Algebraic Solution of the Coincidence Problem in Two and Three Dimensions

Michael Baake[a1] and Peter A. B. Pleasants[b]

[a] Institut für Theoretische Physik, Universität Tübingen, D–72076 Tübingen, Germany
[b] Department of Mathematics, Macquarie University, Sydney, NSW 2109, Australia

Z. Naturforsch. **50a**, 711–717 (1995); received March 27, 1995

Dedicated to Wolfram Prandl on the occasion of his 60th birthday

The coincidence problem is analyzed in an illustrative fashion for some lattices and modules in two and three dimensions which are important for crystals and quasicrystals. We give a complete description of the groups of coincidence rotations with their associated indices and encapsulate their statistics by means of generating functions.

Introduction

The concept of coincidence site lattice (CSL) arises in the crystallography of grain and twin boundaries [1]. Different domains of a crystal across a boundary are related by having a sublattice (of full rank) in common. This is the CSL. It can be viewed as the intersection of a lattice with a rotated copy of itself, where the points in common form a sublattice of finite index (and we will not discuss any situation other than that). So far CSLs have been investigated only for true lattices, for example cubic or hexagonal crystals [2, 3, 4]. With the advent of quasicrystals infinitely many new cases arise, since quasicrystals also have grain boundaries and one would like to know the coincidence site quasilattices [5, 6] and, more specifically, which of them can form twins (or multiple twins, where the angle between the grains is a rational multiple of π). Added impetus is given by the experimental progress made in recent years [7, 8], in particular on the reconstruction of fine structure details. So an extension of the CSL analysis to *all* discrete structures is desirable. We will attack this problem in two steps.

In this paper, we shall present an algebraic approach to the coincidence problem for planar structures with 4-, 6- and 12-fold rotation symmetry and for 3D structures with cubic and icosahedral symmetry. This extends existing work [5, 9, 6] and puts it in a simpler, more unified setting. The results on non-crystalline symmetries are needed for quasicrystalline T-phases which are quasiperiodic in a plane and periodically stacked in the third dimension and for 3D quasicrystals with icosahedral symmetry. Both require a two stage treatment: not only do we have to find the coincidence isometries (the universal part of the problem) but also the specific modifications of the atomic surfaces (also called windows or acceptance domains) that are needed to describe the set of coinciding points. While we present the universal part in detail, we only briefly comment on the acceptance corrections.

In Part 1 of the article we set the scene by starting with the coincidence problem for the square lattice $\mathbb{Z}^2$. The set of coincidence transformations for $\mathbb{Z}^2$ forms a group, the generators of which can be given explicitly through their connection with Gaussian integers [10]. Simultaneously, the so-called Σ-factor or coincidence index can be calculated for an arbitrary CSL isometry. We then show how a completely analogous procedure gives the results for the triangular lattice A_2. Though this is not new, the approach we use here can be generalized to quasiperiodic planar patterns with N-fold symmetry [11]. We give explicitly the results for twelvefold symmetry and discuss their relation to the previous two cases.

Part 2 of the article deals with the 3D case. Again we start with the known case, in this instance the cubic lattices [12, 2, 3], but formulate the results in an algebraic way that allows an immediate generalization to the coincidence problem for the 3D icosahedral

[1]Heisenberg-fellow
Reprint requests to Dr. M. Baake.

0932-0784 / 95 / 0800-0711 $ 06.00 © – Verlag der Zeitschrift für Naturforschung, D-72072 Tübingen

modules of rank 6, the most important ones for the description of icosahedral quasicrystals [10]. As 3D rotations do not commute in general, the coincidence rotations form a non-Abelian group whose structure is more complicated than in the 2D case. Nevertheless the main results are simple and are given below.

Part 1: The two-dimensional case

A lattice (or module) Γ may admit certain rotations R (special point symmetries) which bring $R\Gamma$ into perfect coincidence with Γ. In addition to these one can also find rotations such that $R\Gamma \cap \Gamma$ is a sublattice of Γ of finite index, the so-called coincidence site lattice [5, 13, 2, 3], CSL. The index is called the *coincidence index* (or *Σ-factor*) of the rotation R:

$$\Sigma(R) = [\Gamma : (\Gamma \cap R\Gamma)] \,. \tag{1}$$

One has $\Sigma(R) = \Sigma(R^{-1})$. The set of all such rotations forms a group which we call SOC(Γ). In the planar case this group is a subgroup of SO(2), so Abelian. All this is illustrated in the three examples to follow. The extension to reflections (and thus general point isometries) is straightforward but not discussed here.

