72, Thm. 3] and [8, Thm. 1]). *Let n be one of the 29 numbers from Eq. (5.11). Then, the generating function for the number $c_n^{\infty}(k) = c_{\mathbb{Z}[\xi_n]}^{\infty}(k)$ of CSMS of $\mathbb{Z}[\xi_n]$ of index k is given by*

$$\Psi_{\mathbb{Z}[\xi_n]}^{\infty}(s) = \sum_{k=1}^{\infty} \frac{c_n^{\infty}(k)}{k^s} = \prod_{p \in \mathcal{C}_n} \left(\frac{1}{1 - p^{-\ell_p s}} \right)^{m_p},$$

where \mathcal{C}_n denotes the set of complex splitting primes for the field extension \mathbb{K}_n/\mathbb{Q} and the integers ℓ_p and m_p are those from Theorem 8.1. \square

This nice generating function is due to the fact that we actually count all ideals whose index m factors into primes contained in \mathcal{C}_n . As $\Psi_{\mathbb{Z}[\xi_n]}^{\infty}(s)$ still has a simple pole at $s = 1$, using Theorem 4.1 once more, we get a linear growth behaviour again. The determination of the residue is a bit more complicated here, as $\Psi_{\mathbb{Z}[\xi_n]}^{\infty}(s)$ cannot be represented via zeta functions in a simple way. Still, one has the following result.

Corollary 8.4 ([8, Cor. 1]). *The summatory function $\sum_{k \leq x} c_n^{\infty}(k)$ has the asymptotic behaviour*

$$\sum_{k \leq x} c_n^{\infty}(k) \sim \beta_n x$$

as $x \rightarrow \infty$, with the growth constant $\beta_n = \text{res}_{s=1}(\Psi_{\mathbb{Z}[\xi_n]}^{\infty}(s)) = q_n \gamma_n$. Here, γ_n is defined as in Corollary 8.2, and q_n is given by

$$q_n := \lim_{s \rightarrow 1} \frac{\Psi_{\mathbb{Z}[\xi_n]}^{\infty}(s)}{\Psi_{\mathbb{Z}[\xi_n]}(s)} = \prod_{\ell=1}^{\infty} (\Psi_{\mathbb{Z}[\xi_n]}(2^{\ell}))^{2^{-\ell}}. \quad \square$$

The last formula in Corollary 8.4 is a consequence of the representation

$$(8.9) \quad \begin{aligned} \Psi_{\mathbb{Z}[\xi_n]}^{\infty}(s) &= (\Psi_{\mathbb{Z}[\xi_n]}^{\infty}(2^{L+1}s))^{2^{-(L+1)}} \prod_{\ell=0}^L (\Psi_{\mathbb{Z}[\xi_n]}(2^{\ell}s))^{2^{-\ell}} \\ &= \Psi_{\mathbb{Z}[\xi_n]}(s) \prod_{\ell=1}^{\infty} (\Psi_{\mathbb{Z}[\xi_n]}(2^{\ell}s))^{2^{-\ell}}, \end{aligned}$$

which holds for any integer $L \geq 0$; compare [8, Prop. 2]. As the infinite product converges rapidly, q_n , and thus β_n , can be calculated numerically in an efficient way; see [8, Table 3] for a list of values of β_n .

Example 8.5. Let us once more consider the square lattice for illustration. Theorem 8.3 implies that the generating function for its MCSLs reads

$$\begin{aligned} \Psi_{\square}^{\infty}(s) &= \sum_{m=1}^{\infty} \frac{c_{\square}^{\infty}(k)}{k^s} = (1 + 2^{-s})^{-1} \frac{\zeta_K(s)}{\zeta(2s)} \\ &= \prod_{p \equiv 1(4)} \frac{1}{(1 - p^{-s})^2} = \Psi_{\square}(s) \prod_{p \equiv 1(4)} \frac{1}{1 - p^{-2s}}, \end{aligned}$$

where we have employed the notation $c_{\square}^{\infty}(k) = c_4^{\infty}(k)$ for the number of MCSLs. The latter is a multiplicative function, whose values for (positive) prime powers are given by

$$c_{\square}^{\infty}(p^r) = \begin{cases} r + 1, & \text{if } p \equiv 1 \pmod{4}, \\ 0, & \text{otherwise.} \end{cases}$$

The first terms of the expansion read

$$\Psi_{\square}^{\infty}(s) = 1 + \frac{2}{5^s} + \frac{2}{13^s} + \frac{2}{17^s} + \frac{3}{25^s} + \frac{2}{29^s} + \frac{2}{37^s} + \frac{2}{41^s} + \frac{2}{53^s} + \dots,$$

and a comparison with $\Psi_{\square}(s)$ from Eq. (3.5) yields

$$\Psi_{\square}^{\infty}(s) - \Psi_{\square}(s) = \frac{1}{25^s} + \frac{2}{125^s} + \frac{1}{169^s} + \frac{1}{289^s} + \frac{2}{325^s} + \frac{2}{425^s} + \frac{3}{625^s} + \dots;$$

compare [8, Table 5]. Note that no additional MCSLs exist for square-free indices. The first terms of $\Psi_{\square}^{\infty}(s) - \Psi_{\square}(s)$ indicate that most MCSLs actually are simple CSLs, which is confirmed by the asymptotic growth rates of the summatory functions,

$$\gamma_{\square} := \gamma_4 = \frac{1}{\pi} \approx 0.318310 \quad \text{and} \quad \beta_{\square} := \beta_4 \approx 0.336193,$$

of the simple and multiple CSLs, respectively; compare [8, Table 3].

Furthermore, note that the simple CSLs are all primitive SSLs, whereas the additional MCSLs are all non-primitive SSLs. In fact, an SSL is an MCSL if and only if its index factors into primes $p \equiv 1 \pmod{4}$ only.

The possible coincidence indices are precisely the positive odd integers that are products of primes $p \equiv 1 \pmod{4}$ only. In other words, the coincidence spectra of the square lattice are given by

$$\sigma(\mathbb{Z}^2) = \sigma_{\infty}(\mathbb{Z}^2) = \{\text{all finite products of primes } \equiv 1 \pmod{4}\}$$

and thus agree in this case. \diamond

Let us now turn our attention to some important examples in three and four dimensions, where quaternions will play a fundamental role; compare Section 4.1. On the one hand, following Cayley, rotations in three and four dimensions can be parametrised conveniently by

quaternions, which allows us to exploit the algebraic structure of certain rings of quaternions, including the rings \mathbb{J} , \mathbb{L} and \mathbb{I} . On the other hand, these rings are either four-dimensional lattices themselves, like \mathbb{J} and \mathbb{L} , or they are related to lattices. For instance, the lattice A_4 is related to the icosian ring \mathbb{I} ; see Section 11.1. Likewise, the projections of \mathbb{J} and \mathbb{L} onto the three-dimensional imaginary subspace yield the body-centred and primitive cubic lattices, respectively. Moreover, \mathbb{I} is a $\mathbb{Z}[\tau]$ -lattice of rank 4 in the sense of Definition 6.2.

9. THE CUBIC LATTICES

The three-dimensional cubic lattices are among the most important lattices in crystallography, and the study of their coincidences is a classic problem [75, 47, 50, 48]. Later, these lattices have been revisited in a more mathematical context [4, 93]. Here, the key tool is the ring \mathbb{J} of Hurwitz quaternions, since it turns out that any coincidence rotation of a three-dimensional cubic lattice can be parametrised by a Hurwitz quaternion; compare [9, Sec. 2.5.4] as well as [14] and references therein for some general background.

Let us first define our setting. We use the conventions of [9, Ex. 3.2] and define

$$(9.1) \quad \Gamma_{\text{pc}} := \mathbb{Z}^3, \quad \Gamma_{\text{bcc}} := \mathbb{Z}^3 \cup (u + \mathbb{Z}^3), \quad \Gamma_{\text{fcc}} := \Gamma_{\text{bcc}}^*$$

with $u = \frac{1}{2}(1, 1, 1)$. Here, the index **pc** indicates that this lattice is a primitive cubic lattice, and likewise **bcc** and **fcc** denote the body-centred and the face-centred cubic lattices, respectively.

Traditionally, one starts with the primitive cubic lattice, partly due to the fact that this lattice allows the easiest treatment with elementary methods. We will deviate from this tradition here, as the body-centred lattice allows for the nicest description of its coincidence site lattices.

Fact 9.1. *One has $\Gamma_{\text{bcc}} \simeq \text{Im}(\mathbb{J})$ and $\Gamma_{\text{pc}} \simeq \text{Im}(\mathbb{L})$.* □

Recall that \mathbb{J} is a maximal order and a principal ideal ring, whereas \mathbb{L} is neither. This indicates that Γ_{bcc} is easier to deal with, because we can exploit the arithmetic properties of \mathbb{J} while relying on its ideal structure.

The first step in determining the CSLs of Γ is the determination of $\text{OC}(\Gamma)$. Since the point reflection $I: x \mapsto -x$ is a symmetry operation of all three-dimensional lattices, it is actually sufficient to determine $\text{SOC}(\Gamma)$. We get the following well-known result; compare [4, 15, 98].

Theorem 9.2. *Let $\Gamma_{\text{pc}}, \Gamma_{\text{bcc}}, \Gamma_{\text{fcc}} \subset \mathbb{R}^3$ be the primitive, the body-centred, and the face-centred cubic lattice of Eq. (9.1), respectively. Then, one has $\text{OC}(\Gamma_{\text{pc}}) = \text{OC}(\Gamma_{\text{bcc}}) = \text{OC}(\Gamma_{\text{fcc}}) = \text{O}(3, \mathbb{Q})$ together with*

$$\Sigma_{\text{pc}}(R) = \Sigma_{\text{bcc}}(R) = \Sigma_{\text{fcc}}(R)$$

for all $R \in \text{O}(3, \mathbb{Q})$.

Proof. The equality of the three OC-groups is a consequence of the fact that the three cubic lattices are mutually commensurate. The explicit form of the OC-group is most easily seen for the lattice $\Gamma_{\text{pc}} = \mathbb{Z}^3$, since the standard basis of \mathbb{R}^3 is also a lattice basis of \mathbb{Z}^3 .

Note that $\Gamma_{\text{pc}} \subset \Gamma_{\text{bcc}}$ is a sublattice of index 2. One easily verifies that $|x|^2$ is an integer for all $x \in \Gamma_{\text{pc}}$ and that $4|x|^2 \equiv 3 \pmod{4}$ for all $x \in \Gamma_{\text{bcc}} \setminus \Gamma_{\text{pc}}$. Hence, an application of Lemma 7.10 shows that $\Sigma_{\text{pc}}(R)$ divides $\Sigma_{\text{bcc}}(R)$. The reverse divisibility property can be obtained by considering the dual lattice $\Gamma_{\text{bcc}}^* = \Gamma_{\text{fcc}}$. In particular, $|x|^2$ is even for all $x \in \Gamma_{\text{bcc}}^*$ and odd for all $x \in \Gamma_{\text{pc}} \setminus \Gamma_{\text{bcc}}^*$. \square

Note that this result was already proved by Grimmer, Bollmann and Warrington [50]. Actually, they used a similar method in their proof, and Lemma 7.10 is a natural generalisation of their approach.

Remark 9.3. Let us note that $\text{OC}(\Gamma) = \text{OS}(\Gamma) = \text{O}(3, \mathbb{Q})$ holds for all cubic lattices of Eq. (9.1). We have determined $\text{OC}(\Gamma)$ explicitly above, but we could have argued more abstractly by using the connection of $\text{OS}(\Gamma)$ and $\text{OC}(\Gamma)$ as laid out in Section 7.6. It follows from Theorem 7.32 that all elements of $\text{OS}(\Gamma)/\text{OC}(\Gamma)$ have an order that divides 3. On the other hand, the cubic lattices are rational lattices, which implies that all elements of $\text{OS}(\Gamma)/\text{OC}(\Gamma)$ have an order at most 2. Thus, we indeed have $\text{OC}(\Gamma) = \text{OS}(\Gamma)$. Moreover, as Γ is commensurate to \mathbb{Z}^3 , the elements of $\text{OC}(\Gamma)$ are exactly the rational orthogonal matrices, $\text{O}(3, \mathbb{Q})$. \diamond

As any rotation in $\text{O}(3, \mathbb{Q})$ can be parametrised by a rational quaternion, we can parametrise the coincidence rotations by primitive Lipschitz or Hurwitz quaternions. Contrary to the traditional approach in crystallography, we opt for primitive Hurwitz quaternions here; compare [4]. In particular, via Eq. (4.1), one finds

$$(9.2) \quad \text{SOC}(\Gamma_{\text{bcc}}) = \{R(q) \mid q \in \mathbb{J}\} = \{R(q) \mid q \in \mathbb{J} \text{ is primitive}\}.$$

The first step in determining the coincidence index is the calculation of the denominator $\text{den}_\Gamma(R(q))$. From Eq. (4.1), we see that $\text{den}_\Gamma(R(q))$ must be a divisor of $|q|^2$. Taking into account that the greatest common divisor of all matrix entries of $R(q)$ is a power of 2, we get the following result.

Corollary 9.4. *For any cubic lattice Γ in the setting of Eq. (9.1), we have $\text{den}_\Gamma(R(q)) = \frac{|q|^2}{2^\ell}$, where q is a primitive Hurwitz quaternion and ℓ is the maximal exponent such that $2^\ell \mid |q|^2$. \square*

Note that ℓ is either 0 or 1, depending on whether $|q|^2$ is odd or even. If one chooses to use primitive Lipschitz quaternions, one gets $\ell \in \{0, 1, 2\}$ instead. Furthermore, note that the denominators for any similarity rotation R and its inverse are the same, $\text{den}_\Gamma(R^{-1}) = \text{den}_\Gamma(R)$, as $R^{-1}(q) = R(\bar{q})$.

Proposition 9.5. *For any cubic lattice $\Gamma \subset \mathbb{R}^3$ as in Eq. (9.1), we have*

$$\Sigma_\Gamma(R(q)) = \text{den}_\Gamma(R(q)) = \frac{|q|^2}{2^\ell},$$

where q is a primitive Hurwitz quaternion and ℓ is the maximal exponent such that $2^\ell \mid |q|^2$.

Proof. From Theorem 7.29, we know that the index $\Sigma_\Gamma(R(q))$ is a multiple of $\text{den}_\Gamma(R(q)) = \frac{|q|^2}{2^\ell}$ and a divisor of $\text{den}_\Gamma(R(q))^2$. As the latter is odd, so is $\Sigma_\Gamma(R(q))$, and it is thus sufficient to show that $\Sigma_\Gamma(R(q))$ divides $|q|^2$.

By Theorem 9.2, the coincidence indices are the same for all cubic lattices. Hence, it suffices to prove that $\Sigma_{\text{bcc}}(R(q))$ divides $|q|^2$. We observe $R(q)\text{Im}(xq) = \text{Im}(qx)$, which implies that $R(q)\text{Im}(\mathbb{J}q) = \text{Im}(q\mathbb{J})$, from which we infer that $\text{Im}(q\mathbb{J}) \subseteq \Gamma_{\text{bcc}}(R(q))$. Consequently, $\Sigma_{\text{bcc}}(R(q))$ divides the index $[\text{Im}(\mathbb{J}) : \text{Im}(q\mathbb{J})]$.

In order to determine the latter, we note that $[\mathbb{J} : q\mathbb{J}] = |q|^4$ for any $q \in \mathbb{J}$. Moreover, one has

$$[(\mathbb{J} \cap \text{Re}(\mathbb{H})) : ((q\mathbb{J}) \cap \text{Re}(\mathbb{H}))] = |q|^2,$$

where $\text{Re}(\mathbb{H})$ is to be understood as the real axis. Hence $[\text{Im}(\mathbb{J}) : \text{Im}(q\mathbb{J})] = \frac{[\mathbb{J} : q\mathbb{J}]}{[\text{Re}(\mathbb{J}) : \text{Re}(q\mathbb{J})]} = |q|^2$, and $\Sigma_{\text{bcc}}(R(q))$ thus divides $|q|^2$. \square

If $\text{den}_\Gamma(R(q))$ is square-free, there also exists a simple alternative proof. Since we have $\text{den}_\Gamma(R) = \text{den}_\Gamma(R^{-1})$ for the cubic lattices, Theorem 7.29 tells us that $\Sigma_\Gamma(R)^2$ divides $\text{den}_\Gamma(R)^3$, and if $\text{den}_\Gamma(R)$ is square-free, we may infer that $\Sigma_\Gamma(R) = \text{den}_\Gamma(R)$.

Remark 9.6. It follows from Proposition 9.5 that the coincidence indices are odd positive integers. Moreover, Lagrange's four-square theorem [52] tells us that any positive integer is a sum of four squares. Hence, for any odd n , there exists a Hurwitz quaternion q such that $n = |q|^2$. This implies that any odd positive integer is realised as a coincidence index, or in other words, the coincidence spectrum of any cubic lattice is precisely the set of positive odd integers, so $\sigma(\Gamma_{\text{bcc}}) = \sigma(\Gamma_{\text{pc}}) = \sigma(\Gamma_{\text{fcc}}) = 2\mathbb{N}_0 + 1$. \diamond

Proposition 9.7. *If q is a primitive Hurwitz quaternion with $|q|^2$ odd, one has the relation $\Gamma_{\text{bcc}}(R(q)) = \text{Im}(q\mathbb{J})$.*

Proof. We have seen $\text{Im}(q\mathbb{J}) \subseteq \Gamma_{\text{bcc}}(R(q))$ in the proof of Proposition 9.5. If $|q|^2$ is odd, then both sublattices have the same index,

$$\Sigma_{\text{bcc}}(R(q)) = |q|^2 = [\text{Im}(\mathbb{J}) : \text{Im}(q\mathbb{J})],$$

and hence $\text{Im}(q\mathbb{J}) = \Gamma_{\text{bcc}}(R(q))$. \square

If $|q|^2$ is even, q can be written as $q = rs$ with $r, s \in \mathbb{J}$, where $|r|^2$ is odd and $|s|^2 = 2^\ell$. As $R(s)$ is a symmetry operation of Γ_{bcc} , we see that $\Gamma_{\text{bcc}}(R(q)) = \Gamma_{\text{bcc}}(R(r)) = \text{Im}(r\mathbb{J})$.