1.1. Coincidence rotations for the square lattice

The square lattice $\mathbb{Z}^2$ consists of all integral linear combinations of the two vectors e_1 and e_2. A rotated copy $R\,\mathbb{Z}^2$, with

$$R = R(\varphi) = \begin{pmatrix} \cos(\varphi) & -\sin(\varphi) \\ \sin(\varphi) & \cos(\varphi) \end{pmatrix} \in \mathrm{SO}(2, \mathbb{R}), \tag{2}$$

results in a CSL of finite index if and only if both $\cos(\varphi)$ and $\sin(\varphi)$ are rational. This gives the well-known relation between coincidence rotations and primitive Pythagorean triples [13]. The group of coincidence rotations is thus given by

$$\mathrm{SOC}(\mathbb{Z}^2) \;=\; \mathrm{SO}(2, \mathbb{Q}) \,. \tag{3}$$

To investigate this group, we notice that, with $i = \sqrt{-1}$, we can identify $\mathbb{Z}^2$ with the ring of Gaussian integers (the integers of the quadratic field $\mathbb{Q}(i)$):

$$\mathbb{Z}^2 \;=\; \mathbb{Z}[i] \;=\; \{m + ni \mid m, n \in \mathbb{Z}\} \,, \tag{4}$$

The ring $\mathbb{Z}[i]$ has a finite group of units isomorphic to C_4 (namely, i and its powers) and has unique prime factorization up to units [14].

In this setting, a rotation $R(\varphi) \in \mathrm{SOC}(\mathbb{Z}^2)$ corresponds to multiplication by a complex number $e^{i\varphi} \in \mathbb{Q}(i)$. This number can be written as $e^{i\varphi} = \alpha/\beta$ with $\alpha, \beta \in \mathbb{Z}[i]$ coprime and of equal norm. As a consequence of the unique factorization one can show [11] that every coincidence rotation can be factorized as

$$e^{i\varphi} \;=\; \varepsilon \cdot \prod_{p \equiv 1\,(4)} \left(\frac{\omega_p}{\overline{\omega}_p}\right)^{n_p} \tag{5}$$

where $n_p \in \mathbb{Z}$ (only finitely many of them $\neq 0$), ε is a unit in $\mathbb{Z}[i]$ (a power of i), p runs through the rational primes congruent to 1 (mod 4) and the $\omega_p, \overline{\omega}_p$ are the (complex conjugate) Gaussian prime factors of p (i.e., $\omega_p\overline{\omega}_p \;=\; p$). We thus have

$$\mathrm{SOC}(\mathbb{Z}^2) \;=\; \mathrm{SO}(2, \mathbb{Q}) \;\simeq\; C_4 \otimes \mathbb{Z}^{\aleph_0} \tag{6}$$

with generators i for C_4 and $\omega_p/\overline{\omega}_p$ with $p \equiv 1\,(4)$ for the infinite cyclic groups.

The coincidence index $\Sigma(R)$ is the norm of the denominator of (5), that is,

$$\Sigma(R) \;=\; \prod_{p \equiv 1\,(4)} p^{|n_p|} \,. \tag{7}$$

In particular, it is 1 for the units (i.e. true symmetry rotations) and p for the generator $\omega_p/\overline{\omega}_p$. The first few generators with $\Sigma > 1$ are

$$\frac{4+3i}{5}\,,\quad \frac{12+5i}{13}\,,\quad \frac{15+8i}{17}\,,\quad \frac{21+20i}{29}\,,\quad \frac{35+12i}{37}\,,\quad \frac{40+9i}{41}\,,\ \text{etc.}$$

These have been normalized to have denominator Σ (a prime $\equiv 1$ (mod 4)) and argument in $(0, \pi/4)$. All other CSL rotations are obtained by combinations, as indicated in eq. (5). We have dealt here with rotation coincidences only. For the easy extension to reflections see [11].

It is convenient to summarize the possible coincidence indices and the number of rotations with a given index by means of a generating function. To do so, let $4f(m)$ denote the number of CSL rotations of index m. It turns out [11] that $f(m)$ is a multiplicative function (i.e., $f(m_1m_2) = f(m_1)f(m_2)$ for coprime m_1, m_2) so a Dirichlet series $\Phi(s)$ is an appropriate generating function. We find $f(p^r) = 2$ for a prime power p^r ($p \equiv 1 \pmod 4$, $r \geq 1$) and obtain

$$\begin{aligned}\Phi(s) &= \sum_{m=1}^{\infty} \frac{f(m)}{m^s} \\ &= \prod_{p\equiv 1(4)} \left(1 + \frac{2}{p^s} + \frac{2}{p^{2s}} + \cdots\right) = \prod_{p\equiv 1(4)} \frac{1+p^{-s}}{1-p^{-s}} \\ &= 1 + \frac{2}{5^s} + \frac{2}{13^s} + \frac{2}{17^s} + \frac{2}{25^s} + \frac{2}{29^s} + \frac{2}{37^s} \\ &\quad + \frac{2}{41^s} + \frac{2}{53^s} + \frac{2}{61^s} + \frac{4}{65^s} + \frac{2}{73^s} + \cdots .\end{aligned}$$

This generating function is not only a succinct way of representing the statistics of CSL indices, it is also a powerful tool for determining their asymptotic properties [11]. For example, we have used it to show that the number of CSL rotations of $\mathbb{Z}^2$ with index $< X$ is asymptotically $4X/\pi$. The possible CSL indices are precisely the numbers m with all prime factors $\equiv 1 \pmod 4$ and we have $f(m) = 2^a$, where a is the number of distinct prime divisors of m. Each CSL is itself a square lattice, with the index as the area of its fundamental domain.

1.2. Coincidence rotations for sixfold symmetry

Before treating twelvefold symmetry (the main aim of Part 1 of this article) we look at sixfold symmetry. The triangular (or hexagonal) lattice consists of all integral linear combinations of the two vectors e_1 and $\frac{1}{2}(e_1 + \sqrt{3}\, e_2)$. It is (up to a scale factor $\sqrt{2}$) the root lattice A_2 [15]. A rotated copy $R A_2$ with $R \in \mathrm{SO}(2)$ results in a CSL of finite index if and only if $\cos(\varphi) \in \mathbb{Q}$ and $\sin(\varphi) \in \sqrt{3}\,\mathbb{Q}$. This defines $\mathrm{SOC}(A_2)$ as a subgroup of $\mathrm{SO}(2, \mathbb{Q}(\sqrt{3}))$. To further describe $\mathrm{SOC}(A_2)$ we notice that A_2 can be written as

$$\frac{1}{\sqrt{2}} A_2 = \{m + n\varrho \mid m, n \in \mathbb{Z}\} = \mathbb{Z}[\varrho] \qquad (8)$$

with $\varrho = \frac{1}{2}(1 + i\sqrt{3})$. The lattice $A_2/\sqrt{2}$ is therefore the ring of integers of the imaginary quadratic field $\mathbb{Q}(\sqrt{-3})$, the so-called Eisenstein (or Eisenstein-Jacobi) integers [14]. It has a finite group of units isomorphic to C_6 (namely, ϱ and its powers) and unique prime factorization up to units.

A rotation $R(\varphi) \in \mathrm{SOC}(A_2)$ corresponds to multiplication by a complex number $e^{i\varphi} \in \mathbb{Q}(\sqrt{-3})$. That number can be written as $e^{i\varphi} = \alpha/\beta$ with $\alpha, \beta \in \mathbb{Z}[\varrho]$ coprime and of equal norm. As a consequence of the unique factorization one can again show [11] that every coincidence rotation can be factorized, this time as

$$e^{i\varphi} = \varepsilon \cdot \prod_{p\equiv 1\,(3)} \left(\frac{\omega_p}{\overline{\omega}_p}\right)^{n_p} \qquad (9)$$

where $n_p \in \mathbb{Z}$ (only finitely many of them $\neq 0$), ε is a unit in $\mathbb{Z}[\varrho]$ (a power of ϱ), p runs through the rational primes congruent to 1 (mod 3) and the $\omega_p, \overline{\omega}_p$ are the (complex conjugate) Eisenstein prime factors of p (i.e., $\omega_p\overline{\omega}_p = p$). We thus have

$$\begin{aligned}\mathrm{SOC}(A_2) &= \{R \in \mathrm{SO}(2) \mid \cos(\varphi) \in \mathbb{Q}, \\ &\qquad\qquad \sin(\varphi) \in \sqrt{3}\,\mathbb{Q}\} \qquad (10) \\ &\simeq C_6 \otimes \mathbb{Z}^{\aleph_0}\end{aligned}$$

with generators ϱ for C_6 and $\omega_p/\overline{\omega}_p$ with $p \equiv 1$ (3) for the infinite cyclic groups.