An analogous result exists for the primitive cubic lattice \mathbb{Z}^3 and can be stated as follows; compare [98, Thm. 3.5.5].

Proposition 9.8. *If q is a primitive Lipschitz quaternion with $|q|^2$ odd, one has the relation $\Gamma_{\text{pc}}(R(q)) = \text{Im}(q\mathbb{L})$.*

Proof. From Proposition 9.7, we infer that

$$\Gamma_{\text{bcc}}(R(q)) \cap \text{Im}(\mathbb{L}) = \text{Im}(q\mathbb{J}) \cap \text{Im}(\mathbb{L}).$$

As $\Gamma_{\text{pc}}(R(q)) \subseteq \Gamma_{\text{bcc}}(R(q)) \cap \text{Im}(\mathbb{L})$, and both $\Gamma_{\text{pc}}(R(q))$ and $\Gamma_{\text{bcc}}(R(q)) \cap \text{Im}(\mathbb{L})$ have index 2 in $\Gamma_{\text{bcc}}(R(q))$, we also infer $\Gamma_{\text{pc}}(R(q)) = \Gamma_{\text{bcc}}(R(q)) \cap \text{Im}(\mathbb{L})$. A similar argument applied to $\text{Im}(q\mathbb{L}) \subseteq \text{Im}(q\mathbb{J}) \cap \text{Im}(\mathbb{L})$ shows that one has $\text{Im}(q\mathbb{L}) = \text{Im}(q\mathbb{J}) \cap \text{Im}(\mathbb{L})$, which completes the proof. \square

Again, in analogy to the situation for Γ_{bcc} , we can find a quaternion $r \in \mathbb{L}$ such that $\Gamma_{\text{pc}}(R(q)) = \text{Im}(r\mathbb{L})$ if $|q|^2$ is even.

Let us return to the CSLs of Γ_{bcc} . Proposition 9.7 shows that any CSL of Γ_{bcc} is the projection $\text{Im}(q\mathbb{J})$ of an ideal $q\mathbb{J}$ of \mathbb{J} . On the other hand, whenever q is an odd primitive quaternion, $\text{Im}(q\mathbb{J})$ is a CSL of Γ_{bcc} . If we can show that there is a bijection between the set of ideals $\{q\mathbb{J} \mid q \text{ is primitive and odd}\}$ and the set of CSLs, then we can easily count the CSLs of a given index, as the number of ideals of a fixed index is well known [87]. The first step into this direction is the following result.

Lemma 9.9. *Let $q, r \in \mathbb{J}$ such that $|q|^2$ and $|r|^2$ are odd. Then, one has $\text{Im}(q\mathbb{J}) \subseteq \text{Im}(r\mathbb{J})$ if and only if $q\mathbb{J} \subseteq r\mathbb{J}$.*

Proof. Only the ‘only if’ part is non-trivial. $\text{Im}(q\mathbb{J}) \subseteq \text{Im}(r\mathbb{J})$ implies that $|r|^2$ divides $|q|^2$. Now,

$$\text{Im}(r\mathbb{J}) = \text{Im}(r\mathbb{J}) + \text{Im}(q\mathbb{J}) = \text{Im}(r\mathbb{J} + q\mathbb{J}) = \text{Im}(s\mathbb{J}),$$

which shows that $|r|^2 = |s|^2$, where s is the greatest common left divisor of r and q . Hence $s^{-1}r \in \mathbb{J}$, but as $|s^{-1}r| = 1$, it must be a unit. Thus $q\mathbb{J} \subseteq s\mathbb{J} = r\mathbb{J}$. \square

From this, we infer the following result; compare [15] for a similar result in a more general context.

Corollary 9.10. *Let $q, r \in \mathbb{J}$ such that $|q|^2$ and $|r|^2$ are odd. Then, one has $\text{Im}(q\mathbb{J}) = \text{Im}(r\mathbb{J})$ if and only if $q\mathbb{J} = r\mathbb{J}$.* \square

In other words, putting the previous steps together, we have proved the following result.

Lemma 9.11. *The mapping $q\mathbb{J} \mapsto \Gamma_{\text{bcc}}(R(q))$, which maps the set of left ideals generated by primitive quaternions with $|q|^2$ odd onto the set of CSLs of Γ_{bcc} , is a bijection.* \square

An analogous result can be proved for the other cubic lattices as well.

Theorem 9.12. *The mapping $q\mathbb{J} \mapsto \Gamma_a(R(q)) = \text{Im}(q\mathbb{J}) \cap \Gamma_a$, with fixed type $a \in \{\text{pc}, \text{bcc}, \text{fcc}\}$, defines a bijection between the set of left ideals generated by primitive quaternions with $|q|^2$ odd and the set of CSLs of Γ_a .*

Proof. From $\Gamma_a(R(q)) \subseteq \Gamma_a$ and $\Gamma_a(R(q)) \subseteq \Gamma_{\text{bcc}}(R(q)) = \text{Im}(q\mathbb{J})$, we see that we must have $\Gamma_a(R(q)) \subseteq \text{Im}(q\mathbb{J}) \cap \Gamma_a$. As $[\Gamma_{\text{bcc}} : \Gamma_a]$ is a power of 2 and the coincidence indices are always odd, index considerations show that we even have $\Gamma_a(R(q)) = \text{Im}(q\mathbb{J}) \cap \Gamma_a$. Now, the theorem is a consequence of the bijection in Lemma 9.11, where index considerations confirm that $\text{Im}(q\mathbb{J}) = \text{Im}(q'\mathbb{J})$ holds if and only if $\text{Im}(q\mathbb{J}) \cap \Gamma_a = \text{Im}(q'\mathbb{J}) \cap \Gamma_a$. \square

So far, we get the following result for the arithmetic functions that count the number of CSLs and coincidence isometries for a given index, where we use $c_{\text{bcc}}(n) := c_{\Gamma_{\text{bcc}}}(n)$ for simplicity.

Corollary 9.13. *For the cubic lattices according to Eq. (9.1), one has*

$$c_{\text{bcc}}^{\text{iso}}(n) = c_{\text{bcc}}(n) = c_{\text{pc}}^{\text{iso}}(n) = c_{\text{pc}}(n) = c_{\text{fcc}}^{\text{iso}}(n) = c_{\text{fcc}}(n).$$

Proof. It follows from Theorem 9.12 that the number of CSLs of any cubic lattice for a given index is given by the number of left ideals generated by primitive q with $|q|^2$ odd, hence $c_{\text{bcc}}(n) = c_{\text{pc}}(n) = c_{\text{fcc}}(n)$. As the coincidence indices of a given coincidence isometry are the same for all cubic lattices, we also have $c_{\text{bcc}}^{\text{iso}}(n) = c_{\text{pc}}^{\text{iso}}(n) = c_{\text{fcc}}^{\text{iso}}(n)$.

It remains to show $c_{\text{bcc}}(n) = c_{\text{bcc}}^{\text{iso}}(n)$. By Section 7.4, $c^{\text{iso}}(n) = c^{\text{rot}}(n)$ holds for any lattice in odd dimensions and for any $n \in \mathbb{N}$. It thus suffices to show that $c_{\text{bcc}}(n) = c_{\text{bcc}}^{\text{rot}}(n)$. Recall that any coincidence rotation can be parametrised either by an odd primitive quaternion q or by a primitive quaternion $q(1+i)$, where q is again odd. As the rotation $R(1+i)$ is a symmetry operation of all three cubic lattices, q and $q(1+i)$ generate the same CSL. As all symmetry rotations are generated by quaternions u or $(1+i)u$, where u is a unit, Theorem 9.12 implies $c_{\text{bcc}}(n) = c_{\text{bcc}}^{\text{rot}}(n) = c_{\text{bcc}}^{\text{iso}}(n)$. \square

Actually, we can calculate $c_{\Gamma}(n)$ explicitly. We first note that $c_{\Gamma}(n)$ is multiplicative, as \mathbb{J} is a principal ideal ring and thus has an essentially unique prime factorisation. Let us recall that uniqueness is a bit subtle here, since \mathbb{J} is not Abelian, and the prime factorisation depends on the ordering of the factors in general. But, if we fix an ordering (by requiring that the norm of the prime factors should increase monotonically, say), the prime factors are unique up to units. Thus, $c_{\Gamma}(n)$ is determined by its values for prime powers, and, in particular, we have

$$(9.3) \quad c_{\text{bcc}}(p^r) = (p+1)p^{r-1}$$

if p is an odd prime, as $c_{\text{bcc}}(p^r)$ is the number of primitive ideals of norm p^{2r} ; see [59, Ch. 10]. Furthermore, note that $24c_{\text{bcc}}(p^r)$ is the number of primitive quaternions of norm p^r and $8c_{\text{bcc}}(p^r)$ is the number of primitive representations of p^r as a sum of four squares, which follows easily from the total number of representations; compare [52, 55]. Thus, $8c_{\text{bcc}}(m)$ is the number of primitive representations of m as a sum of four squares, if m is odd,¹⁰ and

¹⁰This is part of Jacobi's four-square theorem [52], which states that the number of ways to represent m as the sum of four squares is 8 times the sum of its divisors (if m is odd) and 24 times the sum of its odd divisors (if m is even).

$c_{\text{bcc}}(m) = 0$ for m even. Hence, we obtain an explicit expression for the generating function; see also [4] and [15, Sec. 2].

Theorem 9.14 ([4, Props. 3.2 and 3.3]). *For any cubic lattice $\Gamma \subset \mathbb{R}^3$ in the setting of Eq. (9.1), we have*

$$\text{OC}(\Gamma) = \text{OS}(\Gamma) = \text{OC}(\Gamma_{\text{bcc}}) = \text{O}(3, \mathbb{Q}).$$

In particular, if q is a primitive Hurwitz quaternion and ℓ is the maximal exponent such that $2^\ell \mid |q|^2$, then the coincidence index is given by

$$\Sigma_\Gamma(R(q)) = \Sigma_{\text{bcc}}(R(q)) = \text{den}_\Gamma(R(q)) = \frac{|q|^2}{2^\ell}.$$

Moreover, we have $\Psi_\Gamma(s) = \Psi_\Gamma^{\text{iso}}(s) = \Psi_{\text{bcc}}(s)$, which is given by the equation

$$\begin{aligned} \Psi_{\text{bcc}}(s) &= \sum_{m=1}^{\infty} \frac{c_\Gamma(m)}{m^s} = \prod_{p \neq 2} \frac{1 + p^{-s}}{1 - p^{1-s}} \\ &= \frac{1}{1 + 2^{-s}} \frac{\zeta_{\mathbb{J}}(s/2)}{\zeta(2s)} = \frac{1 - 2^{1-s}}{1 + 2^{-s}} \frac{\zeta(s) \zeta(s-1)}{\zeta(2s)} \\ &= 1 + \frac{4}{3^s} + \frac{6}{5^s} + \frac{8}{7^s} + \frac{12}{9^s} + \frac{12}{11^s} + \frac{14}{13^s} + \frac{24}{15^s} + \frac{18}{17^s} + \frac{20}{19^s} + \frac{32}{21^s} + \dots, \end{aligned}$$

where all positive odd integers appear in the denominator. □

Here, we have made use of the zeta function $\zeta_{\mathbb{J}}$ of the Hurwitz ring from Eq. (5.21), which counts the non-trivial left ideals of \mathbb{J} . We observe that $\zeta_{\mathbb{J}}(s)$ and $\Psi_{\text{bcc}}(s)$ differ by the factors $\frac{1}{1+2^{-s}}$ and $\frac{1}{\zeta(2s)}$. Note that the term $(1+2^{-s})\zeta(2s)$ is the generating function for the two-sided ideals of \mathbb{J} . But as the two-sided ideals only generate the trivial CSL $\Gamma(R) = \Gamma$, they do not contribute to $\Psi_{\text{bcc}}(s)$, hence their contribution to $\zeta_{\mathbb{J}}(s)$ has to be factored out to obtain the generating function $\Psi_{\text{bcc}}(s)$.

It follows from the properties of Riemann's zeta function that $\Psi_{\text{bcc}}(s)$ is a meromorphic function of s . In particular, Ψ_{bcc} is analytic in the half-plane $\{\text{Re}(s) \geq 2\}$, and its rightmost pole is located at $s = 2$. Using Delange's theorem (Theorem 4.1), we find the asymptotic growth behaviour (compare [4] and [15, Sec. 2])

$$(9.4) \quad \sum_{n \leq x} c_{\text{bcc}}(n) = \frac{3x^2}{\pi^2} + \mathcal{O}(x^2), \quad \text{as } x \rightarrow \infty.$$

In contrast to the CSLs of the square and the triangular lattice in the plane, the CSLs of the cubic lattice generally fail to be similar sublattices, and usually have lower symmetries; see [93] for details.

Remark 9.15. It is an interesting question what kind of grain boundaries are compatible with CSLs of cubic lattices, as the geometric situation in 3-space is certainly richer than in the plane. Now, a large number of CSLs for cubic lattices can be written as $\Gamma(R)$, where R

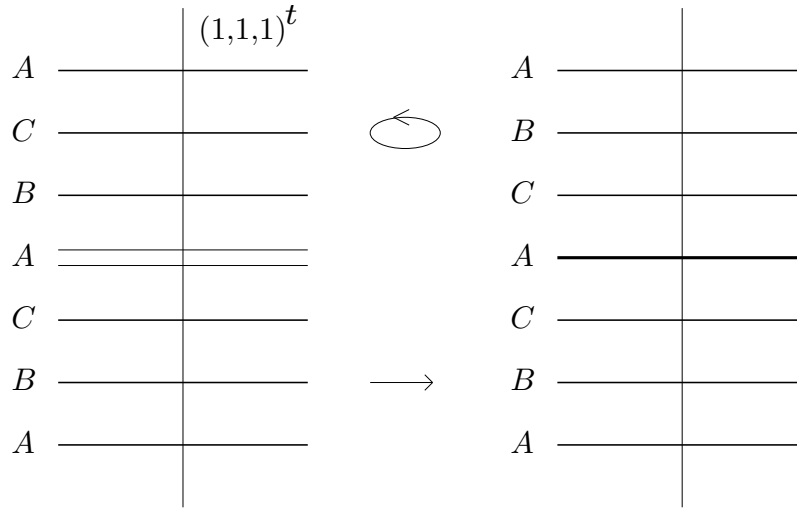


FIGURE 2. Sketch of a stacking fault in a cubic crystal. The upper half is rotated through an angle π about the $(1, 1, 1)^t$ -axis. This keeps the A layers fixed and interchanges layers of types B and C .

is actually a rotation through π around an axis in a lattice direction v . These are precisely the rotations parametrised by a quaternion $q = (0, v)$; compare [46].

The lattice planes perpendicular to v through a point nv with $n \in \mathbb{Z}$ are invariant under a rotation about v through π . Any of these can act as a defect-free (or perfect) grain boundary between two crystal halves, and the entire configuration appears as a stacking fault; see Figure 2 for an illustration of a stacking sequence that corresponds to a CSL with index $\Sigma = 3$ and hexagonal symmetry. Note that the order of the layers is reversed in the rotated half.

In contrast to cubic lattices, a rotation R through π about a lattice vector v is not necessarily a coincidence rotation for a general lattice. However, if R is a coincidence rotation, the corresponding lattice planes orthogonal to v are invariant under R , and analogous stacking faults may occur.

Apart from their obvious relevance to the twinning structure of cubic crystals, coincidence isometries in the form of rotations through π or simple reflections are useful generators for more complicated coincidence isometries in higher dimensions. In fact, this leads to one of the few approaches to higher dimensions known so far; see Section 13 below for more. \diamond

Remark 9.16. The results for the cubic lattices can be generalised to certain embedded \mathbb{Z} -modules of the form $\text{Im}(\mathcal{O})$, where \mathcal{O} is a maximal order in a quaternion algebra [15]. The situation is quite convenient in the case of quaternion algebras $\mathbb{H}(K)$ over a real algebraic number field K such that both K and $\mathbb{H}(K)$ have class number 1. In particular, apart from the Hurwitz ring \mathbb{J} , this includes the icosian ring $\mathbb{I} \subset \mathbb{H}(\mathbb{Q}(\sqrt{5}))$ and the cubian ring $\mathbb{K} \subset \mathbb{H}(\mathbb{Q}(\sqrt{2}))$; see [14, 15] for details.

The counterpart to the odd primitive quaternions are the so-called \mathcal{O} -reduced quaternions. If q is \mathcal{O} -reduced, many of our results for the cubic lattices can be reformulated for $\mathcal{O} \subset \mathbb{H}(K)$. In particular, the coincidence index is given by $\Sigma_{\mathcal{O}}(R(q)) = N(|q|^2)$, where N is the norm in the number field K ; compare [15, Prop. 5]. This follows from the explicit expression for the CSMs

$$\mathrm{Im}(\mathcal{O}) \cap \mathrm{Im}(q\mathcal{O}q^{-1}) = \mathrm{Im}(\mathcal{O} \cap q\mathcal{O}q^{-1}) = \mathrm{Im}(q\mathcal{O});$$

compare [15, Lemmas 4, 5 and 6]. Moreover, there still is a bijection between the CSMs $\mathrm{Im}(q\mathcal{O})$ and the left ideals $q\mathcal{O}$; see [15, Thm. 1]. This makes it possible to count the CSMs and to write down an explicit expression for the generating function [15, Thm. 2], namely

$$\Psi_{\mathcal{O}}^{\mathrm{iso}}(s) = \Psi_{\mathcal{O}}(s) = \frac{\zeta_{\mathcal{O}}(s/2)}{\zeta_{\mathcal{O},\mathcal{O}}(s/2)} = E(s) \frac{\zeta_K(s) \zeta_K(s-1)}{\zeta_K(2s)}.$$

Here, $\zeta_{\mathcal{O}}(s)$ and $\zeta_{\mathcal{O},\mathcal{O}}(s)$ denote the zeta functions of the left and the two-sided ideals of \mathcal{O} , respectively, whereas $\zeta_K(s)$ is the zeta function of K and $E(s)$ is either 1 or an additional analytic factor that takes care of the extra contributions from (finitely many) ramified primes. As a consequence, one gets the asymptotic behaviour [15, Cor. 1]

$$\sum_{n \leq x} c_{\mathcal{O}}(n) \sim \rho_{\mathcal{O}} \frac{x^2}{2}, \quad \text{as } x \rightarrow \infty$$

for some $\rho_{\mathcal{O}} \in \mathbb{R}_+$. ◇

10. THE FOUR-DIMENSIONAL HYPERCUBIC LATTICES

Let us continue with some examples in 4-space, and let us start with the hypercubic lattices. So far, in all our examples, the generating functions for the number of coincidence rotations (modulo symmetries) and the number of CSLs coincided, as two different coincidence rotations generated the same CSL if and only if they were symmetry related. This is no longer the case in the examples to come.