As in the previous example, the coincidence index is 1 for the units and p for the other generators, so for a rotation $R(\varphi)$ factorized as in (9), we have

$$\Sigma(R) = \prod_{p\equiv 1\,(3)} p^{|n_p|} . \qquad (11)$$

The first three generators with $\Sigma > 1$, normalized to have denominator Σ (a prime $\equiv 1 \pmod 3$) and argument in $(0, \pi/6)$, are

$$\frac{5+3\varrho}{7}, \quad \frac{8+7\varrho}{13}, \quad \frac{16+5\varrho}{19}.$$

Finally, if $6f(m)$ denotes the number of CSL rotations of index m, $f(m)$ is multiplicative and one finds the Dirichlet series generating function [11]

$$\begin{aligned}\Phi(s) &= \sum_{m=1}^{\infty} \frac{f(m)}{m^s} = \prod_{p\equiv 1\,(3)} \frac{1+p^{-s}}{1-p^{-s}} \\ &= 1 + \frac{2}{7^s} + \frac{2}{13^s} + \frac{2}{19^s} + \frac{2}{31^s} + \frac{2}{37^s} + \frac{2}{43^s} \\ &\quad + \frac{2}{49^s} + \cdots + \frac{2}{79^s} + \frac{4}{91^s} + \frac{2}{97^s} + \cdots\end{aligned}$$

The possible coincidence indices are precisely the numbers m with all prime factors $\equiv 1 \pmod 3$ and we have $f(m) = 2^a$, where a is the number of distinct prime divisors of m. Each CSL $A_2 \cap RA_2$ is itself a scaled version of A_2, the scale factor being the square root of its index $\Sigma(R)$. The number of CSL rotations with index $< X$ is asymptotically $3\sqrt{3}X/\pi$.

1.3. Coincidence rotations for twelvefold symmetry

Let us consider a 2D quasicrystal with twelvefold symmetry, the Stampfli [16] or the square triangle tiling [17], say. As mentioned earlier, the coincidence problem splits into two parts: first the coincidence problem for the underlying $\mathbb{Z}$-module $\mathcal{M}_{12}$ and second the correction, due to the acceptance domain, of the coincidence indices obtained in this way [11]. Here we discuss in detail only the first part.

In the complex plane, the twelvefold module [18] (of rank 4 over $\mathbb{Z}$) can be written as the direct sum $\mathcal{M}_{12} = \mathbb{Z}\cdot 1 \oplus \mathbb{Z}\cdot\xi \oplus \mathbb{Z}\cdot\xi^2 \oplus \mathbb{Z}\cdot\xi^3$ with $\xi = e^{2\pi i/12}$. Thus $\mathcal{M}_{12}$ is the ring of integers in the cyclotomic field $K = \mathbb{Q}(\xi)$. Again prime factorization is unique up to units. Every coincidence rotation (written as $e^{i\varphi} \in K$) can be factorized as [11]

$$e^{i\varphi} = \varepsilon \cdot \prod_{p\equiv 1(12)} \left(\frac{\omega_p^{(1)}}{\overline{\omega_p^{(1)}}}\right)^{n_p^{(1)}} \left(\frac{\omega_p^{(2)}}{\overline{\omega_p^{(2)}}}\right)^{n_p^{(2)}} \prod_{p\equiv\pm 5(12)} \left(\frac{\omega_p}{\overline{\omega_p}}\right)^{n_p}, \tag{12}$$

where ε is one of the 12 roots of unity in K. The factorization is more complicated than before, and we have two independent generators of index p when $p \equiv 1\,(12)$ since these primes have four prime factors in K which form two pairs of complex conjugates.

The index of a rotation R is

$$\Sigma(R) = \prod_{p\equiv 1\,(12)} p^{(|n_p^{(1)}|+|n_p^{(2)}|)} \prod_{p\equiv\pm 5\,(12)} p^{2|n_p|} \tag{13}$$

and the group of coincidence rotations has the form

$$\mathrm{SOC}(\mathcal{M}_{12}) \simeq C_{12} \otimes \mathbb{Z}^{\aleph_0}. \tag{14}$$

Thus, in spite of the more complicated factorization, the structure of the coincidence group remains simple, as indeed it does for all other planar symmetries [11].

If $12f(m)$ denotes the number of coincidence rotations of index m, the Dirichlet series generating function for $f(m)$ is

$$\begin{aligned}\Phi(s) &= \sum_{m=1}^{\infty} \frac{f(m)}{m^s} \\ &= \prod_{p\equiv 1(12)} \left(\frac{1+p^{-s}}{1-p^{-s}}\right)^2 \prod_{p\equiv\pm 5(12)} \left(\frac{1+p^{-2s}}{1-p^{-2s}}\right) \\ &= 1 + \frac{4}{13^s} + \frac{2}{25^s} + \frac{4}{37^s} + \frac{2}{49^s} + \frac{4}{61^s} + \frac{4}{73^s} \\ &\quad + \frac{4}{97^s} + \frac{4}{109^s} + \frac{4}{157^s} + \frac{8}{169^s} + \frac{4}{181^s} + \cdots .\end{aligned}$$

All coincidence modules are scaled versions of $\mathcal{M}_{12}$ and the number of CSL rotations with index $< X$ is asymptotically $12\sqrt{3}\ln(2+\sqrt{3})X/\pi^2$.