10.1. The centred hypercubic lattice D_4^* . As we have already seen in Section 5.5, any similarity rotation can be parametrised by a pair of \mathbb{J} -primitive Hurwitz quaternions, where $\mathbb{J} = D_4^*$ as lattices in our setting. In fact, it follows from Corollary 7.28 and Eq. (5.23) that $R = R(p, q)$ is a coincidence rotation of \mathbb{J} if and only if $|pq| \in \mathbb{N}$. A pair $(p, q) \in \mathbb{J} \times \mathbb{J}$ with $|pq| \in \mathbb{N}$ is called *admissible*. Thus, $R(p, q)$ is a coincidence rotation of \mathbb{J} if and only if $R(p, q)$ can be parametrised by an admissible pair of \mathbb{J} -primitive Hurwitz quaternions. As a consequence, we have the following result.

Fact 10.1. $\mathrm{SOC}(\mathbb{J}) = \mathrm{SO}(4, \mathbb{Q})$. □

However, it turns out that primitive quaternions are not an optimal choice in this case, and we prefer a suitably scaled pair. To find such a pair, note first that $|pq|^2$ is a square in \mathbb{N}

for any admissible pair, and so is $|pq|^2 / \gcd(|p|^2, |q|^2)^2$. As the two factors

$$\frac{|q|^2}{\gcd(|p|^2, |q|^2)} \quad \text{and} \quad \frac{|p|^2}{\gcd(|p|^2, |q|^2)}$$

are coprime, they must be squares as well. Hence, we can define the (coprime) integers

$$(10.1) \quad \alpha_p := \sqrt{\frac{|q|^2}{\gcd(|p|^2, |q|^2)}} \quad \text{and} \quad \alpha_q := \sqrt{\frac{|p|^2}{\gcd(|p|^2, |q|^2)}}.$$

Of course, $(x, y) = (\alpha_p p, \alpha_q q)$ defines the same rotation as (p, q) . However, we can deal more easily with (x, y) since $|x|^2 = |y|^2$. Moreover, the octuple $(x, y) = (\alpha_p p, \alpha_q q)$ is primitive for primitive p and q , in the sense that $\frac{1}{n}(\alpha_p p, \alpha_q q) \in \mathbb{J} \times \mathbb{J}$ if and only if $n \in \{\pm 1\}$. This guarantees that there exist quaternions $v, w \in \mathbb{J}$ such that $\langle x|v \rangle + \langle y|w \rangle = 1$. We shall call a pair of quaternions with these two properties an *extended admissible pair*, and denote it by $(p_\alpha, q_\alpha) = (\alpha_p p, \alpha_q q)$.

Clearly, scaling quaternions does not change the rotation $R(p, q)$. On the other hand, there are a lot of rotations that yield the same CSL, namely all rotations that only differ by a symmetry operation of \mathbb{J} . Let us denote the corresponding group by

$$\text{SO}(\mathbb{J}) := \{R \in \text{SO}(4, \mathbb{R}) \mid R\mathbb{J} = \mathbb{J}\},$$

which is a group of order $24^2 = 576$. Recall that we call two coincidence rotations R, R' symmetry related if there exists an $S \in \text{SO}(\mathbb{J})$ such that $R' = RS$ holds.

Let us have a closer look at symmetry-related rotations. It follows from $R(p, q)\mathbb{J} = \frac{1}{|pq|}p\mathbb{J}\bar{q}$ that $R(p, q)\mathbb{J} = R(p', q')\mathbb{J}$ if and only if

$$\frac{1}{|pp'|}\bar{p}p'\mathbb{J} = \frac{1}{|qq'|}\mathbb{J}\bar{q}q'.$$

This means that (p, q) and (pr, qr) are symmetry related if and only if r is a quaternion such that $r\mathbb{J}$ is a two-sided ideal. Apart from scaling factors and units, the only non-trivial such quaternion is $r = 1 + i$; see [87, 61, 36, 59]. Thus, $R(p, q)\mathbb{J} = R(pr, qr)\mathbb{J}$, and, as r is the only prime quaternion (up to units) of norm $|r|^2 = 2$, we can find, for any rotation $R \in \text{SOC}(\mathbb{J})$, a pair of quaternions (p, q) with $|p|^2$ and $|q|^2$ odd such that R is symmetry related to $R(p, q)$. We can thus confine our considerations to the latter rotations, and we will call an extended admissible pair (p, q) with $|p|^2$ and $|q|^2$ odd an *odd extended admissible pair*.

In fact, we can express all CSLs in terms of odd extended admissible pairs as follows.

Lemma 10.2. *If (p, q) is an odd extended admissible pair, one has*

$$p\mathbb{J} + \mathbb{J}\bar{q} \subseteq \mathbb{J} \cap \frac{p\mathbb{J}\bar{q}}{|pq|}.$$

Proof. Clearly, $p\mathbb{J} \subseteq \mathbb{J}$ and $\mathbb{J}\bar{q} \subseteq \mathbb{J}$, thus giving $p\mathbb{J} + \mathbb{J}\bar{q} \subseteq \mathbb{J}$. On the other hand, since $|p|^2 = |q|^2$, one has

$$(10.2) \quad p\mathbb{J} = \frac{p\mathbb{J}q\bar{q}}{|q|^2} \subseteq \frac{p\mathbb{J}\bar{q}}{|q|^2} = \frac{p\mathbb{J}\bar{q}}{|pq|},$$

and a similar argument for $\mathbb{J}\bar{q}$ yields $p\mathbb{J} + \mathbb{J}\bar{q} \subseteq \frac{p\mathbb{J}\bar{q}}{|pq|}$. \square

The first step for the converse inclusion is the following result, where we return to the more general case of extended admissible pairs for a moment.

Lemma 10.3. *If (p, q) is an extended admissible pair, one has*

$$2 \left(\mathbb{J} \cap \frac{p\mathbb{J}\bar{q}}{|pq|} \right) \subseteq p\mathbb{J} + \mathbb{J}\bar{q}.$$

Proof. Let $x \in \mathbb{J} \cap \frac{p\mathbb{J}\bar{q}}{|pq|}$. Then, there exists a $y \in \mathbb{J}$ such that $x = \frac{py\bar{q}}{|pq|}$. Since (p, q) is an extended admissible pair, there exist quaternions $v, w \in \mathbb{J}$ such that $\langle p|v \rangle + \langle q|w \rangle = 1$. Consequently,

$$\begin{aligned} 2x &= 2(\langle p|v \rangle + \langle q|w \rangle)x = 2\langle p|v \rangle x + 2x\langle q|w \rangle = p\bar{v}x + v\bar{p}x + xq\bar{w} + xw\bar{q} \\ &= p\bar{v}x + vy\bar{q} + py\bar{w} + xw\bar{q} \in p\mathbb{J} + \mathbb{J}\bar{q}, \end{aligned}$$

where we have made use of the identity $\langle a|b \rangle = \frac{1}{2}(a\bar{b} + b\bar{a})$. \square

Trivially, since $|p|^2 = |q|^2$, one has

$$|p|^2 \left(\mathbb{J} \cap \frac{p\mathbb{J}\bar{q}}{|pq|} \right) = |p|^2 \mathbb{J} \cap p\mathbb{J}\bar{q} \subseteq p\mathbb{J} + \mathbb{J}\bar{q}.$$

If we restrict again to odd extended admissible pairs, we get

$$\mathbb{J} \cap \frac{p\mathbb{J}\bar{q}}{|pq|} = 2 \left(\mathbb{J} \cap \frac{p\mathbb{J}\bar{q}}{|pq|} \right) + |p|^2 \left(\mathbb{J} \cap \frac{p\mathbb{J}\bar{q}}{|pq|} \right) \subseteq p\mathbb{J} + \mathbb{J}\bar{q},$$

since $|p|^2$ is odd. Hence, we have proved the following result.

Theorem 10.4. *Let (p, q) be an odd extended admissible pair. Then,*

$$\mathbb{J} \cap \frac{p\mathbb{J}\bar{q}}{|pq|} = p\mathbb{J} + \mathbb{J}\bar{q},$$

so each CSL of the centred hypercubic lattice is of the form $p\mathbb{J} + \mathbb{J}\bar{q}$ for a suitable odd extended admissible pair. \square

This explicit expression of the CSLs of \mathbb{J} in terms of a sum of ideals of \mathbb{J} is very useful, as it does not only help to calculate their indices, but it also allows us to determine which coincidence rotations yield the same CSL.

Let us first state the result for the index.

Theorem 10.5 ([98, Theorem 4.1.6]). *If (p, q) is an odd extended admissible pair, one has $\Sigma(R(p, q)) = |p|^2$.*

Sketch of proof. The idea of the proof is to exploit the equation

$$p\mathbb{J} \subseteq p\mathbb{J} + \mathbb{J}\bar{q} = \mathbb{J} \cap \frac{p\mathbb{J}\bar{q}}{|pq|} \subseteq \mathbb{J}$$

to show $\Sigma(R(\bar{p}, q))\Sigma(R(p, q)) = |p|^4$. By proving that the index $\Sigma(R(p, q))$ divides $|p|^2$, one then infers $\Sigma(R(p, q)) = |p|^2$. For the rather technical details, we refer to [98]. \square

Remark 10.6. It may be useful to formulate the index in terms of primitive admissible pairs. Let p, q be primitive odd quaternions with associated extended pair $(p_\alpha, q_\alpha) = (\alpha_p p, \alpha_q q)$. Then,

$$\begin{aligned}\Sigma(R(p, q)) &= \alpha_p^2 |p|^2 = \alpha_q^2 |q|^2 = \alpha_p \alpha_q |pq| \\ &= \text{lcm}(|p|^2, |q|^2) = \alpha_p^2 \alpha_q^2 \text{gcd}(|p|^2, |q|^2).\end{aligned}$$

Note that $|pq|$ is the denominator of $R(p, q)$. This shows that, in general, $\text{den}(R)$ and $\Sigma(R)$ do *not* coincide for the lattice D_4^* , which is in contrast to the three-dimensional cubic lattices. In fact, $\text{den}(R) = \Sigma(R)$ holds if and only if $\alpha_p = \alpha_q = 1$. \diamond

Remark 10.7. This explicit expression for the coincidence indices allows us to determine the coincidence spectrum. As in Remark 9.6, we conclude that $|p|^2$ and $|q|^2$ run through all odd positive integers, and the possible coincidence indices thus are exactly the odd positive integers. In other words, the coincidence spectrum of D_4^* and D_4 , which we know to be similar lattices, is the set of all odd positive integers,

$$\Sigma(\text{SOC}(D_4^*)) = \Sigma(\text{SOC}(D_4)) = 2\mathbb{N}_0 + 1.$$

This is exactly the same spectrum we have found for the three-dimensional cubic lattices; compare Remark 9.6. As D_4^* has reflections among its symmetry operations, this is also the full spectrum $\Sigma(\text{OC}(D_4^*)) = \Sigma(\text{SOC}(D_4^*))$ by Remark 7.8. \diamond

Our next task is to enumerate the coincidence isometries of D_4^* . Since the point group of D_4^* contains $24^2 = 576$ rotations, the number of coincidence rotations of a given index n can be written as $576 c_{D_4^*}^{\text{rot}}(n)$. As the point group contains also reflections, the number of coincidence isometries is twice this number, $1152 c_{D_4^*}^{\text{rot}}(n)$.

By Theorem 10.5, counting the number of coincidence rotations is equivalent to counting the number of odd extended admissible pairs. We first observe that $c_{D_4^*}^{\text{rot}}(n)$ is a multiplicative function, which follows from the essentially unique prime factorisation in \mathbb{J} . Indeed, if (p, q) and (r, s) are odd extended admissible pairs with $|p|^2 = m$ and $|r|^2 = n$ for m, n coprime, (pr, qs) is an odd extended admissible pair with $|pr|^2 = mn$. Conversely, any odd extended admissible pair (p, q) with $|p|^2 = mn$ can be decomposed into odd extended admissible pairs with index m and n , respectively. As this decomposition is unique up to units, multiplicativity follows.

Thus, we only need to compute $c_{D_4^*}^{\text{rot}}(n)$ for n being a prime power. In the following, let π denote a rational prime (we choose π here as we have used p for quaternions already). As odd extended admissible pairs consist of odd quaternions only, $c_{D_4^*}^{\text{rot}}(2^r) = 0$. Hence, π is always odd in what follows. It is now a purely combinatorial task to determine $c_{D_4^*}^{\text{rot}}(\pi^r)$. The number of primitive quaternions p with norm $|p|^2 = \pi^r$ is given by $24f(\pi^r)$ with $f(\pi^r) = (\pi + 1)\pi^{r-1}$

for $r \geq 1$; compare Eq. (9.3). Any odd extended admissible pair (p, q) with $|p|^2 = \pi^r$ can be obtained from a primitive admissible pair (p_1, q_1) with $|p_1|^2 = \pi^{r'}$, $|q_1|^2 = \pi^{r''}$, $r = \max(r', r'')$, and $r' - r''$ even. Hence,

$$(10.3) \quad \begin{aligned} c_{D_4^*}^{\text{rot}}(\pi^r) &= f(\pi^r)^2 + 2 \sum_{s=1}^{\lfloor r/2 \rfloor} f(\pi^r) f(\pi^{r-2s}) \\ &= \frac{\pi+1}{\pi-1} \pi^{r-1} (\pi^{r+1} + \pi^{r-1} - 2). \end{aligned}$$

Let us summarise this result in the following theorem, where we change the notation and use p to denote a rational prime.

Theorem 10.8. *The number of coincidence rotations of D_4^* of index n is given by $576 c_{D_4^*}^{\text{rot}}(n)$, where $c_{D_4^*}^{\text{rot}}(n)$ is a multiplicative arithmetic function. It is determined by $c_{D_4^*}^{\text{rot}}(2^r) = 0$ for $r \geq 1$ together with*

$$c_{D_4^*}^{\text{rot}}(p^r) = \frac{p+1}{p-1} p^{r-1} (p^{r+1} + p^{r-1} - 2)$$

if p is an odd prime and $r \geq 1$. □

The multiplicativity of $c_{D_4^*}^{\text{rot}}(n)$ guarantees that the corresponding Dirichlet series generating function can be written as an Euler product,

$$(10.4) \quad \begin{aligned} \Psi_{D_4^*}^{\text{rot}}(s) &= \sum_{n=1}^{\infty} \frac{c_{D_4^*}^{\text{rot}}(n)}{n^s} = \prod_{p \neq 2} \frac{(1+p^{-s})(1+p^{1-s})}{(1-p^{1-s})(1-p^{2-s})} \\ &= \frac{1-2^{1-s}}{1+2^{-s}} \frac{1-2^{2-s}}{1+2^{1-s}} \frac{\zeta(s)\zeta(s-1)^2\zeta(s-2)}{\zeta(2s)\zeta(2s-2)}, \end{aligned}$$

where the first few terms read as follows,

$$\Psi_{D_4^*}^{\text{rot}}(s) = 1 + \frac{16}{3^s} + \frac{36}{5^s} + \frac{64}{7^s} + \frac{168}{9^s} + \frac{144}{11^s} + \frac{196}{13^s} + \frac{576}{15^s} + \frac{324}{17^s} + \frac{400}{19^s} + \frac{1024}{21^s} + \dots$$

It is remarkable that $\Psi_{D_4^*}^{\text{rot}}(s)$ can be expressed in terms of the cubic generating function $\Psi_{\text{bcc}}(s)$ from Theorem 9.14, which follows immediately from its explicit expression in terms of zeta functions from Eq. (10.4). In particular, one has

$$(10.5) \quad \Psi_{D_4^*}^{\text{rot}}(s) = \Psi_{\text{bcc}}(s)\Psi_{\text{bcc}}(s-1).$$

This explicit expression shows that $\Psi_{D_4^*}^{\text{rot}}(s)$ is a meromorphic function in the complex plane. Its rightmost pole is at $s = 3$, with residue $\frac{630}{\pi^6}\zeta(3)$. Using Theorem 4.1, we obtain the asymptotic behaviour

$$\sum_{n \leq x} c_{D_4^*}^{\text{rot}}(n) \sim \frac{210}{\pi^6} \zeta(3) x^3 \approx 0.262570 x^3$$

as $x \rightarrow \infty$.

Next, we want to calculate the number $c_{D_4^*}(n)$ of distinct CSLs of a given index n . In contrast to the three-dimensional cubic lattices, where we have $c^{\text{rot}}(n) = c(n)$, it turns out

that $c_{D_4^*}(n)$ and $c_{D_4^*}^{\text{rot}}(n)$ generally differ. Clearly, we have the upper bound $c_{D_4^*}(n) \leq c_{D_4^*}^{\text{rot}}(n)$. To calculate $c_{D_4^*}(n)$, we must determine which coincidence rotations generate the same CSL.

One knows from Lemma 7.33 that two CSLs can only agree if the corresponding coincidence indices are the same. In addition, the denominators of the inverses must be equal, but as $\text{den}(R) = \text{den}(R^{-1})$, we infer that the denominators must be the same as well. However, these conditions are not yet sufficient. In fact, we need additional conditions, which are a bit technical; compare [19] and see [98, Thm. 4.1.12] for a proof.