Let us compare these findings with those of the previous two cases. One would expect the CSL rotations of 4- and 6-fold symmetry to reappear here (though possibly with a different index), and this is indeed so since $\mathbb{Q}(i)$ and $\mathbb{Q}(\sqrt{-3})$ are subfields of K. To go into more detail, except for 2 and 3, all primes are $\equiv \pm 1$ or ± 5 (mod 12). For the square lattice, the generators of coincidence rotations come from primes $p \equiv 1\,(4)$, therefore $\equiv 1$ or 5 (mod 12). And for the triangular lattice, the generators of coincidence rotations come from primes $p \equiv 1\,(3)$, therefore $\equiv 1$ or -5 (mod 12). It turns out that $\mathrm{SOC}(\mathbb{Z}^2)$ and $\mathrm{SOC}(A_2)$ together generate the subgroup of $\mathrm{SOC}(\mathcal{M}_{12})$ consisting of all coincidences whose indices are squares.

How do these results apply to the coincidence problem for twelvefold symmetric tilings? Let us assume that such a tiling is obtained through projection with a certain window, a dodecagon say [16]. A coincidence in the set of vertex points occurs if there is a coincidence in the module $\mathcal{M}_{12}$ such that the image point in internal space lies both in the original window *and* in an appropriately rotated window. A consequence of this is that the coincidence group of the tiling is still $\mathrm{SOC}(\mathcal{M}_{12})$ but the index of each group element is normally larger than its index in $\mathcal{M}_{12}$ by a correction factor close to 1 (depending on the group element). It also explains why the set of coinciding points forms a tiling of slightly different type from the original one, a small proportion of the points of the original tiling being missing from it. In fact the term "index" for the reciprocal of the fraction of coinciding points is perhaps inappropriate in this setting as it no longer has a purely algebraic interpretation and is no longer an integer. Details of this and the determination of the rotation angle in internal space by means of algebraic conjugation are given in [11].

Part 2: Examples in three dimensions

The coincidence problem in three dimensions is more involved. In particular, the SOC-group, being a subgroup of SO(3), is in general no longer Abelian. In what follows, we present two examples where we can give a complete description of the SOC-group and its indices through Cayley's parametrization of O(3). Since $\mathrm{O}(3) = \mathrm{SO}(3) \otimes \{\pm \mathbb{1}\}$, the extension to reflections is trivial and will not be discussed below.

2.1. Coincidence rotations for cubic lattices

The simplest object to start with is the primitive cubic lattice, $\mathbb{Z}^3$. (The *bcc* and *fcc* lattices require only a minimal modification mentioned at the end of the section.) If we write $\mathbb{Z}^3 = \mathbb{Z}e_1 \oplus \mathbb{Z}e_2 \oplus \mathbb{Z}e_3$ it is immediate that the coincidence group is

$$\mathrm{SOC}(\mathbb{Z}^3) = \mathrm{SO}(3, \mathbb{Q}) . \tag{15}$$

(other rotations might also lead to coincidences, but not to a CSL of full rank 3). The subgroup of rotations with index 1 is the rotation group of the cube [20] of order 24, $\mathcal{O} = \mathrm{SO}(3, \mathbb{Z})$.

To determine the index of a rotation $R \in \mathrm{SO}(3, \mathbb{Q})$, we use quaternions [21, 22] and Cayley's parametrization [22] with 4 *coprime* integers $\kappa, \lambda, \mu, \nu$

$$R(\kappa, \lambda, \mu, \nu) = \frac{1}{\sigma} \begin{pmatrix} \delta_\lambda & -2\kappa\nu + 2\lambda\mu & 2\kappa\mu + 2\lambda\nu \\ 2\kappa\nu + 2\lambda\mu & \delta_\mu & -2\kappa\lambda + 2\mu\nu \\ -2\kappa\mu + 2\lambda\nu & 2\kappa\lambda + 2\mu\nu & \delta_\nu \end{pmatrix}$$

where $\sigma = \kappa^2 + \lambda^2 + \mu^2 + \nu^2$, $\delta_\lambda = \kappa^2 + \lambda^2 - \mu^2 - \nu^2$, $\delta_\mu = \kappa^2 - \lambda^2 + \mu^2 - \nu^2$, and $\delta_\nu = \kappa^2 - \lambda^2 - \mu^2 + \nu^2$. This gives a double cover of $\mathrm{SO}(3, \mathbb{Q})$ (since $R(q) = R(-q)$). One can show [23] that the coincidence index $\Sigma(R)$ is the denominator of R, defined as $\mathrm{den}(R) = \gcd(r \in \mathbb{N} \mid rR \text{ integral})$. It is the "odd part" of σ:

$$\Sigma(R) = \mathrm{den}(R(\kappa, \lambda, \mu, \nu)) = \sigma / 2^s, \tag{16}$$

where s is the largest integer such that 2^s divides σ. In particular, we reproduce the result [12, 2] that $\Sigma(R)$ runs precisely through all odd integers.

Cayley's parametrization has the nice property that (λ, μ, ν) gives the rotation axis of $R(\kappa, \lambda, \mu, \nu)$,

$$R(\kappa, \lambda, \mu, \nu) \cdot (\lambda, \mu, \nu)^t = (\lambda, \mu, \nu)^t , \tag{17}$$

while the rotation angle follows from $\mathrm{tr}(R) = 1 + 2\cos(\varphi)$, so

$$\cos(\varphi) = \frac{\kappa^2 - \lambda^2 - \mu^2 - \nu^2}{\kappa^2 + \lambda^2 + \mu^2 + \nu^2} . \tag{18}$$

One can easily construct all solutions for small indices explicitly [3, 4, 23], while the case $\kappa = 0$ gives all CSL rotations through 180° as described by Lück [13]. If $24f(m)$ is the number of CSL rotations of index m, it is known [24, 23] that $f(1) = 1$, $f(2n) = 0$, $f(p^r) = (p+1)p^{r-1}$ for odd primes, and $f(mn) = f(m)f(n)$ for m, n coprime (multiplicativity of f). The corresponding generating function reads

$$\begin{aligned} \Phi(s) = \sum_{m=1}^{\infty} \frac{f(m)}{m^s} &= \prod_{p \text{ odd}} \frac{1 + p^{-s}}{1 - p^{1-s}} \\ &= 1 + \frac{4}{3^s} + \frac{6}{5^s} + \frac{8}{7^s} + \frac{12}{9^s} + \frac{12}{11^s} + \frac{14}{13^s} + \frac{24}{15^s} \\ &\quad + \frac{18}{17^s} + \frac{20}{19^s} + \frac{32}{21^s} + \frac{24}{23^s} + \frac{30}{25^s} + \cdots , \end{aligned}$$

and the number of CSL rotations with index $< X$ is asymptotically $72X^2/\pi^2$.

This is not the end of the story. Coincidence rotations of given index m can be collected into equivalence classes of rotations related by the action of $\mathcal{O}$ [24]. This double coset analysis will be described in [23]. For example, truly different CSL's of $\mathbb{Z}^3$ with the same index occur for the first time at $\Sigma = 13$.

Also, describing the fine structure of a coincidence rotation requires an analysis of the lattice planes perpendicular to the rotation axis. For example, the (unique) equivalence class for $\Sigma = 3$ can be represented by $\boldsymbol{q} = (0, 1, 1, 1)$, i.e. a rotation through π around $(1, 1, 1)^t$. Here, three layers are stacked periodically, with perfect coincidence in one (which is therefore an ideal grain boundary), but none in the other two. So this coincidence rotation represents a change in the stacking sequence.

Finally, let us mention that it is precisely in this layer structure that the three cubic lattices (primitive, *bcc* and *fcc*) differ, although the SOC-group and the index formula are the same for all three.

2.2. 3D icosahedral modules of rank 6

Icosahedral quasicrystals are of particular interest, and one would like to know their coincidence structure in detail [6, 25]. We restrict our discussion to the investigation of the 3 different 3D icosahedral modules [26] (of rank 6 over $\mathbb{Z}$) and again omit the determination of the window correction [23]. We will call the modules $\mathcal{M}_B$, $\mathcal{M}_P$, $\mathcal{M}_F$ for body-centred, primitive and face-centred, respectively. They are spanned by the orthonormal basis e_1, e_2, e_3 with coefficients $\alpha_i \in \mathbb{Z}[\tau]$, $\tau = (1+\sqrt{5})/2$, as follows:

$$\begin{aligned} \mathcal{M}_B &= \{\textstyle\sum_{i=1}^{3} \alpha_i e_i \mid \tau^2\alpha_1 + \tau\alpha_2 + \alpha_3 \equiv 0\,(2)\}, \\ \mathcal{M}_P &= \{x \in \mathcal{M}_B \mid \alpha_1+\alpha_2+\alpha_3 \equiv 0 \text{ or } \tau\,(2)\}, \\ \mathcal{M}_F &= \{x \in \mathcal{M}_B \mid \alpha_1+\alpha_2+\alpha_3 \equiv 0\,(2)\}. \end{aligned} \tag{19}$$