Theorem 10.9. *Let (q_1, p_1) and (q_2, p_2) be two primitive admissible pairs of odd quaternions. Then, the relation*

$$\mathbb{J} \cap \frac{p_1 \mathbb{J} \bar{q}_1}{|p_1 q_1|} = \mathbb{J} \cap \frac{p_2 \mathbb{J} \bar{q}_2}{|p_2 q_2|}$$

holds if and only if the following conditions are satisfied (up to units):

- (1) $|p_1 q_1| = |p_2 q_2|$,
- (2) $\text{lcm}(|p_1|^2, |q_1|^2) = \text{lcm}(|p_2|^2, |q_2|^2)$,
- (3) $\text{gcd}(p_1, |p_1 q_1|) = \text{gcd}(p_2, |p_2 q_2|)$, and
- (4) $\text{gcd}(q_1, |p_1 q_1|) = \text{gcd}(q_2, |p_2 q_2|)$. □

Note that the first two conditions correspond to the aforementioned condition that the coincidence indices and the denominator are the same (recall from Remark 10.6 that $\Sigma(R(p, q)) = \text{lcm}(|p|^2, |q|^2)$ and $\text{den}(R(p, q)) = |pq|$, if (p, q) is a primitive admissible pair of odd quaternions).

Remark 10.10. One gets an equivalent set of conditions for the equality of two CSLs if one replaces conditions (1) and (2) in Theorem 10.9 by $|p_1|^2 = |p_2|^2$ and $|q_1|^2 = |q_2|^2$. It is obvious that the two conditions $|p_1|^2 = |p_2|^2$ and $|q_1|^2 = |q_2|^2$ imply that the denominators $|p_1 q_1| = |p_2 q_2|$ and the coincidence indices $\text{lcm}(|p_1|^2, |q_1|^2) = \text{lcm}(|p_2|^2, |q_2|^2)$ are the same. The reverse direction is more complicated, as the two conditions $|p_1 q_1| = |p_2 q_2|$ and $\text{lcm}(|p_1|^2, |q_1|^2) = \text{lcm}(|p_2|^2, |q_2|^2)$ alone only yield $\text{gcd}(|p_1|^2, |q_1|^2) = \text{gcd}(|p_2|^2, |q_2|^2)$, but not $|p_1|^2 = |p_2|^2$ and $|q_1|^2 = |q_2|^2$ directly. In fact, we need both of the other two conditions, $\text{gcd}(p_1, |p_1 q_1|) = \text{gcd}(p_2, |p_2 q_2|)$ and $\text{gcd}(q_1, |p_1 q_1|) = \text{gcd}(q_2, |p_2 q_2|)$, to establish $|p_1|^2 = |p_2|^2$ and $|q_1|^2 = |q_2|^2$ as well; compare [98, Proof of Thm. 4.1.12 and Rem. 4.1.13]. ◇

We are now ready to count the number $c_{D_4^*}(n)$ of CSLs. It follows from Theorem 7.18 that $c_{D_4^*}(n)$ is multiplicative, since $c_{D_4^*}^{\text{iso}}(n)$ is multiplicative. As there are no CSLs of even index, $c_{D_4^*}(n)$ is completely determined by $c_{D_4^*}(\pi^r)$ for odd rational primes π and $r \in \mathbb{N}$. The latter can be calculated by counting the number of odd primitive admissible pairs that satisfy the conditions in Theorem 10.9 or in Remark 10.10. Thus,

$$(10.6) \quad c_{D_4^*}(\pi^r) = f(\pi^r)^2 + 2 \sum_{s=1}^{\lfloor r/2 \rfloor} f(\pi^{r-s}) f(\pi^{r-2s}),$$

where $f(\pi^r) = (\pi + 1)\pi^{r-1}$ for $r \geq 1$ as above. Note that this expression is very similar to Eq. (10.3), the only difference being that one factor $f(\pi^r)$ is replaced by $f(\pi^{r-s})$, where the latter counts the number of distinct $\text{gld}(p, |pq|)$ with $|p|^2 = \pi^r$ and $|q|^2 = \pi^{r-2s}$.

Evaluating the sum yields the following result, where we again switch to p to denote a rational prime.

Theorem 10.11. *The number of distinct CSLs of D_4^* of index n is given by $c_{D_4^*}(n)$. Here, $c_{D_4^*}(n)$ is a multiplicative arithmetic function, which is completely determined by $c_{D_4^*}(2^r) = 0$ for $r \geq 1$ together with*

$$c_{D_4^*}(p^r) = \begin{cases} \frac{(p+1)^2}{p^3-1} (p^{2r+1} + p^{2r-2} - 2p^{\frac{r-1}{2}}), & \text{if } r \geq 1 \text{ is odd,} \\ \frac{(p+1)^2}{p^3-1} (p^{2r+1} + p^{2r-2} - 2\frac{p^2+1}{p+1}p^{\frac{r-2}{2}}), & \text{if } r \geq 2 \text{ is even,} \end{cases}$$

for odd primes p . Then,

$$\begin{aligned} \Psi_{D_4^*}(s) &= \sum_{n=1}^{\infty} \frac{c_{D_4^*}(n)}{n^s} = \prod_{p \neq 2} \frac{1 + p^{-s} + 2p^{1-s} + 2p^{-2s} + p^{1-2s} + p^{1-3s}}{(1 - p^{2-s})(1 - p^{1-2s})} \\ &= 1 + \frac{16}{3^s} + \frac{36}{5^s} + \frac{64}{7^s} + \frac{152}{9^s} + \frac{144}{11^s} + \frac{196}{13^s} + \frac{576}{15^s} + \frac{324}{17^s} + \frac{400}{19^s} + \frac{1024}{21^s} + \dots \end{aligned}$$

is the corresponding Dirichlet series. \square

Unfortunately, unlike before, there is no nice representation of $\Psi_{D_4^*}(s)$ as a product of zeta functions. Nevertheless, we can use Theorem 4.1 to calculate the asymptotic behaviour as follows.

Note that $\Psi_{D_4^*}(s)$ is quite similar to $\Psi_{D_4^{\text{rot}}}^{\text{rot}}(s)$; compare Eq. (10.4). In fact, differences between the corresponding counting functions occur only for those integers that are divisible by the square of an odd prime. Thus, the rightmost pole of $\Psi_{D_4^*}(s)$ is still at $s = 3$, which is the same as for $\Psi_{D_4^{\text{rot}}}^{\text{rot}}(s)$. This implies the asymptotic behaviour $\sum_{n \leq x} c_{D_4^*}(n) \sim cx^3$ as $x \rightarrow \infty$ for some positive constant c . To be more specific, we consider the ratio

$$(10.7) \quad \frac{\Psi_{D_4^*}(s)}{\Psi_{D_4^{\text{rot}}}^{\text{rot}}(s)} = \prod_{p \neq 2} \left(1 - \frac{2(p^2 - 1)p^{-2s}}{(1 + p^{-s})(1 + p^{1-s})(1 - p^{1-2s})} \right),$$

where the right-hand side defines an analytic function in the open half-plane $\{\text{Re}(s) > \frac{3}{2}\}$ with

$$(10.8) \quad \begin{aligned} \gamma &:= \lim_{s \rightarrow 3} \frac{\Psi_{D_4^*}(s)}{\Psi_{D_4^{\text{rot}}}^{\text{rot}}(s)} = \prod_{p \neq 2} \left(1 - \frac{2(p^2 - 1)p^{-6}}{(1 + p^{-2})(1 + p^{-3})(1 - p^{-5})} \right) \\ &\approx 0.976966019 < 1. \end{aligned}$$

Hence, $\sum_{n \leq x} c_{D_4^*}(n)$ grows by a factor γ slower than $\sum_{n \leq x} c_{D_4^{\text{rot}}}^{\text{rot}}(n)$. In particular, we obtain

$$\sum_{n \leq x} c_{D_4^*}(n) \sim \frac{210}{\pi^6} \zeta(3) \gamma x^3 \approx 0.256522 x^3,$$

as $x \rightarrow \infty$. This shows that $\sum_{n \leq x} c_{D_4^*}^{\text{rot}}(n)$ and $\sum_{n \leq x} c_{D_4^*}(n)$ differ by less than 2.5% asymptotically, which means that it is quite rare that two coincidence rotations that are not symmetry related generate the same CSL.

As we have enumerated the distinct CSLs, we might ask the question of how many non-equivalent CSLs there are, where we call two CSLs Λ_1 and Λ_2 *equivalent* if there is an $R \in O(\mathbb{J})$ such that $\Lambda_2 = R\Lambda_1$. This question has not completely been answered yet, but some partial results can be found in [94].

10.2. The primitive hypercubic lattice \mathbb{Z}^4 . Let us move on to the primitive hypercubic lattice, which we identify with \mathbb{Z}^4 or, in terms of quaternions, with the ring of Lipschitz quaternions \mathbb{L} . As \mathbb{Z}^4 and D_4^* are commensurate, they have the same group of coincidence rotations, which means

$$\text{SOC}(\mathbb{Z}^4) = \text{SOC}(D_4^*) = \text{SO}(4, \mathbb{Q}).$$

Moreover, we have $D_4 \subset \mathbb{Z}^4 \subset D_4^*$, where \mathbb{Z}^4 is a sublattice of D_4^* of index 2. Thus, by Theorem 7.25, the coincidence indices of the two lattices can differ at most by a factor of 2. This implies that we have either $\Sigma_{\mathbb{Z}^4}(R) = \Sigma_{D_4^*}(R)$ or $\Sigma_{\mathbb{Z}^4}(R) = 2\Sigma_{D_4^*}(R)$ for a given coincidence rotation R . Actually, both cases do occur.

This becomes immediately clear if we recall that the primitive hypercubic lattice \mathbb{Z}^4 has a smaller symmetry group than D_4^* . In particular, $\text{SO}(\mathbb{Z}^4)$ contains only 192 rotations, so that

$$[\text{SO}(D_4^*) : \text{SO}(\mathbb{Z}^4)] = [\text{O}(D_4^*) : \text{O}(\mathbb{Z}^4)] = 3.$$

As a consequence, every class of symmetry-related coincidence rotations of D_4^* splits into three classes of \mathbb{Z}^4 . In particular, all rotations in $\text{SO}(D_4^*) \setminus \text{SO}(\mathbb{Z}^4)$ are coincidence rotations for \mathbb{Z}^4 of index 2, so we have one class with coincidence index 1 and two classes with index 2.

The same pattern also emerges for the other coincidence rotations — and, more generally, for coincidence isometries as well. In particular, every class of symmetry-related coincidence rotations of D_4^* 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 $\Sigma_{\mathbb{Z}^4}(R) = 2\Sigma_{D_4^*}(R)$. To see this, we recall from Theorem 7.29 that $\text{den}_{\mathbb{Z}^4}(R)$ divides $\Sigma_{\mathbb{Z}^4}(R)$, while $\Sigma_{\mathbb{Z}^4}(R)$ divides $\text{den}_{\mathbb{Z}^4}(R)^4$. Consequently, $\Sigma_{\mathbb{Z}^4}(R)$ is even if and only if $\text{den}_{\mathbb{Z}^4}(R)$ is. In other words,

$$(10.9) \quad \Sigma_{\mathbb{Z}^4}(R) = \text{lcm}(\Sigma_{D_4^*}(R), \text{den}_{\mathbb{Z}^4}(R));$$

compare [4]. If (p, q) is an odd primitive admissible pair, we have

$$(10.10) \quad \text{den}_{\mathbb{Z}^4}(R(p, q)) = \begin{cases} |pq|, & \text{if } \langle p|q \rangle \in \mathbb{Z}, \\ 2|pq|, & \text{if } \langle p|q \rangle \notin \mathbb{Z}, \end{cases}$$

while, if (p, q) is an even primitive admissible pair, one gets

$$(10.11) \quad \text{den}_{\mathbb{Z}^4}(R(p, q)) = \begin{cases} \frac{|pq|}{2}, & \text{if } \langle p|q \rangle \text{ is even,} \\ |pq|, & \text{if } \langle p|q \rangle \text{ is odd.} \end{cases}$$

Checking for all possible combinations of units, we see that every class of symmetry-related coincidence rotations of D_4^* indeed splits into three classes, one of which has odd denominator and coincidence index $\Sigma_{\mathbb{Z}^4}(R) = \Sigma_{D_4^*}(R)$, while the other two classes have even denominator and coincidence index $\Sigma_{\mathbb{Z}^4}(R) = 2\Sigma_{D_4^*}(R)$.

Remark 10.12. These relations mean that the coincidence spectrum of \mathbb{Z}^4 is larger than the coincidence spectrum of D_4^* and D_4 . In particular, we conclude from Remark 10.7 that the coincidence spectrum of \mathbb{Z}^4 is the set

$$\Sigma(\text{OC}(\mathbb{Z}^4)) = \Sigma(\text{SOC}(\mathbb{Z}^4)) = (2\mathbb{N}_0 + 1) \cup (4\mathbb{N}_0 + 2). \quad \diamond$$

In order to also get an explicit expression for the CSLs, we consider the following chain of inclusions

$$(10.12) \quad D_4 \cap RD_4 \subseteq \mathbb{Z}^4 \cap R\mathbb{Z}^4 \subseteq D_4^* \cap RD_4^* \cap \mathbb{Z}^4 \subset D_4^* \cap RD_4^*$$

for any $R \in \text{SOC}(D_4^*)$. As $\Sigma_{D_4}(R) = \Sigma_{D_4^*}(R)$ by Lemma 7.4, and also $[D_4^* : D_4] = 4$, we conclude that $[(D_4^* \cap RD_4^*) : (D_4 \cap RD_4)] = 4$. Moreover, with $[D_4^* : \mathbb{Z}^4] = 2$, this shows $[(D_4^* \cap RD_4^* \cap \mathbb{Z}^4) : (D_4 \cap RD_4)] = 2$, as $\Sigma_{D_4^*}(R)$ is always odd. Thus, we are left with two possibilities, namely either with $\mathbb{Z}^4 \cap R\mathbb{Z}^4 = D_4^* \cap RD_4^* \cap \mathbb{Z}^4 = \mathbb{Z}^4 \cap RD_4^*$, in which case $\Sigma_{\mathbb{Z}^4}(R) = \Sigma_{D_4^*}(R)$, or with $\mathbb{Z}^4 \cap R\mathbb{Z}^4 = D_4 \cap RD_4$, where we have $\Sigma_{\mathbb{Z}^4}(R) = 2\Sigma_{D_4^*}(R)$ instead.

Let us summarise these results as follows.

Proposition 10.13. *For any coincidence rotation $R \in \text{SOC}(\mathbb{Z}^4)$, the coincidence index is*

$$\Sigma_{\mathbb{Z}^4}(R) = \text{lcm}(\Sigma_{D_4^*}(R), \text{den}_{\mathbb{Z}^4}(R)),$$

which is even if and only if $\text{den}_{\mathbb{Z}^4}(R)$ is even. Moreover,

$$\mathbb{Z}^4 \cap R\mathbb{Z}^4 = \begin{cases} (D_4^* \cap RD_4^*) \cap \mathbb{Z}^4 = \mathbb{Z}^4 \cap RD_4^*, & \text{if } \Sigma_{\mathbb{Z}^4}(R) \text{ is even,} \\ D_4 \cap RD_4, & \text{if } \Sigma_{\mathbb{Z}^4}(R) \text{ is odd,} \end{cases}$$

is the corresponding CSL. □

This allows us to determine the number of coincidence rotations, which is $192 c_{\mathbb{Z}^4}^{\text{rot}}(n)$, as the symmetry group $\text{SO}(\mathbb{Z}^4)$ has order 192. By the above considerations, each class of symmetry-related coincidence rotations splits into three classes, one with coincidence index $\Sigma_{\mathbb{Z}^4}(R) = \Sigma_{D_4^*}(R)$, and two with index $\Sigma_{\mathbb{Z}^4}(R) = 2\Sigma_{D_4^*}(R)$. This gives

$$(10.13) \quad c_{\mathbb{Z}^4}^{\text{rot}}(n) = \begin{cases} c_{D_4^*}^{\text{rot}}(n), & \text{if } n \text{ is odd,} \\ 2 c_{D_4^*}^{\text{rot}}\left(\frac{n}{2}\right), & \text{if } n \text{ is even.} \end{cases}$$

As $c_{D_4^*}^{\text{rot}}(n)$ is multiplicative, so is $c_{\mathbb{Z}^4}^{\text{rot}}(n)$, and the corresponding Dirichlet series again admits an Euler product expansion. In particular, we have the following result; compare [4, 94].

Theorem 10.14. *The generating function for the number $c_{\mathbb{Z}^4}^{\text{rot}}(n)$ of coincidence rotations of \mathbb{Z}^4 is given by*

$$\begin{aligned} \Psi_{\mathbb{Z}^4}^{\text{rot}}(s) &= \sum_{n=1}^{\infty} \frac{c_{\mathbb{Z}^4}^{\text{rot}}(n)}{n^s} = (1 + 2^{1-s}) \Psi_{D_4^*}^{\text{rot}}(s) \\ &= \frac{(1 - 2^{1-s})(1 - 2^{2-s}) \zeta(s) \zeta(s-1)^2 \zeta(s-2)}{1 + 2^{-s} \zeta(2s) \zeta(2s-2)} \\ &= (1 + 2^{1-s}) \prod_{p \neq 2} \frac{(1 + p^{-s})(1 + p^{1-s})}{(1 - p^{1-s})(1 - p^{2-s})} \end{aligned}$$

with the first terms being given by

$$\begin{aligned} \Psi_{\mathbb{Z}^4}^{\text{rot}}(s) &= 1 + \frac{2}{2^s} + \frac{16}{3^s} + \frac{36}{5^s} + \frac{32}{6^s} + \frac{64}{7^s} + \frac{168}{9^s} + \frac{72}{10^s} + \frac{144}{11^s} + \frac{196}{13^s} \\ &\quad + \frac{128}{14^s} + \frac{576}{15^s} + \frac{324}{17^s} + \frac{336}{18^s} + \frac{400}{19^s} + \frac{1024}{21^s} + \frac{288}{22^s} + \dots \end{aligned}$$

It is a meromorphic function in the complex plane, whose rightmost pole is located at $s = 3$, with residue $\frac{1575}{2\pi^6} \zeta(3)$. Consequently, as $x \rightarrow \infty$, we have the asymptotic behaviour

$$\sum_{n \leq x} c_{\mathbb{Z}^4}^{\text{rot}}(n) \sim \frac{525}{2\pi^6} \zeta(3) x^3 \approx 0.328212 x^3.$$

Proof. It follows from Eq. (10.13) that $\Psi_{\mathbb{Z}^4}^{\text{rot}}(s)$ is obtained from $\Psi_{D_4^*}^{\text{rot}}(s)$ by adding a factor $1 + 2^{1-s}$. As the latter is analytic, the analytic structure of $\Psi_{\mathbb{Z}^4}^{\text{rot}}(s)$ is the same as that of $\Psi_{D_4^*}^{\text{rot}}(s)$ (see Theorem 10.8 and the comments thereafter), except for poles located at $s = 1 + \frac{(2n+1)\pi}{\log(2)}i$, which are cancelled by the factor $1 + 2^{1-s}$. An application of Theorem 4.1 finally yields the asymptotic behaviour. \square

In a similar way, we can enumerate the CSLs. It follows from Proposition 10.13 that each CSL of D_4^* corresponds to exactly one pair of CSLs of \mathbb{Z}^4 , one of which has odd index, while the other one has even index. Note that the explicit expressions for the CSLs in Proposition 10.13 guarantee that two CSLs of \mathbb{Z}^4 are only equal if the corresponding CSLs of D_4^* are equal. This implies that the number of CSLs of \mathbb{Z}^4 is given by

$$(10.14) \quad c_{\mathbb{Z}^4}(n) = \begin{cases} c_{D_4^*}(n), & \text{if } n \text{ is odd,} \\ c_{D_4^*}(\frac{n}{2}), & \text{if } n \text{ is even.} \end{cases}$$

This yields the following result.