Cayley's parametrization can again be used. Our first assertion is that the coincidence group is the same for all three modules [23], namely

$$\begin{aligned} \mathrm{SOC}(\mathcal{M}_B) = \mathrm{SOC}(\mathcal{M}_P) &= \mathrm{SOC}(\mathcal{M}_F) \\ &= \mathrm{SO}(3, \mathbb{Q}(\tau)). \end{aligned} \tag{20}$$

The unit quaternions (1, 0, 0, 0), $\frac{1}{2}(1, 1, 1, 1)$, and $\frac{1}{2}(\tau, 1, -1/\tau, 0)$ together with all even permutations and arbitrary sign flips form a group [27, 19] $\widehat{Y}$ of order 120 which is the usual double cover of the icosahedral group $Y = \{R \in \mathrm{SO}(3,\mathbb{Q}(\tau)) \mid \Sigma(R) = 1\}$. The icosian ring [19] $\mathbf{I}$ consists of all integral linear combinations of elements in $\widehat{Y}$ and is a maximal order with unique (left- or right-) factorization. One finds the relation $\mathrm{SO}(3,\mathbb{Q}(\tau)) = \{R(q) \mid q \in \mathbf{I}\}$, and our second assertion is the index formula for a coincidence rotation $R_0 \in \mathrm{SO}(3, \mathbb{Q}(\tau))$, again for all three modules:

$$\Sigma(R_0) = \min\{N(|q|^2) \mid q \in \mathbf{I},\ R(q) = R_0\} \tag{21}$$

where the argument $|q|^2$ on the right hand side is always a number in $\mathbb{Z}[\tau]$ and its norm is defined by $N(m+n\tau) = m^2+mn-n^2$. The indices Σ run through all positive integers of the form m^2+mn-n^2 with integral m and n. These are the numbers all of whose prime factors congruent to 2 or 3 (mod 5) occur with even exponent only. (They can also be characterized as the positive numbers of the form $5x^2 - y^2$ with integral x and y, as used in [25].) For $\Sigma \le 100$, one finds the list of the numbers 1, 4, 5, 9, 11, 16, 19, 20, 25, 29, 31, 36, 41, 44, 45, 49, 55, 59, 61, 64, 71, 76, 79, 80, 81, 89, 95, 99, 100 – which covers the known cases [6].

If $60f(m)$ is the number of coincidence rotations of index m, the generating function for the multiplicative function $f(m)$ starts as

$$\begin{aligned} \Phi(s) = \sum_{m=1}^{\infty} \frac{f(m)}{m^s} &= 1 + \frac{5}{4^s} + \frac{6}{5^s} + \frac{10}{9^s} + \frac{24}{11^s} \\ &+ \frac{20}{16^s} + \frac{40}{19^s} + \frac{30}{20^s} + \frac{30}{25^s} + \frac{60}{29^s} + \frac{64}{31^s} \\ &+ \frac{50}{36^s} + \frac{84}{41^s} + \frac{120}{44^s} + \frac{60}{45^s} + \frac{50}{49^s} + \cdots \end{aligned}$$

(where the denominators show all indices ≤ 50) and the number of CSL rotations with index $< X$ is asymptotically $1350\sqrt{5}\ln(\tau)X^2/\pi^4$. A more complete description of the icosahedral case, which requires a more mathematical treatment, will be given in [23].

Concluding remarks

Various examples of coincidence problems in two and three dimensions have been presented together with their solutions in algebraic terms. Although proofs have been omitted, we hope this illustrates the usefulness of the algebraic approach. Many more cases can be treated similarly though there are open questions concerning the detailed way a coincidence is realized in three dimensions (e.g., its layer structure).

There remains the question of what can be said in higher dimensions. In dimensions > 4 orthogonal transformations can no longer be parametrized by quaternions. Nevertheless, two problems look solvable: the cubic lattices in arbitrary dimension and the module $H4$ in 4-space which is related to a highly symmetric 4D quasicrystal [28, 29]. We hope to report on these soon.

[1] S. L. Sass, "Grain Boundary Structure", in: Encyclopedia of Materials Science and Engineering, ed. M. B. Bever, Vol. 3, Pergamon, Oxford 1985.

[2] H. Grimmer, "Disorientations and Coincidence Rotations for Cubic Lattices", Acta Cryst. **A30**, 685 (1974).

[3] H. Grimmer, W. Bollmann, and D. H. Warrington, "Coincidence-Site Lattices and Complete Pattern-Shift Lattices in Cubic Crystals", Acta Cryst. **A30**, 197 (1974).