Theorem 10.15. *The generating function for the number $c_{\mathbb{Z}^4}(n)$ of CSLs of \mathbb{Z}^4 is given by*

$$\begin{aligned} \Psi_{\mathbb{Z}^4}(s) &= (1 + 2^{-s})\Psi_{D_4^*}(s) \\ &= (1 + 2^{-s}) \prod_{p \neq 2} \frac{1 + p^{-s} + 2p^{1-s} + 2p^{-2s} + p^{1-2s} + p^{1-3s}}{(1 - p^{2-s})(1 - p^{1-2s})} \\ &= 1 + \frac{1}{2^s} + \frac{16}{3^s} + \frac{36}{5^s} + \frac{16}{6^s} + \frac{64}{7^s} + \frac{152}{9^s} + \frac{36}{10^s} + \frac{144}{11^s} + \frac{196}{13^s} \\ &\quad + \frac{64}{14^s} + \frac{576}{15^s} + \frac{324}{17^s} + \frac{152}{18^s} + \frac{400}{19^s} + \frac{1024}{21^s} + \frac{144}{22^s} + \dots \end{aligned}$$

It is a meromorphic function in the half-plane $\{\operatorname{Re}(s) > \frac{3}{2}\}$, whose rightmost pole is located at $s = 3$, with residue $\frac{2835}{4\pi^6} \zeta(3)\gamma$, where γ is the constant from Eq. (10.8). Consequently, we have the asymptotic behaviour

$$\sum_{n \leq x} c_{\mathbb{Z}^4}(n) \sim \frac{945}{4\pi^6} \zeta(3)\gamma x^3 \approx 0.288587 x^3,$$

as $x \rightarrow \infty$. □

Let us now turn our attention to the corresponding problem of embedded modules, with special focus on the golden ratio.

11. MORE ON THE ICOSIAN RING

The icosian ring, which is a maximal order in the quaternion algebra $\mathbb{H}(\mathbb{Q}(\sqrt{5}))$, is an interesting example of a \mathbb{Z} -module of rank 8 that is embedded in \mathbb{R}^4 . At the same time, it is a $\mathbb{Z}[\tau]$ -module of rank 4, and thus an interesting object in our context in its own right. Beyond this, as we already saw in the context of SSLs, it is a powerful tool for the description of the root lattice A_4 . Here, we analyse the coincidence structure, first via the CSLs for A_4 and then via the CSMs for \mathbb{I} itself.

11.1. Coincidences of the root lattice A_4 . Recall from Section 5.4 that A_4 can be represented as

$$L = \{x \in \mathbb{I} \mid x = \tilde{x}\},$$

which brings in the icosian ring, \mathbb{I} . As \mathbb{J} and \mathbb{I} share a lot of properties, we expect the calculation of the CSLs to be similar. Indeed, this is true, and we may thus skip various details; see [11, 56, 98] for details. However, recall that we needed a pair of quaternions to characterise the CSLs of \mathbb{J} . Here, we only need a *single* quaternion q , as the coincidence rotations of A_4 can be parametrised by admissible pairs of the form (q, \tilde{q}) . Consequently, we call a quaternion $q \in \mathbb{I}$ *admissible*, if $|q\tilde{q}|^2 = \operatorname{nr}(|q|^2)$ is a square in \mathbb{N} . In fact, $x \mapsto \frac{1}{|q\tilde{q}|}qx\tilde{q}$ defines a coincidence rotation of A_4 in the above representation if and only if $q \in \mathbb{I}$ is admissible.

In the case of the hypercubic lattices in four dimensions, it was useful to deal with an extended admissible pair of primitive quaternions. Here, we define the notion of an extended primitive admissible quaternion as follows. Let $q \in \mathbb{I}$ be primitive and admissible. Then,

$\frac{|q\tilde{q}|^2}{\gcd(|q|^2, |\tilde{q}|^2)^2}$ is a square in $\mathbb{Z}[\tau]$. Here, \gcd refers to the greatest common divisor in $\mathbb{Z}[\tau]$, which is well defined up to a unit as $\mathbb{Z}[\tau]$ is a Euclidean domain. Now, $\frac{|q|^2}{\gcd(|q|^2, |\tilde{q}|^2)} \in \mathbb{Z}[\tau]$ and $\frac{|\tilde{q}|^2}{\gcd(|q|^2, |\tilde{q}|^2)} \in \mathbb{Z}[\tau]$ are relatively prime in $\mathbb{Z}[\tau]$. Since their product is a square, they must be squares (up to units) in $\mathbb{Z}[\tau]$, too (we have unique prime factorisation). If the units have been chosen appropriately, we may assume that $\frac{|q|^2}{\gcd(|q|^2, |\tilde{q}|^2)} \in \mathbb{Z}[\tau]$ and $\frac{|\tilde{q}|^2}{\gcd(|q|^2, |\tilde{q}|^2)} \in \mathbb{Z}[\tau]$ are squares in $\mathbb{Z}[\tau]$. Hence, we may take the root (where we may choose the positive one) and define

$$(11.1) \quad \alpha_q := \sqrt{\frac{|\tilde{q}|^2}{\gcd(|q|^2, |\tilde{q}|^2)}}, \quad \alpha_{\tilde{q}} := \alpha'_q = \sqrt{\frac{|q|^2}{\gcd(|q|^2, |\tilde{q}|^2)}},$$

which are unique up to units. Note further that the last equality only holds up to a unit.

Definition 11.1. Let $q \in \mathbb{I}$ be a primitive admissible quaternion. Then, $q_\alpha := \alpha_q q$ is called an *extended admissible quaternion* (corresponding to q).

Of course, this definition is unique only up to units in $\mathbb{Z}[\tau]$, but this does not matter as units of $\mathbb{Z}[\tau]$ cancel out in the definition of the coincidence rotations. The key result in the determination of the CSLs is the following characterisation.

Theorem 11.2 ([11, Thms. 2 and 3]). *Let $q \in \mathbb{I}$ be a primitive admissible quaternion and q_α its extension. Then,*

$$L \cap \frac{qL\tilde{q}}{|q\tilde{q}|} = L_{q_\alpha} := (q_\alpha \mathbb{I} + \mathbb{I}\tilde{q}_\alpha) \cap L.$$

Moreover, its coincidence index $\Sigma_{A_4}(q)$ is given by

$$\Sigma_{A_4}(q) = |q_\alpha|^2 = \text{lcm}(|q|^2, |\tilde{q}|^2). \quad \square$$

This allows us to determine the multiplicative counting function $c_{A_4}^{\text{rot}}$, which is explicitly given by [98, Eq. (5.29)]

$$(11.2) \quad c_{A_4}^{\text{rot}}(p^r) = \begin{cases} 6 \cdot 5^{2r-1}, & \text{if } p = 5, \\ \frac{p+1}{p-1} p^{r-1} (p^{r+1} + p^{r-1} - 2), & \text{if } p \equiv \pm 1 \pmod{5}, \\ p^{2r} + p^{2r-2}, & \text{if } p \equiv \pm 2 \pmod{5}. \end{cases}$$

The result now reads as follows.

Theorem 11.3 ([11, Thm. 4]). *Let $120 c_{A_4}^{\text{rot}}(m)$ be the number of coincidence rotations of index m of the root lattice A_4 , as specified by Eq. (11.2). Then, with $K = \mathbb{Q}(\sqrt{5})$, the*

Dirichlet series generating function for $c_{A_4}^{\text{rot}}(m)$ reads

$$\begin{aligned} \Psi_{A_4}^{\text{rot}}(s) &= \sum_{n \in \mathbb{N}} \frac{c_{A_4}^{\text{rot}}(n)}{n^s} = \frac{\zeta_K(s-1)}{1+5^{-s}} \frac{\zeta(s)\zeta(s-2)}{\zeta(2s)\zeta(2s-2)} \\ &= \frac{1+5^{1-s}}{1-5^{2-s}} \prod_{p \equiv \pm 1(5)} \frac{(1+p^{-s})(1+p^{1-s})}{(1-p^{1-s})(1-p^{2-s})} \prod_{p \equiv \pm 2(5)} \frac{1+p^{-s}}{1-p^{2-s}} \\ &= 1 + \frac{5}{2^s} + \frac{10}{3^s} + \frac{20}{4^s} + \frac{30}{5^s} + \frac{50}{6^s} + \frac{50}{7^s} + \frac{80}{8^s} + \frac{90}{9^s} + \frac{150}{10^s} + \frac{144}{11^s} + \dots, \end{aligned}$$

and the coincidence spectrum is \mathbb{N} . □

The function $\Psi_{A_4}^{\text{rot}}$ is meromorphic in the entire complex plane, and its rightmost pole is a simple pole at $s = 3$, with residue

$$\begin{aligned} (11.3) \quad \rho_{A_4}^{\text{rot}} &= \text{res}_{s=3}(\Psi_{A_4}^{\text{rot}}(s)) = \frac{125}{126} \frac{\zeta_K(2)\zeta(3)}{\zeta(6)\zeta(4)} \\ &= \frac{450\sqrt{5}}{\pi^6} \zeta(3) \approx 1.258124, \end{aligned}$$

where the last equation follows by inserting the special values

$$\zeta(4) = \frac{\pi^4}{90}, \quad \zeta(6) = \frac{\pi^6}{945}, \quad \zeta_K(2) = \frac{2\pi^4}{75\sqrt{5}}, \quad L(1, \chi_5) = \frac{2 \log(\tau)}{\sqrt{5}},$$

and Apéry's constant $\zeta(3) \approx 1.202056903$; see [14, 11] and references therein.

A familiar argument based on Theorem 4.1 gives us the asymptotic growth rate of $c_{A_4}^{\text{rot}}(m)$ as follows.

Corollary 11.4. *With the residue $\rho_{A_4}^{\text{rot}}$ from Eq. (11.3), the summatory asymptotic behaviour of $c_{A_4}^{\text{rot}}(m)$ is given by*

$$\sum_{m \leq x} c_{A_4}^{\text{rot}}(m) \sim \rho_{A_4}^{\text{rot}} \frac{x^3}{3} \approx 0.419375 x^3,$$

as $x \rightarrow \infty$. □

As we shall see later in Corollary 11.7, the number of coincidence rotations and the number of CSLs of a given index grow much faster than the number of SSLs. This is due to the fact that the index of a primitive SSL is $\text{den}_{A_4}(q)^4$, whereas the coincidence index $\Sigma_{A_4}(q)$ is much smaller and satisfies the inequality $\text{den}_{A_4}(q) \leq \Sigma_{A_4}(q) \leq (\text{den}_{A_4}(q))^2$.

The key result in counting the number of distinct CSLs is the following.

Theorem 11.5 ([56, Thm. 7]). *Assume that q_1 and q_2 are admissible. Then, one has $L(R(q_1)) = L(R(q_2))$ if and only if $|q_1|^2 = |q_2|^2$ and $\text{gcd}(q_1, |q_1 \tilde{q}_1|/c) = \text{gcd}(q_2, |q_2 \tilde{q}_2|/c)$, where $c = \sqrt{5}$ if $|q_1|^2 = |q_2|^2$ is divisible by 5, and $c = 1$ otherwise. □*

From this result, one can derive the following explicit expression for the counting function [98, Eq. (5.93)]

$$c_{A_4}(p^r) = \begin{cases} 6 \cdot 5^{2r-2}, & \text{if } p = 5, \\ \frac{(p+1)^2}{p^3-1} (p^{2r+1} + p^{2r-2} - 2p^{\frac{r-1}{2}}), & \text{if } p \equiv \pm 1 \pmod{5}, r \text{ odd}, \\ \frac{(p+1)^2}{p^3-1} (p^{2r+1} + p^{2r-2} - 2\frac{p^2+1}{p+1}p^{\frac{r-2}{2}}), & \text{if } p \equiv \pm 1 \pmod{5}, r \text{ even}, \\ p^{2r} + p^{2r-2}, & \text{if } p \equiv \pm 2 \pmod{5}. \end{cases}$$

We can now summarise as follows.

Theorem 11.6 ([98, Thm. 5.5.6]). *Let $c_{A_4}(m)$ be the number of CSLs of the root lattice A_4 of index m . The Dirichlet series generating function for $c_{A_4}(m)$ reads*

$$\begin{aligned} \Psi_{A_4}(s) &= \sum_{n \in \mathbb{N}} \frac{c_{A_4}(n)}{n^s} = \left(1 + \frac{6 \cdot 5^{-s}}{1 - 5^{2-s}}\right) \prod_{p \equiv \pm 2 \pmod{5}} \frac{1 + p^{-s}}{1 - p^{2-s}} \\ &\quad \times \prod_{p \equiv \pm 1 \pmod{5}} \frac{1 + p^{-s} + 2p^{1-s} + 2p^{-2s} + p^{1-2s} + p^{1-3s}}{(1 - p^{2-s})(1 - p^{1-2s})} \\ &= 1 + \frac{5}{2^s} + \frac{10}{3^s} + \frac{20}{4^s} + \frac{6}{5^s} + \frac{50}{6^s} + \frac{50}{7^s} + \frac{80}{8^s} + \frac{90}{9^s} + \frac{30}{10^s} + \frac{144}{11^s} + \frac{200}{12^s} + \frac{170}{13^s} + \dots \quad \square \end{aligned}$$

In order to compare $\Psi_{A_4}(s)$ and $\Psi_{A_4}^{\text{rot}}(s)$, we consider the function

$$\psi_{A_4}(s) := \frac{\Psi_{A_4}(s)}{\Psi_{A_4}^{\text{rot}}(s)} = \left(1 - \frac{24 \cdot 5^{-s}}{1 + 5^{1-s}}\right) \prod_{p \equiv \pm 1 \pmod{5}} \left(1 - \frac{2(p^2 - 1)p^{-2s}}{(1 + p^{-s})(1 + p^{1-s})(1 - p^{1-2s})}\right).$$

It is analytic in the open half-plane $\{\text{Re}(s) > \frac{3}{2}\}$, as the Euler product converges there. This proves that $\Psi_{A_4}(s)$ is a meromorphic function in the open half-plane $\{\text{Re}(s) > \frac{3}{2}\}$. Its rightmost pole is a simple pole at $s = 3$ with residue

$$(11.4) \quad \rho_{A_4} = \text{res}_{s=3}(\Psi_{A_4}(s)) = \psi_{A_4}(3) \rho_{A_4}^{\text{rot}} \approx 1.025695,$$

where $\psi_{A_4}(3) \approx 0.815257622 < 1$ has been calculated numerically. Finally, we apply Theorem 4.1, which gives us the asymptotic growth rate as follows.

Corollary 11.7. *With the residue ρ_{A_4} from Eq. (11.4), the summatory asymptotic behaviour of $c_{A_4}(m)$ is given by*

$$\sum_{m \leq x} c_{A_4}(m) \sim \rho_{A_4} \frac{x^3}{3} \approx 0.341898 x^3,$$

as $x \rightarrow \infty$. □

Comparing the growth rate of the number of CSLs with that of the coincidence rotations, we see that the former is roughly 20% lower than the latter. As we shall see shortly, this difference is much bigger than in the case of the icosian ring. Yet, it is still more an exception than a rule that two coincidence rotations that are not symmetry related generate the same CSL.

11.2. Coincidences of \mathbb{I} . Here, we want to consider the CSMs of the icosian ring \mathbb{I} itself, which is an interesting example of an embedded module in 4-space. It is also a $\mathbb{Z}[\tau]$ -lattice in \mathbb{R}^4 in the sense of Definition 6.2.

The methods to find the CSMs are basically a combination of the tools we used in Sections 10 and 11.1, as we deal with admissible pairs of quaternions in \mathbb{I} here. Thus, we will keep the presentation concise and refer to [98] for details.

As \mathbb{I} is a $\mathbb{Z}(\tau)$ -lattice, we have $\text{scal}_{\mathbb{I}}(\mathbb{1}) = \mathbb{Q}(\tau)^\times$ and $\text{Scal}_{\mathbb{I}}(\mathbb{1}) = \mathbb{Z}(\tau)$. Correspondingly, we call a pair $(p, q) \in \mathbb{I} \times \mathbb{I}$ *primitive admissible* if p, q are primitive and $|pq|^2$ is a square in $\mathbb{Z}[\tau]$. It follows that the coincidence rotations are precisely those rotations $R(q, p)x = qxp/|pq|$ that can be parametrised by a primitive admissible pair; compare [98].

As before, it makes sense to define

$$(11.5) \quad \alpha_q := \sqrt{\frac{|p|^2}{\gcd(|q|^2, |p|^2)}} \quad \text{and} \quad \alpha_p := \sqrt{\frac{|q|^2}{\gcd(|q|^2, |p|^2)}}$$

for any primitive admissible pair (q, p) , where α_q and α_p are again defined up to a unit (now in $\mathbb{Z}[\tau]$). Correspondingly, we call $(q_\alpha, p_\alpha) = (\alpha_q q, \alpha_p p)$ the extension of the primitive admissible pair (q, p) . This implies

$$(11.6) \quad |q_\alpha|^2 = |p_\alpha|^2 = |q_\alpha p_\alpha| \quad (\text{up to a unit}).$$

The CSMs of \mathbb{I} can now completely be characterised as follows, which is the analogue of Theorem 10.4 for the Hurwitz ring \mathbb{J} .

Theorem 11.8 ([98, Thm. 5.4.2 and 5.4.4]). *Let (q_α, p_α) be the extension of the primitive admissible pair (q, p) . Then, one has*

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

The index of this CSM in \mathbb{I} is given by

$$\Sigma_{\mathbb{I}}(R(q, p)) = \text{nr}(\text{lcm}(|q|^2, |p|^2)) = \text{nr}(|q_\alpha|^2) = \text{nr}(|p_\alpha|^2). \quad \square$$

This allows us to calculate the number of coincidence rotations of a given index m , which is given by $7200 c_{\mathbb{I}}^{\text{rot}}(m)$, where the factor 7200 is the order of $\text{SO}(\mathbb{I})$, the rotation symmetry group of \mathbb{I} , and $c_{\mathbb{I}}^{\text{rot}}(m)$ is a multiplicative function which is completely determined by

$$c_{\mathbb{I}}^{\text{rot}}(p^r) = \begin{cases} 3 \cdot 5^{r-1} (13 \cdot 5^{r-1} - 1), & \text{if } p = 5, r \geq 1, \\ h(p, r), & \text{if } p \equiv \pm 1 \pmod{5} \text{ and } r \geq 1, \\ \frac{p^2+1}{p^2-1} p^{2r-2} (p^{2r+2} + p^{2r-2} - 2), & \text{if } p \equiv \pm 2 \pmod{5} \text{ and } r \geq 2 \text{ even,} \\ 0, & \text{if } p \equiv \pm 2 \pmod{5} \text{ and } r \geq 1 \text{ odd,} \end{cases}$$

with

$$(11.7) \quad \begin{aligned} h(p, r) &= 2p^{2r-2}(p+1)^2 - 4p^{r-2} \frac{p^{r-1} - 1}{(p-1)^3} (3p^2 + 1)(p+1) \\ &\quad + (r-1) \frac{(p+1)^2}{(p-1)^2} p^{r-2} (p^{r-2}(p^2+1)^2 + 4). \end{aligned}$$

Thus, we can calculate the corresponding generating function.

Theorem 11.9 ([98, Thm. 5.4.5]). *Let $7200 c_{\mathbb{I}}^{\text{rot}}(m)$ be the number of coincidence rotations of the icosian ring \mathbb{I} . Then, the Dirichlet series generating function for $c_{\mathbb{I}}^{\text{rot}}(m)$ reads*

$$\begin{aligned} \Psi_{\mathbb{I}}^{\text{rot}}(s) &= \sum_{n \in \mathbb{N}} \frac{c_{\mathbb{I}}^{\text{rot}}(n)}{n^s} = \zeta_{\mathbb{I}}^{\text{pr}}(s) \zeta_{\mathbb{I}}^{\text{pr}}(s-1) \\ &= \frac{(1+5^{-s})(1+5^{1-s})}{(1-5^{1-s})(1-5^{2-s})} \prod_{p \equiv \pm 1(5)} \left(\frac{(1+p^{-s})(1+p^{1-s})}{(1-p^{1-s})(1-p^{2-s})} \right)^2 \prod_{p \equiv \pm 2(5)} \frac{(1+p^{-2s})(1+p^{2-2s})}{(1-p^{2-2s})(1-p^{4-2s})} \\ &= 1 + \frac{25}{4^s} + \frac{36}{5^s} + \frac{100}{9^s} + \frac{288}{11^s} + \frac{440}{16^s} + \frac{400}{19^s} + \frac{900}{20^s} + \frac{960}{25^s} + \frac{1800}{29^s} + \frac{2048}{31^s} + \frac{2500}{36^s} + \dots \end{aligned}$$

with $\zeta_{\mathbb{I}}^{\text{pr}}(s)$ as given in Eq. (5.18). In particular, the possible coincidence indices are exactly those numbers that can be represented by the quadratic form $k^2 + k\ell - \ell^2 = \text{nr}(k + \ell\tau)$. \square

$\Psi_{\mathbb{I}}^{\text{rot}}(s)$ is a meromorphic function in the entire complex plane, whose rightmost pole is a simple pole at $s = 3$ with residue (see [98, Eq. (5.61)])

$$(11.8) \quad \begin{aligned} \rho_{\mathbb{I}}^{\text{rot}} &:= \text{res}_{s=3}(\Psi_{\mathbb{I}}^{\text{rot}}(s)) = \frac{\zeta_K(2)^2 \zeta_K(3)}{\zeta_K(4) \zeta_K(6)} L(1, \chi_5) \\ &= \frac{3^5 5^7 7 \sqrt{5}}{268 \pi^{12}} \log(\tau) \zeta_K(3) \approx 0.593177. \end{aligned}$$

Using Theorem 4.1, we get the following asymptotic behaviour.

Corollary 11.10 ([98, Cor. 5.4.6]). *The asymptotic behaviour of the summatory function of $c_{\mathbb{I}}^{\text{rot}}(m)$, as $x \rightarrow \infty$, is*

$$\sum_{m \leq x} c_{\mathbb{I}}^{\text{rot}}(m) \sim \rho_{\mathbb{I}}^{\text{rot}} \frac{x^3}{3} \approx 0.197726 x^3,$$

with $\rho_{\mathbb{I}}^{\text{rot}}$ as given in Eq. (11.8). \square

In order to enumerate the CSMs themselves, we need a criterion that tells us which rotations generate the same CSM. This is given by the following result, which is the analogue of Theorem 10.9 for \mathbb{J} , and of Theorem 11.5 for the lattice A_4 .

Theorem 11.11 ([98, Thm. 5.4.13]). *Let (q_1, p_1) and (q_2, p_2) be two primitive admissible pairs. Then, the identity*

$$\mathbb{I} \cap \frac{q_1 \mathbb{I} p_1}{|q_1 p_1|} = \mathbb{I} \cap \frac{q_2 \mathbb{I} p_2}{|q_2 p_2|}$$

holds if and only if the following conditions are satisfied (up to units).

$$(1) \quad |q_1 p_1| = |q_2 p_2|,$$

$$(2) \operatorname{lcm}(|q_1|^2, |p_1|^2) = \operatorname{lcm}(|q_2|^2, |p_2|^2),$$

$$(3) \operatorname{gcd}(|q_1|, |p_1 q_1|) = \operatorname{gcd}(|q_2|, |p_2 q_2|), \text{ and}$$

$$(4) \operatorname{gcd}(|p_1|, |p_1 q_1|) = \operatorname{gcd}(|p_2|, |p_2 q_2|). \quad \square$$

The effect of these criteria is that it is now a purely combinatorial task to calculate $c_{\mathbb{I}}(m)$ and the corresponding Dirichlet series. For explicit expressions for $c_{\mathbb{I}}(m)$, see [98, Eq. 5.79].

Theorem 11.12 ([98, Thm. 5.4.14]). *Let $c_{\mathbb{I}}(m)$ be the number of CSMs of the icosian ring \mathbb{I} of index m . Then, the Dirichlet series generating function for $c_{\mathbb{I}}(m)$ reads*

$$\begin{aligned} \Psi_{\mathbb{I}}(s) &= \sum_{n \in \mathbb{N}} \frac{c_{\mathbb{I}}(n)}{n^s} = \frac{1 + 11 \cdot 5^{-s} + 7 \cdot 5^{-2s} + 5^{1-3s}}{(1 - 5^{2-s})(1 - 5^{1-2s})} \\ &\quad \times \prod_{p \equiv \pm 1(5)} \left(\frac{1 + p^{-s} + 2p^{1-s} + 2p^{-2s} + p^{1-2s} + p^{1-3s}}{(1 - p^{2-s})(1 - p^{1-2s})} \right)^2 \\ &\quad \times \prod_{p \equiv \pm 2(5)} \frac{1 + p^{-2s} + 2p^{2-2s} + 2p^{-4s} + p^{2-4s} + p^{2-6s}}{(1 - p^{4-2s})(1 - p^{2-4s})} \\ &= 1 + \frac{25}{4^s} + \frac{36}{5^s} + \frac{100}{9^s} + \frac{288}{11^s} + \frac{410}{16^s} + \frac{400}{19^s} + \frac{900}{20^s} + \frac{912}{25^s} + \frac{1800}{29^s} + \frac{2048}{31^s} + \dots \quad \square \end{aligned}$$

We are not aware of a representation of $\Psi_{\mathbb{I}}(s)$ in terms of zeta functions. Nevertheless, we can determine its analytic properties. We note that the Euler product

$$\begin{aligned} (11.9) \quad \psi_{\mathbb{I}}(s) &:= \frac{\Psi_{\mathbb{I}}(s)}{\Psi_{\mathbb{I}}^{\operatorname{rot}}(s)} = \left(1 - \frac{48 \cdot 5^{-2s}}{(1 + 5^{-s})(1 + 5^{1-s})(1 - 5^{1-2s})} \right) \\ &\quad \times \prod_{p \equiv \pm 1(5)} \left(1 - \frac{2(p^2 - 1)p^{-2s}}{(1 + p^{-s})(1 + p^{1-s})(1 - p^{1-2s})} \right)^2 \\ &\quad \times \prod_{p \equiv \pm 2(5)} \left(1 - \frac{2(p^4 - 1)p^{-4s}}{(1 + p^{-2s})(1 + p^{2-2s})(1 - p^{2-4s})} \right) \end{aligned}$$

converges for $\operatorname{Re}(s) > \frac{3}{2}$, which implies that $\Psi_{\mathbb{I}}(s)$ is meromorphic in the half-plane given by $\{\operatorname{Re}(s) > \frac{3}{2}\}$. Moreover, the rightmost pole of $\Psi_{\mathbb{I}}(s)$ is a simple pole located at $s = 3$, with residue

$$(11.10) \quad \rho_{\mathbb{I}} := \operatorname{res}_{s=3}(\Psi_{\mathbb{I}}(s)) = \psi_{\mathbb{I}}(3)\rho_{\mathbb{I}}^{\operatorname{rot}} \approx 0.587063.$$

Here, $\psi_{\mathbb{I}}(3) \approx 0.989691798 < 1$ was calculated numerically. Finally, we apply Theorem 4.1 to obtain the asymptotic behaviour.

Corollary 11.13 ([98, Cor. 5.4.15]). *The asymptotic behaviour of the summatory function of $c_{\mathbb{I}}(m)$, as $x \rightarrow \infty$, is*

$$(11.11) \quad \sum_{m \leq x} c_{\mathbb{I}}(m) \sim \rho_{\mathbb{I}} \frac{x^3}{3} \approx 0.195688 x^3,$$

with $\rho_{\mathbb{I}}$ as given above. □

Note that $\rho_{\mathbb{I}}$ and $\rho_{\mathbb{I}}^{\text{rot}}$ differ by just about 1%. Thus, in most cases, two coincidence rotations that are not symmetry related generate different CSMs.

12. MULTIPLE CSLS OF THE CUBIC LATTICES

So far, we have mostly considered ordinary (or simple) CSLs and CSMs. The problem of finding all *multiple* CSLs (MCSLs) is more difficult than determining all CSLs. In fact, there are only few cases where the problem of multiple coincidences has been solved so far. These include the two-dimensional lattices and modules of n -fold symmetry [4], which we discussed in Section 8, and the three-dimensional cubic lattices, which we want to discuss here; compare [95, 98].

Let us recall from Section 9 that any coincidence rotation R of the cubic lattices can be parametrised by primitive Hurwitz quaternions. Moreover, there is a bijection between the CSLs of the body-centred cubic lattice and the ideals $q\mathbb{J}$ generated by odd primitive quaternions. In particular, we have $\Gamma_{\text{bcc}} = \text{Im}(\mathbb{J})$ and $\Gamma_{\text{bcc}}(R(q)) = \text{Im}(q\mathbb{J})$ with $\Sigma(R(q)) = |q|^2$ if q is a primitive odd quaternion. If q is an even primitive quaternion, then $\Sigma(R(q)) = \frac{|q|^2}{2}$. In this case, q can be written as the product $r(1, 1, 0, 0)$ of an odd primitive quaternion with an even one, and the corresponding CSL can be written as $\Gamma_{\text{bcc}}(R(q)) = \text{Im}(r\mathbb{J})$.

Consequently, it is sufficient to consider CSLs generated by primitive odd quaternions. Just as in the case of ordinary CSLs, we start with the analysis of the body-centred cubic lattice and later derive the MCSLs of the other cubic lattices in the setting of Eq. (9.1).

Let us first discuss the coincidence spectrum. We know from Remark 9.6 that the ordinary coincidence spectrum for all three types of cubic lattices is $2\mathbb{N}_0 + 1$. Moreover, we have seen in Section 7.2 that $\Sigma(R_1, \dots, R_m)$ divides the product $\Sigma(R_1) \cdot \dots \cdot \Sigma(R_m)$. Thus, the spectrum of indices of MCSLs is again the set of positive odd integers.

Proposition 12.1. *Let Γ be any cubic lattice. The (multiple) coincidence spectrum of Γ is given by $2\mathbb{N}_0 + 1$. □*

Hence, no new indices occur. Nevertheless, additional lattices emerge and the multiplicity of the corresponding index will increase. We have seen that $c_{\Gamma}(m)$ is a multiplicative function. By Theorem 7.19, this implies that any ordinary CSL can be written as

$$\Gamma(R) = \Gamma(R_1) \cap \dots \cap \Gamma(R_n),$$

where the indices $\Sigma_{\Gamma}(R_i)$ are powers of distinct primes. In this case, we know that the MCSL $\Gamma(R_1) \cap \dots \cap \Gamma(R_n)$ agrees with an ordinary CSL. However, if the indices of the $\Gamma(R_i)$ are not relatively prime, the corresponding MCSL is, in general, not equal to an ordinary CSL.

More generally, by an application of Theorem 7.19, the multiplicativity of $c_{\Gamma}(m)$ guarantees that *any* MCSL $\Gamma(R_1, \dots, R_n)$ can be written as the intersection of MCSLs Γ_k of prime power index. Furthermore, the Γ_k can be chosen in such a way that they are intersections of at most

n ordinary CSLs. Thus, we may restrict our analysis of MCSLs to those MCSLs whose index is a prime power.

To become more concrete, we mention that the decomposition of CSLs into CSLs of prime power index corresponds to the prime factorisation in \mathbb{J} . In particular, if $|q|^2 = \pi_1^{\alpha_1} \cdots \pi_k^{\alpha_k}$ is the prime factorisation of $|q|^2$ in \mathbb{N} and $p_i := \text{gcd}(q, \pi_i^{\alpha_i})$, the aforementioned decomposition is now given by $\Gamma(R(q)) = \Gamma(R(p_1)) \cap \cdots \cap \Gamma(R(p_k))$. Note that q is a common right multiple of all p_i . Conversely, if the p_i are primitive odd quaternions such that all $|p_i|^2$ are relatively prime, then any least common right multiple q is primitive and odd, and we have $\Gamma(R(q)) = \Gamma(R(p_1)) \cap \cdots \cap \Gamma(R(p_k))$. Likewise, if we define $p_{ij} = \text{gcd}(q_i, \pi_j^{\alpha_{ij}})$, where the α_{ij} are the exponents in the prime factorisation $|q_i|^2 = \pi_1^{\alpha_{i1}} \cdots \pi_k^{\alpha_{ik}}$, then the corresponding decomposition of the MCSL reads $\Gamma(R(q_1), \dots, R(q_n)) = \Gamma_1 \cap \cdots \cap \Gamma_k$ with the lattices $\Gamma_\ell = \Gamma(R(p_{1\ell})) \cap \cdots \cap \Gamma(R(p_{n\ell}))$.

Moreover, this guarantees the multiplicativity of the corresponding counting functions $c^{(\infty)}(m)$ and $c^{(k)}(m)$, where $c^{(\infty)}(m)$ is the number of all MCSLs of a given index m and $c^{(k)}(m)$ the corresponding number of all MCSLs that can be written as the intersection of at most k ordinary CSLs.

As we want to enumerate the distinct MCSLs, it is an essential question under what condition two MCSLs are equal. A preliminary result is the following, which generalises Lemma 7.33 to the present situation.

Lemma 12.2 ([98, Lemma 6.1.2]). *Let Γ be any cubic lattice and assume that*

$$\Gamma(R(q_1), \dots, R(q_n)) = \Gamma(R(q'_1), \dots, R(q'_m)),$$

where q_i and q'_j are primitive odd quaternions. Then, we have

$$\Sigma_\Gamma(R(q_1), \dots, R(q_n)) = \Sigma_\Gamma(R(q'_1), \dots, R(q'_m))$$

together with $\text{lcm}(|q_1|^2, \dots, |q_n|^2) = \text{lcm}(|q'_1|^2, \dots, |q'_m|^2)$. \square

The conditions of the lemma are necessary, but by no means sufficient. For ordinary CSLs, we have the much stronger condition $q\mathbb{J} = q'\mathbb{J}$, and we expect additional conditions for MCSLs. Let us start with the case $n = 2$.