[4] H. Grimmer, "Tables of all coincidence orientations with low multiplicity for arbitrary hexagonal and rhombohedral lattices", Scripta Met. **23**, 1407 (1989).

[5] D. H. Warrington, "Coincidence site lattices in quasicrystal tilings", Mat. Science Forum **126-128**, 57 (1993).

[6] D. H. Warrington and R. Lück, "The use of the Wieringa roof to examine coincidence site quasilattices in quasicrystals", in: Aperiodic 94, ed. G. Chapuis, World Scientific, Singapore, in press.

[7] R. J. Papoular, W. Prandl, and P. Schiebel, The maximum entropy reconstruction of Patterson and Fourier densities in orientationally disordered molecular crystals: A systematic test for crystallographic interpolation models, in: Maximum Entropy and Bayesian Methods, eds. C. R. Smith et al., Kluwer, Dordrecht 1992, p. 359–76.

[8] W. Prandl, "Phase determination from X-ray powder diffraction data. II. Partial Patterson maps and the localization of anomalously scattering atoms", Acta Cryst. **A50**, 52 (1994).

[9] O. Radulescu and D. H. Warrington, Arithmetic Properties of Module Directions in Quasicrystals, Coincidence Modules and Coincidence Quasilattices, preprint (1994), to appear in Acta Cryst. **A**.

[10] M. Baake and P. A. B. Pleasants, "The coincidence problem for crystals and quasicrystals", in: Aperiodic 94, ed. G. Chapuis, World Scientific, Singapore 1995, in press.

[11] P. A. B. Pleasants, M. Baake, and J. Roth, "Planar coincidences for N-fold symmetry", Tübingen preprint TPT-QC-94-05-1, to appear in J. Math. Phys.

[12] H. Grimmer, "Coincidence Rotations for Cubic Lattices", Scripta Met. **7**, 1295 (1973).

[13] R. Lück, "Pythagoreische Zahlen für den dreidimensionalen Raum", Phys. Blätter **35**, 72 (1979).

[14] G. H. Hardy and E. M. Wright, An Introduction to the Theory of Numbers, 5th ed., Clarendon Press, Oxford 1979.

[15] J. H. Conway and N. J. A. Sloane, Sphere Packings, Lattices and Groups, 2nd ed., Springer, New York 1993.

[16] P. Stampfli, "New Quasiperiodic Lattices from the Grid Method", in: Quasicrystals, Networks, and Molecules of Fivefold Symmetry, ed. I. Hargittai, VCH, New York 1990.

[17] M. Baake, R. Klitzing, and M. Schlottmann, "Fractally shaped acceptance domains of quasiperiodic square-triangle tilings with dodecagonal symmetry", Physica **A191**, 554 (1992).

[18] N. D. Mermin, D. S. Rokhsar, and D. C. Wright, "Beware of 46-fold symmetry: the classification of two-dimensional quasicrystallographic lattices", Phys. Rev. Lett. **58**, 2099 (1987).

[19] R. V. Moody and J. Patera, "Quasicrystals and icosians", J. Phys. **A26**, 2829 (1993).

[20] M. Baake, "Structure and representations of the hyperoctahedral group", J. Math. Phys. **25**, 3171 (1984).

[21] A. Hurwitz, Vorlesungen über die Zahlentheorie der Quaternionen, Springer, Berlin 1919.

[22] M. Koecher and R. Remmert, "HAMILTONsche Quaternionen", in: Zahlen, eds. H.-D. Ebbinghaus et al., 3rd ed., Springer, Berlin 1992, p. 155–81.

[23] M. Baake, R. Lück, and P. A. B. Pleasants, "The coincidence problem for cubic and icosahedral patterns", in preparation.

[24] H. Grimmer, "The Generating Function for Coincidence Site Lattices in the Cubic System", Acta Cryst. **A40**, 108 (1984).

[25] O. Radulescu, "A Simple Approach to the Crystallography of Twins in Icosahedral Quasicrystals", preprint (1995), to appear in J. Phys. I (France).

[26] D. S. Rokhsar, N. D. Mermin, and D. C. Wright, "Rudimentary quasicrystallography: The icosahedral and decagonal reciprocal lattices", Phys. Rev. **B35**, 5487 (1987).

[27] J. E. Humphreys, Reflection Groups and Coxeter Groups, C. U. P., Cambridge 1990.

[28] V. Elser and N. J. A. Sloane, "A highly symmetric four-dimensional quasicrystal", J. Phys. **A20**, 6161 (1987).

[29] R. V. Moody and A. Weiss, "On Shelling E_8 Quasicrystals", J. Number Theory **47**, 405 (1994).