12.1. Intersections of two CSLs. As the body-centred cubic lattice $\Gamma = \Gamma_{\text{bcc}} = \text{Im}(\mathbb{J})$ has the most convenient representation in terms of quaternions, we start with this lattice. The first step to determine all possible MCSLs $\Gamma(R_1, R_2)$ that can be written as the intersection of at most two ordinary CSLs is the calculation of their indices. We note that

$$\Gamma_+(R_1, R_2) := \Gamma(R_1) + \Gamma(R_2) = \text{Im}(q_1\mathbb{J} + q_2\mathbb{J}) = \text{Im}(q\mathbb{J}),$$

where $q = \text{gcd}(q_1, q_2)$. Hence, recalling that we may assume $|q_i|^2$ to be odd, we have

$$(12.1) \quad \Sigma(R_1, R_2) = \frac{|q_1|^2 |q_2|^2}{|q|^2}.$$

In the case that $|q_1|^2$ and $|q_2|^2$ are relatively prime, this reduces to $\Sigma(R_1, R_2) = |q_1|^2|q_2|^2$. This is the aforementioned case where the MCSL is equal to an ordinary CSL. Another special case occurs when q_1 is a left divisor of q_2 . Here, we have $\Gamma(R_2) \subseteq \Gamma(R_1)$, and the MCSL $\Gamma(R_1, R_2) = \Gamma(R_2)$ is again an ordinary CSL. In order to understand the general situation, we start with the case that both $|q_i|^2$ are powers of the same rational prime p .

Actually, the case of MCSLs of prime power index is sufficient, because we can recover the general case from this one, as we have mentioned before. We are mainly interested in the case of two different CSLs none of which is a sublattice of the other one, so neither q_1 nor q_2 is a right multiple of the other one. Fortunately, we do not need to exclude the latter case explicitly, as all formulas include the case of ordinary CSLs implicitly.

Recall that we have an explicit expression for ordinary CSLs, namely $\Gamma_{\text{bcc}}(R(q)) = \text{Im}(q\mathbb{J})$. An analogous expression for MCSLs is given by the following result.

Lemma 12.3 ([98, Lemma 6.2.2]). *Let q_1 and q_2 be primitive quaternions with $|q_i|^2 = p^{\alpha_i}$, where p is the same odd prime for both quaternions. Let q be a least common right multiple of q_1 and q_2 . Then, we have*

$$\Gamma_{\text{bcc}}(R_1, R_2) = \text{Im}(q\mathbb{J} + q_1\mathbb{J}\bar{q}_2) = \text{Im}(q\mathbb{J} + q_2\mathbb{J}\bar{q}_1). \quad \square$$

Note that $q\mathbb{J} + q_1\mathbb{J}\bar{q}_2$ need not be an ideal. If not, $\Gamma_{\text{bcc}}(R_1, R_2)$ is neither an ordinary CSL nor a multiple of one. Further, note that $\text{Im}(q\mathbb{J})$ is a multiple of an ordinary CSL as q , in general, is not primitive here.

When enumerating MCSLs, we must make sure that we do not count any MCSL twice. Thus, we need a criterion when two MCSLs are equal. This is provided by the following result.

Theorem 12.4 ([98, Thm. 6.2.3]). *Let q_i with $1 \leq i \leq 4$ be primitive quaternions such that $|q_i|^2 = p^{\alpha_i}$, where p is an odd rational prime and where $\alpha_1 \geq \alpha_2 \geq \alpha_4$ and $\alpha_3 \geq \alpha_4$. Let q_{ij} with $|q_{ij}|^2 = p^{\alpha_{ij}}$ be the greatest common left divisor of q_i and q_j . In addition, if $\alpha_1 = \alpha_2$, let $\alpha_{13} \geq \alpha_{23}$, and if $\alpha_3 = \alpha_4$, let $\alpha_{13} \geq \alpha_{14}$. Then, with $R_i = R(q_i)$, we have*

$$\Gamma_{\text{bcc}}(R_1) \cap \Gamma_{\text{bcc}}(R_2) = \Gamma_{\text{bcc}}(R_3) \cap \Gamma_{\text{bcc}}(R_4)$$

if and only if the conditions $\alpha_1 = \alpha_3$, $\alpha_2 - \alpha_{12} = \alpha_4 - \alpha_{34}$, $\alpha_1 - \alpha_{13} \leq \min(\alpha_4 - \alpha_{34}, \alpha_{34})$ and $\alpha_4 - \alpha_{24} \leq \min(\alpha_4 - \alpha_{34}, \alpha_{34})$ are satisfied. \square

Note that the ordering conditions on the α coefficients do not put any restrictions on the applicability of the theorem, since we can always interchange the role of the q_i such that these conditions are met.

Remark 12.5. The two conditions $\alpha_1 = \alpha_3$ and $\alpha_2 - \alpha_{12} = \alpha_4 - \alpha_{34}$ correspond to the two conditions in Lemma 12.2. The first one means that the least common multiples of the denominators must be the same, and the second follows from the equality of the indices,

which gives $\alpha_1 + \alpha_2 - \alpha_{12} = \alpha_3 + \alpha_4 - \alpha_{34}$. Furthermore, the condition $\alpha_1 - \alpha_{13} \leq \alpha_4 - \alpha_{34}$ can easily be understood by considering

$$\begin{aligned} \Gamma_{\text{bcc}}(R_1) \cap \Gamma(R_3) &\supseteq \Gamma_{\text{bcc}}(R_1) \cap \Gamma_{\text{bcc}}(R_2) \cap \Gamma_{\text{bcc}}(R_3) \cap \Gamma_{\text{bcc}}(R_4) \\ &= \Gamma_{\text{bcc}}(R_3) \cap \Gamma_{\text{bcc}}(R_4). \end{aligned} \quad \diamond$$

Theorem 12.4 is not very intuitive, but we can understand it better by comparing the quaternions involved. It basically tells us how different the quaternions q_1, q_3 and q_2, q_4 may be; see [98] for details. This allows us to calculate the counting function for MCSLs that are the intersection of at most two ordinary CSLs.

Theorem 12.6 ([98, Thm. 6.2.4]). *Let p be an odd prime number. Then, the number $c_{\text{bcc}}^{(2)}(p^r)$ of distinct MCSLs of Γ_{bcc} of index p^r that are an intersection of at most two ordinary CSLs is given by*

$$\begin{aligned} c_{\text{bcc}}^{(2)}(p^r) &= \frac{r+1}{2} (p+1) p^{r-1} + \left(\frac{r}{2} - 1\right) p^{r-2} - \left(\frac{r}{2} - \left[\frac{r}{2}\right]\right) p^{r-4} \\ &\quad + \frac{p^{r-1} - p^{r-2[r/3]-1}}{p^2 - 1} + \frac{p^{4[r/3]-r+2} - p^{4[r/2]-r-2}}{2(p^2 - 1)}, \end{aligned}$$

where $[x]$ denotes the Gauß bracket. □

As $c_{\text{bcc}}^{(2)}(n)$ is a multiplicative function, we can find an explicit expression for its Dirichlet series generating function as usual.

Theorem 12.7. *Let $c_{\text{bcc}}^{(2)}(m)$ be the number of distinct MCSLs of index m that are an intersection of at most two ordinary CSLs. Then, $c_{\text{bcc}}^{(2)}(\Sigma)$ is a multiplicative arithmetic function whose Dirichlet series is given by*

$$\begin{aligned} \Psi_{\text{bcc}}^{(2)}(s) &:= \sum_{n=1}^{\infty} \frac{c_{\text{bcc}}^{(2)}(n)}{n^s} = \prod_{p \in \mathbb{P} \setminus \{2\}} \psi_2(p, s) \\ &= \frac{1 - 2^{1-3s}}{1 + 2^{-3s}} \frac{\zeta(3s-1)\zeta(3s)}{\zeta(6s)} \varphi_{\text{bcc}}^{(2)}(s) \Psi_{\text{bcc}}(s) \\ &= \frac{(1 - 2^{1-s})(1 - 2^{1-3s})}{(1 + 2^{-s})(1 + 2^{-3s})} \frac{\zeta(s-1)\zeta(s)\zeta(3s-1)\zeta(3s)}{\zeta(2s)\zeta(6s)} \varphi_{\text{bcc}}^{(2)}(s) \\ &= 1 + \frac{4}{3^s} + \frac{6}{5^s} + \frac{8}{7^s} + \frac{18}{9^s} + \frac{12}{11^s} + \frac{14}{13^s} + \frac{24}{15^s} + \frac{18}{17^s} + \frac{20}{19^s} + \frac{32}{21^s} \\ &\quad + \frac{24}{23^s} + \frac{45}{25^s} + \frac{76}{27^s} + \frac{30}{29^s} + \frac{32}{31^s} + \frac{48}{33^s} + \frac{48}{35^s} + \frac{38}{37^s} + \frac{56}{39^s} + \dots, \end{aligned}$$

where $\psi_2(p, s)$ is the Euler factor corresponding to $c_{\text{bcc}}^{(2)}(p)$, which is given by

$$\psi_2(p, s) := \sum_{r=1}^{\infty} \frac{c_{\text{bcc}}^{(2)}(p^r)}{p^{rs}} = \frac{(1 + p^{-s})(1 + p^{-3s})}{(1 - p^{1-s})(1 - p^{1-3s})} \times C(p, s)$$

with

$$C(p, s) = \left(1 + \frac{p^{-2s}(p^2 + p)}{2(1 + p^{-s})(1 - p^{1-s})} - \frac{p^{-4s}(p + 1)}{(1 + p^{-s})(1 - p^{1-s})(1 + p^{-3s})} \right),$$

while $\varphi_{\text{bcc}}^{(2)}(s)$ is then given by

$$\varphi_{\text{bcc}}^{(2)}(s) = \prod_{p \in \mathbb{P} \setminus \{2\}} C(p, s),$$

where the product runs over all odd rational primes. \square

The explicit knowledge of $\Psi_{\text{bcc}}^{(2)}(s)$ allows us to find its analytic properties. We know from Section 9 that $\Psi_{\text{bcc}}(s)$ is meromorphic function of s , whose rightmost pole is located at $s = 2$. Furthermore, $\varphi_{\text{bcc}}^{(2)}(s)$ converges absolutely in the half-plane $\{\text{Re}(s) > \frac{3}{2}\}$, which guarantees its analyticity there. Thus, we get the following asymptotic behaviour.

Corollary 12.8 ([98, Cor. 6.2.6]). *The asymptotic behaviour of the summatory function of $c_{\text{bcc}}^{(2)}(m)$ is given by*

$$\sum_{m \leq x} c_{\text{bcc}}^{(2)}(m) \sim \frac{\rho_{\text{bcc}}^{(2)}}{2} x^2 \approx 0.356491 x^2,$$

as $x \rightarrow \infty$, with

$$\begin{aligned} \rho_{\text{bcc}}^{(2)} &:= \text{res}_{s=2}(\Psi_{\text{bcc}}^{(2)}(s)) = \frac{124}{325} \frac{\zeta(2)\zeta(6)\zeta(5)}{\zeta(4)\zeta(12)} \varphi_{\text{bcc}}^{(2)}(2) \\ &= \frac{3866940}{691\pi^8} \zeta(5) \varphi_{\text{bcc}}^{(2)}(2) \approx 0.712983. \end{aligned} \quad \square$$

If we compare the asymptotic growth rates for ordinary CSLs and MCSLs, we see that the latter is not much bigger than the former. This shows that most MCSLs are ordinary CSLs. This behaviour is not surprising, since $c_{\text{bcc}}^{(2)}(m) = c_{\text{bcc}}(m)$ for square-free indices m . Thus, all terms n^{-s} with n square-free are missing in the expansion of $\Psi_{\text{bcc}}^{(2)}(s) - \Psi_{\text{bcc}}(s)$, whose first terms are given by

$$\begin{aligned} \Psi_{\text{bcc}}^{(2)}(s) - \Psi_{\text{bcc}}(s) &= \frac{6}{9^s} + \frac{15}{25^s} + \frac{40}{27^s} + \frac{36}{45^s} + \frac{28}{49^s} + \frac{48}{63^s} + \frac{60}{75^s} + \frac{174}{81^s} + \frac{72}{99^s} \\ &\quad + \frac{84}{117^s} + \frac{66}{121^s} + \frac{156}{125^s} + \frac{240}{135^s} + \frac{112}{147^s} + \frac{108}{153^s} + \dots \end{aligned}$$

For the determination of the counting function, it was sufficient to have an explicit expression for $\Gamma_{\text{bcc}}(R_1, R_2)$ for prime power indices. Nevertheless, we can give an explicit expression for MCSLs with general index as well, which generalises Lemma 12.3.

Theorem 12.9 ([98, Thm. 6.2.7]). *Let q_1 and q_2 be primitive odd quaternions and let q be their least common right multiple. Then, one has $\Gamma_{\text{bcc}}(R(q_1), R(q_2)) = \text{Im}(q\mathbb{J} + q_1\mathbb{J}\bar{q}_2) = \text{Im}(q\mathbb{J} + q_2\mathbb{J}\bar{q}_1)$.* \square

12.2. Intersections of three or more CSLs. We can go one step further and analyse MCSLS which are the intersection of at most three ordinary CSLs. Again, it is sufficient to consider only MCSLS of prime power index. Also in this case, we get an explicit expression for the MCSLS as follows.

Theorem 12.10 ([98, Thm. 6.3.7]). *Let q_i with $i \in \{1, 2, 3\}$ be odd primitive quaternions with prime power norm $|q_i|^2 = p^{\alpha_i}$, such that $|q_1|^2 \geq |q_i|^2$. Let $m_{ij} = \text{lcrm}(q_i, q_j)$ and $g_{ij} = \text{gld}(q_i, q_j)$. Let $|m_{12}|^2 \geq |m_{13}|^2$. Then,*

$$\Gamma_{\text{bcc}}(R(q_1), R(q_2), R(q_3)) = \text{Im}(m_{12}\mathbb{J} + nq_1\mathbb{J}\bar{q}_2),$$

where $n = \max\left(1, \frac{|q_3|^2}{|g_{13}|^2|g_{23}|^2}\right)$. □

Note that the expression for the triple CSL in Theorem 12.10 is very similar to the expression for the double CSL in Lemma 12.3. In fact, the only difference is that an additional factor n occurs. If $n = 1$, the triple CSL is just the intersection of two ordinary CSLs, since one has the relation $\Gamma_{\text{bcc}}(R(q_1), R(q_2), R(q_3)) = \Gamma_{\text{bcc}}(R(q_1), R(q_2)) \subseteq \Gamma_{\text{bcc}}(R(q_1), R(q_3))$ in this case. Let us note in passing that this yields a criterion for $\Gamma(R(q_1), R(q_2)) \subseteq \Gamma(R(q_1), R(q_3))$. In particular, under the assumptions of Theorem 12.10, this inclusion holds if and only if

$$\frac{|q_3|^2}{|g_{13}|^2|g_{23}|^2} \leq 1.$$

But even if $n > 1$, the triple CSL is just a multiple of a double CSL, as we have the following result.

Theorem 12.11 ([98, Thm. 6.3.8]). *Let Γ' be a sublattice of Γ_{bcc} of prime power index p^α . Then, Γ' can be represented as the intersection of three ordinary CSLs,*

$$\Gamma' = \Gamma_{\text{bcc}}(R_1) \cap \Gamma_{\text{bcc}}(R_2) \cap \Gamma_{\text{bcc}}(R_3),$$

if and only if there exists $\beta \in \mathbb{N}_0$ together with two coincidence rotations R'_1 and R'_2 such that $\Gamma' = p^\beta(\Gamma_{\text{bcc}}(R'_1) \cap \Gamma_{\text{bcc}}(R'_2))$. The integer β is determined uniquely by Γ' . □

Thus, we have established a one-to-one correspondence between intersections of three ordinary CSLs and multiples of intersections of two ordinary CSLs. This allows us to express $c_{\text{bcc}}^{(3)}(p^r)$ in terms of $c_{\text{bcc}}^{(2)}(p^r)$ as follows.

Corollary 12.12 ([98, Cor. 6.3.9]). *Let p be an odd prime number. Then,*

$$c_{\text{bcc}}^{(3)}(p^r) = \sum_{0 \leq n \leq r/3} c_{\text{bcc}}^{(2)}(p^{r-3n}),$$

where $c_{\text{bcc}}^{(3)}(m)$ and $c_{\text{bcc}}^{(2)}(m)$ denote the number of MCSLS of index m that can be written as an intersection of (up to) three and two ordinary CSLs, respectively. □

As $c_{\text{bcc}}^{(3)}$ is once again multiplicative, we can easily infer its generating function as follows.

Theorem 12.13 ([98, Thm. 6.3.10]). *Let $c_{\text{bcc}}^{(3)}(m)$ be the number of distinct MCSLs of index m that are an intersection of at most three ordinary CSLs. Then, $c_{\text{bcc}}^{(3)}(m)$ is a multiplicative arithmetic function whose Dirichlet series is given by*

$$\Psi_{\text{bcc}}^{(3)}(s) := \sum_{n=1}^{\infty} \frac{c_{\text{bcc}}^{(3)}(n)}{n^s} = (1 - 2^{-3s}) \zeta(3s) \Psi_{\text{bcc}}^{(2)}(s)$$

where $\Psi_{\text{bcc}}^{(2)}(s)$ is given by Theorem 12.7. One finds

$$\begin{aligned} \Psi_{\text{bcc}}^{(3)}(s) = & 1 + \frac{4}{3^s} + \frac{6}{5^s} + \frac{8}{7^s} + \frac{18}{9^s} + \frac{12}{11^s} + \frac{14}{13^s} + \frac{24}{15^s} + \frac{18}{17^s} + \frac{20}{19^s} + \frac{32}{21^s} \\ & + \frac{24}{23^s} + \frac{45}{25^s} + \frac{77}{27^s} + \frac{30}{29^s} + \frac{32}{31^s} + \frac{48}{33^s} + \frac{48}{35^s} + \frac{38}{37^s} + \frac{56}{39^s} + \dots \end{aligned}$$

for the leading terms. □

Familiar arguments involving Theorem 4.1 yield the following asymptotic behaviour.

Corollary 12.14 ([98, Cor. 6.3.11]). *The asymptotic behaviour of the summatory function of $c_{\text{bcc}}^{(3)}(m)$, as $x \rightarrow \infty$, is given by*

$$\sum_{m \leq x} c_{\text{bcc}}^{(3)}(m) = \frac{\rho_{\text{bcc}}^{(3)}}{2} x^2 \approx 0.357007 x^2,$$

where

$$\begin{aligned} \rho_{\text{bcc}}^{(3)} := \text{res}_{s=2} (\Psi_{\text{bcc}}^{(3)}(s)) &= \frac{63}{64} \zeta(6) \rho_{\text{bcc}}^{(2)} = \frac{1953}{5200} \frac{\zeta(2)\zeta(6)^2\zeta(5)}{\zeta(4)\zeta(12)} \varphi_{\text{bcc}}^{(2)}(2) \\ &= \frac{64449}{11056\pi^2} \zeta(5) \varphi_{\text{bcc}}^{(2)}(2) \approx 0.714014. \end{aligned} \quad \square$$

Comparing these results with Corollary 12.8, we see that the difference in the growth rate is significantly below 1%. This small difference is not surprising as genuinely triple CSLs can only occur for indices that are divisible by p^3 for some odd p . In particular, the first such lattice occurs for the index $\Sigma = 27$. The fact that new MCSLs are rather rare is also illustrated by the first terms of the expansion

$$\begin{aligned} \Psi_{\text{bcc}}^{(3)}(s) - \Psi_{\text{bcc}}^{(2)}(s) &= \Psi_{\text{bcc}}^{(2)}(s) ((1 - 2^{-3s})\zeta(3s) - 1) \\ &= \frac{1}{27^s} + \frac{4}{81^s} + \frac{1}{125^s} + \frac{6}{135^s} + \frac{8}{189^s} + \frac{18}{243^s} + \frac{12}{297^s} + \frac{1}{343^s} + \frac{14}{351^s} + \dots \end{aligned}$$

Here, all terms n^{-s} with n cube-free are missing, which is just a reformulation of the fact that $c_{\text{bcc}}^{(3)}(n) = c_{\text{bcc}}^{(2)}(n)$ for these n .

Finally, let us mention that any triple CSL is just a multiple of a double CSL for general index m , as we have the following generalisation of Theorem 12.11.

Theorem 12.15 ([98, Thm. 6.3.12]). *Let R_i with $i \in \{1, 2, 3\}$ be coincidence rotations of Γ_{bcc} . Then, there exist rotations R'_1 and R'_2 together with an integer $n \in \mathbb{N}$ such that $\Gamma_{\text{bcc}}(R_1, R_2, R_3) = n\Gamma_{\text{bcc}}(R'_1, R'_2)$. Conversely, for any sublattice of the form $n\Gamma_{\text{bcc}}(R'_1, R'_2)$,*

there exist coincidence rotations R_i with $i \in \{1, 2, 3\}$ such that one has the coincidence relation $\Gamma_{\text{bcc}}(R_1, R_2, R_3) = n\Gamma_{\text{bcc}}(R'_1, R'_2)$. \square

In fact, this yields all MCSLs, as any MCSL of Γ_{bcc} can be written as the intersection of three ordinary CSLs.

Theorem 12.16 ([98, Thm. 6.4.3]). *Let R_1, \dots, R_n be a finite number of coincidence rotations of Γ_{bcc} . Then, there exist coincidence rotations R'_1, R'_2 and R'_3 such that one has $\Gamma_{\text{bcc}}(R_1, \dots, R_n) = \Gamma_{\text{bcc}}(R'_1, R'_2, R'_3)$.* \square

Consequently, no new MCSLs emerge if we consider intersections of more than three ordinary CSLs. Hence, the total number of MCSLs of given index m is already given by $c_{\text{bcc}}^{(3)}(m)$, which means that, for all $n \geq 3$, we have

$$c_{\text{bcc}}^{(\infty)}(m) = c_{\text{bcc}}^{(n)}(m) = c_{\text{bcc}}^{(3)}(m).$$

A similar phenomenon has been observed in two dimensions, where the set of MCSLs stabilises already for $n = 2$; compare Section 8 and [8].

So far, we have only discussed the body-centred cubic lattice. However, we know from the ordinary CSLs that all three types of cubic lattices have the same group of coincidence rotations, the same spectrum of indices and the same multiplicity function. In fact, this remains true in the case of MCSLs, too; compare [98, Thms. 6.5.2, 6.5.4 and 6.5.5].

Theorem 12.17. *Let R_1, \dots, R_n be coincidence rotations for the cubic lattices in the setting of Eq. (9.1). Then,*

$$\Sigma_{\text{pc}}(R_1, \dots, R_n) = \Sigma_{\text{bcc}}(R_1, \dots, R_n) = \Sigma_{\text{fcc}}(R_1, \dots, R_n).$$

Moreover,

$$\Gamma_{\text{pc}}(R_1, \dots, R_n) = \Gamma_{\text{bcc}}(R_1, \dots, R_n) \cap \Gamma_{\text{pc}} \quad \text{and}$$

$$\Gamma_{\text{fcc}}(R_1, \dots, R_n) = \Gamma_{\text{bcc}}(R_1, \dots, R_n) \cap \Gamma_{\text{fcc}}$$

relate the CSLs of the different cubic lattices. \square

This result implies that the counting functions are equal for all three cubic lattices, too. In particular, we have

$$(12.2) \quad c_{\text{pc}}^{(n)}(m) = c_{\text{fcc}}^{(n)}(m) = c_{\text{bcc}}^{(n)}(m)$$

for any $n \in \mathbb{N} \cup \{\infty\}$, and the corresponding generating functions are equal as well.

Finally, let us mention an application to crystallography. One object of interest to crystallographers are so-called triple junctions [41, 40, 42]. Roughly speaking, *triple junctions* are three crystal grains meeting in a straight line. This means that there are three pairs of grains sharing a common plane (grain boundary). They give rise to three simple CSLs and to a double CSL, which is the intersection of the former. In our terms, the latter is an MCSL

$\Gamma \cap R_1 \Gamma \cap R_2 \Gamma$, whereas the former are the simple CSLs $\Gamma \cap R_1 \Gamma$, $\Gamma \cap R_2 \Gamma$ and $R_1 \Gamma \cap R_2 \Gamma$, respectively. An important question is the relation of the indices of these lattices.

Let us denote the indices of the simple CSLs by $\Sigma_i := \Sigma(R_i)$, where $R_3 := R_1^{-1} R_2$. Let q_1 and q_2 be the quaternions that parametrise R_1 and R_2 , respectively. Then, R_3 is generated by $\bar{q}_1 q_2$, which is not a primitive quaternion in general. The corresponding primitive quaternion is given by $q_3 := \frac{\bar{q}_1 q_2}{|q_{12}|^2}$, where $q_{12} = \text{gcd}(q_1, q_2)$. Hence, we can immediately reproduce Gertsman's result [40] for the index $\Sigma_3 = \frac{\Sigma_1 \Sigma_2}{\Sigma_{12}}$, where $\Sigma_{12} := \Sigma(R(q_{12}))$ is the index that corresponds to the rotation $R(q_{12})$. On the other hand, we know from Lemma 7.14 and Eq. (12.1) that

$$\Sigma(R_1, R_2) = \frac{\Sigma_1 \Sigma_2}{\Sigma_{12}} = \Sigma_{12} \Sigma_3.$$

Now, we define $q'_1 := q_{12}^{-1} q_1$ and $q'_2 := q_{12}^{-1} q_2$. Then, we may write

$$(12.3) \quad q_1 = q_{12} q'_1, \quad q_2 = q_{12} q'_2, \quad q_3 = \bar{q}'_1 q'_2$$

and, correspondingly, we may also decompose the rotations R_i into the 'basic' constituents $R_{12} := R(q_{12})$, $R'_1 := R(q'_1)$ and $R'_2 := R(q'_2)$. We note that the corresponding indices are multiplicative,

$$\Sigma(R_1) = \Sigma(R_{12}) \Sigma(R'_1), \quad \Sigma(R_2) = \Sigma(R_{12}) \Sigma(R'_2), \quad \Sigma(R_3) = \Sigma(R'_1) \Sigma(R'_2).$$

Furthermore, we see $\bar{q}'_1 = \text{gcd}(\bar{q}_1, q_3) =: q_{13}$ and $\bar{q}'_2 = \text{gcd}(\bar{q}_2, \bar{q}_3) =: q_{23}$, whence Eq. (12.3) may be written in a more symmetric way as

$$q_1 = q_{12} \bar{q}_{13} = \frac{q_2 \bar{q}_3}{|q_{23}|^2}, \quad q_2 = q_{12} \bar{q}_{23} = \frac{q_1 q_3}{|q_{13}|^2}, \quad q_3 = \bar{q}_{13} \bar{q}_{23} = \frac{\bar{q}_1 q_2}{|q_{12}|^2}.$$

If we define the corresponding indices in the obvious way, we see that the index $\Sigma(R_1, R_2)$ can be written as

$$\begin{aligned} \Sigma(R_1, R_2) &= \frac{\Sigma_1 \Sigma_2}{\Sigma_{12}} = \frac{\Sigma_1 \Sigma_3}{\Sigma_{13}} = \frac{\Sigma_2 \Sigma_3}{\Sigma_{23}} = \Sigma_{12} \Sigma_3 = \Sigma_{13} \Sigma_2 = \Sigma_{23} \Sigma_1 \\ &= \Sigma_{12} \Sigma_{13} \Sigma_{23} = \Sigma_{12} \Sigma'_1 \Sigma'_2 = (\Sigma_1 \Sigma_2 \Sigma_3)^{\frac{1}{2}}. \end{aligned}$$

The last expression was proved by different methods in [40]. Note that we can express $\Sigma(R_1, R_2)$ either in terms of the simple indices $\Sigma_1, \Sigma_2, \Sigma_3$ or in terms of the 'reduced' indices $\Sigma_{12}, \Sigma_{13}, \Sigma_{23}$, which somehow describe the 'common' part of R_1, R_2 and R_3 . Note that R_{12}, R_{13} and R_{23} contain the complete information about the triple junction. In particular, we can write $\Gamma(R_1, R_2)$ as $\Gamma(R_1, R_2) = R_{12}(R_{12}^{-1} \Gamma \cap R_{13}^{-1} \Gamma \cap R_{23}^{-1} \Gamma)$.

As we have now solved the problem of MCSLs of the cubic lattices, it is natural to ask whether these results can be generalised. Unfortunately, not much is known about MCSLs in dimensions $d > 3$, not even for the A_4 -lattice or the hypercubic lattices. This is not too surprising in view of the fact that the computation of MCSLs is substantially more difficult than the determination of ordinary CSLs. Indeed, even for the 4-dimensional root lattices,

no explicit expression for the MCSLs is known, which makes the corresponding enumeration problem intractable along the explicit route we have taken above.

Still, there are several interesting questions to address. A striking feature of our examples is the stabilisation property of the coincidence spectra and of the MCSLs themselves. For the planar lattices and modules of Section 8, any MCSM can be represented as the intersection of at most two ordinary CSMs, whereas for the cubic lattices up to three ordinary CSLs are needed. One might suspect that, in dimension d , any MCSL can be written as the intersection of at most d ordinary CSLs, but this seems too difficult to decide at the moment.

A somewhat easier problem is the stabilisation phenomenon of the coincidence spectra. For the cubic lattices as well as for the planar lattices and modules of Section 8, we have $\sigma_\infty(\Gamma) = \sigma(\Gamma)$; compare Proposition 12.1 and Eq. (8.8). Similarly, we have $\sigma_\infty(\Gamma) = \sigma(\Gamma)$ for the lattices A_4 , D_4^* and \mathbb{Z}^4 . For A_4 and D_4^* , this follows immediately from $\sigma(\Gamma) = \widehat{\sigma}(\Gamma)$ and Eq. (7.3). For \mathbb{Z}^4 , one has to argue differently, as $\sigma(\Gamma) \neq \widehat{\sigma}(\Gamma)$. Here, index considerations similar to those in Eq. (10.12) do the job.

There are two further (somewhat extremal) situations where we can prove stabilisation. If the simple spectrum is a finite set, which is equivalent to the finiteness of the set of CSLs, the coincidence spectra must stabilise after a finite number of steps, as the set of all MCSLs is finite as well. This happens for the rather large class of planar lattices that have exactly two coincidence reflections; compare [17]. The second situation is the case $\sigma(\Gamma) = \mathbb{N}$, where we obviously have $\sigma_\infty(\Gamma) = \sigma(\Gamma)$. This happens for $\Gamma = \mathbb{Z}^d$ for $d \geq 5$, as we shall see below.

13. RESULTS IN HIGHER DIMENSIONS

For dimensions $d \geq 4$, not much is known about CSLs in general, let alone CSMs. However, if Γ is *rational*, we have some results on the possible indices. In this case, the group $\text{OC}(\Gamma)$ is generated by coincidence reflections. To be more concrete, let $R_v: \mathbb{R}^d \rightarrow \mathbb{R}^d$, $x \mapsto x - 2\frac{\langle v|x \rangle}{\langle v|v \rangle}v$ denote the reflection in the plane perpendicular to $v \in \mathbb{R}^d$. As a first result, we mention the following characterisation of rational lattices.

Theorem 13.1 ([99, Thm. 3.2 and Cor. 3.3]). *A lattice $\Gamma \subset \mathbb{R}^d$ is rational¹¹ if and only if any reflection R_v , with $v \in \Gamma \setminus \{0\}$ is a coincidence reflection.* \square

As we have plenty of coincidence reflections for rational lattices, it is not a surprise that they generate the group $\text{OC}(\Gamma)$. In particular, we have the following analogue of the classic Cartan–Dieudonné theorem (see [23, 39]) for coincidence isometries.

Theorem 13.2 ([99, Thm. 3.1 and Thm. 3.5]). *Let $\Gamma \subset \mathbb{R}^d$ be a rational lattice (in the wider sense). Then, any coincidence isometry of Γ is a product of at most d coincidence reflections generated by lattice vectors of Γ .* \square

¹¹meaning rational in the wider sense; compare Footnote 4 on page 25.

Theorem 13.2 allows us to determine the coincidence spectrum for some rational lattices. As an example, we consider $\Gamma = \mathbb{Z}^d$. In this case, $\text{OC}(\mathbb{Z}^d)$ is generated by the reflections R_v , where v runs through all non-zero primitive lattice vectors. The coincidence index $\Sigma(R_v)$ can be calculated explicitly and, for primitive v , is given by [100, Thm. 3.2] as

$$(13.1) \quad \Sigma(R_v) = \begin{cases} \langle v|v \rangle, & \text{if } \langle v|v \rangle \text{ is odd,} \\ \frac{1}{2}\langle v|v \rangle, & \text{if } \langle v|v \rangle \text{ is even.} \end{cases}$$

As any positive integer n can be written as the sum of four squares, there exists a primitive vector $v \in \mathbb{Z}^d$ with $\langle v|v \rangle = 2n$ for $d \geq 5$ (choose one of the components to be 1, which guarantees the primitivity, and adjust the other components to get length $\langle v|v \rangle = 2n$). Hence, in \mathbb{Z}^d with $d \geq 5$, all positive integers occur as a coincidence index of some reflection, which gives us the coincidence spectrum; compare [100].

Fact 13.3. *The coincidence spectrum of \mathbb{Z}^d for $d \geq 5$ is \mathbb{N} .* □

Remark 13.4. Previously, we have seen that the coincidence spectrum of \mathbb{Z}^d is a proper subset of \mathbb{N} for $2 \leq d \leq 4$; compare Example 8.5 and Remarks 9.6 and 10.12. Although Theorem 13.2 guarantees that the coincidence reflections generate $\text{OC}(\mathbb{Z}^d)$, it is not evident whether they yield the whole coincidence spectrum. But, in fact, this is indeed the case. Moreover, for $2 \leq d \leq 4$, it follows that n is the index of a coincidence reflection if and only if n is the index of a coincidence rotation.

This is obvious for $d = 2$, as there is an index-preserving bijection between coincidence reflections and coincidence rotations (observe that any reflection is the product of complex conjugation with a rotation).

For $d = 3$ or $d = 4$, there is no such bijection. Nevertheless, we get the possible indices for coincidence reflections by evaluating Eq. (13.1). This is straightforward for $d = 4$, where we conclude that exactly all odd positive integers and all positive integers of the form $4n + 2$ occur as coincidence indices for some coincidence reflection. These are the same indices we found for the coincidence rotations of \mathbb{Z}^4 in Section 10; compare Remark 10.12.

For $d = 3$, evaluating Eq. (13.1) is more difficult. Recall that any integer that is not of the form $4^k m$ with $m \equiv 7 \pmod{8}$ can be written as the sum of three squares. Hence, for any odd n , there exists a vector $v \in \mathbb{Z}^3$ such that $\langle v|v \rangle = 2n$. In fact, there even exists a primitive v , since a positive integer $m \not\equiv 0 \pmod{4}$ can be represented as a sum of three integers if and only if it has a primitive representation; see [29] for an explicit formula for the number of primitive representations. Thus, there is a coincidence reflection of index n for any positive odd n . Recall from Section 9 that there are coincidence rotations of index n for all positive odd n as well. ◇

Theorem 13.1 can be generalised to \mathcal{S} -lattices, as its proof is algebraic in nature. The analogue of a rational lattice can be characterised as follows.

Theorem 13.5 ([57, Thm. 3.2]). *Let $M \subseteq \mathbb{R}^d$ be an \mathcal{S} -lattice, and let K be the field of fractions of \mathcal{S} . Then, the following properties are equivalent.*

- (1) *For all $u, v \in M$ and $w \in M \setminus \{0\}$, we have $\frac{\langle u|v \rangle}{\langle w|w \rangle} \in K$;*
- (2) *R_v is a coincidence reflection for any $v \in M \setminus \{0\}$.* □

For any \mathcal{S} -lattice that satisfies the properties of Theorem 13.5, we have the following generalisation of Theorem 13.2, which again is an analogue of the Cartan–Dieudonné theorem.

Theorem 13.6 ([57, Thm. 3.1]). *Let $M \subseteq \mathbb{R}^d$ be an \mathcal{S} -lattice, and let K be the field of fractions of \mathcal{S} . Let M satisfy the conditions of Theorem 13.5. Then, any coincidence isometry of M can be written as the product of at most d coincidence reflections generated by non-zero vectors of M .* □

To get more concrete results in dimensions $d \geq 5$, it would be nice to have an explicit parametrisation for the coincidence isometries. For dimensions $d = 3$ and $d = 4$, we profitted from the parametrisation of rotation by quaternions. An obvious candidate for higher dimensions is Cayley’s parametrisation of rotations in terms of Clifford algebras. At present, however, we are not aware of any concrete results in this direction for $d \geq 5$.

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