

COINCIDENCE INDICES OF SUBLATTICES AND COINCIDENCES OF COLORINGS

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ABSTRACT. Even though a lattice and its sublattices have the same group of coincidence isometries, the coincidence index of a coincidence isometry with respect to a lattice Λ_1 and to a sublattice Λ_2 may differ. Here, we examine the coloring of Λ_1 induced by Λ_2 to identify how the coincidence indices with respect to Λ_1 and to Λ_2 are related. This leads to a generalization of the notion of color symmetries of lattices to what we call color coincidences of lattices. Examples involving the cubic and hypercubic lattices are given to illustrate these ideas.

1. INTRODUCTION

Coincidence site lattices (CSLs) are an important tool to describe grain boundaries in crystals [12, 32, 5] and quasicrystals [38, 39, 31, 40]. In particular one is interested in the so-called coincidence index, which describes how much larger the unit cell of the CSL is compared to the unit cell of the parent lattice. It is a well-known fact that a lattice and all its sublattices share the same group of coincidence isometries, more generally - two commensurate lattices have the same coincidence isometries. However, the coincidence indices of a coincidence isometry with respect to the lattice and its sublattices usually differ. Nevertheless, there is a relationship between the coincidence indices for a parent lattice and its sublattice. The aim of this paper is to give an explicit expression of this relationship by means of colorings of lattices.

Grimmer, Bollmann, and Warrington proved that the coincidence indices for a given coincidence isometry are the same for all three cubic lattices by using a shelling argument [16]. The main idea behind their proof can be rephrased in the terminology of colorings. Consider a body-centered cubic lattice and its maximal primitive cubic sublattice of index 2. Suppose we assign the color black to the lattice points of the primitive cubic lattice and the color white to the other lattice points. Then a rotation about any lattice point can map black points only onto black points and never onto white points, and vice versa - this follows from the fact that black and white points lie on different shells.

The aim of this paper is to generalize this idea. First, we color the lattice points of a sublattice using the same color, and assign suitable colors to the remaining lattice points. By analyzing how these colors are interchanged by the coincidence isometries, we are able to get an explicit formula for the coincidence index of the sublattice in terms of the coincidence index of its parent lattice and some properties of the coloring of the lattice.

This establishes a link between CSLs and colorings of a lattice. Actually, connections between colorings and CSLs have already been observed earlier in [33, 30, 1, 27, 28]. This motivates us to analyze the coincidences of lattice colorings even further. Indeed, there is a long tradition on analyzing colorings of various structures, starting from the context of magnetic structures [36, 24] that led to an extensive analysis of various symmetrically colored symmetrical structures, such as colored lattices [19, 33, 34, 11] and colored tilings [10, 35]. In fact, studies have been done not only on colored periodic tilings, but also on colored quasiperiodic tilings [29, 23, 1, 7].

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Recall that a CSL is the intersection of a lattice with a rotated copy of itself, while its coincidence index is the ratio of the volumes of a (primitive) unit cell of the CSL and a unit cell of the parent lattice. Thus, the coincidence index is a measure of how the two lattices (the lattice and its rotated copy) fit together. Moreover, it also describes how well two crystal grains fit together. Here, it is not so important whether the actual atomic positions at the grain boundary do coincide, as the atoms will rearrange anyhow to minimize energy. What is important is that the grain boundary has a small (two-dimensional) unit cell. The latter is related to the coincidence index and can be calculated by considering the corresponding CSL. By a rule of thumb, grain boundaries with a small coincidence index have low energy and are thus preferred. Of course, this rule of thumb is based on geometric considerations only and cannot replace an actual calculation of the energy of the grain boundary. Nevertheless, it serves as an important tool in the theory of interfaces as it gives a good hint on which grain boundaries are preferred (*cf.* [20, 37]).

Hence, we consider coincidences of lattices only, although coincidences of actual crystals could be considered as well and have been considered [26]. This means that we restrict our attention to coincidence isometries that fix the origin, but see [26] for a treatment of general affine coincidence isometries.

Note that most results of the present paper have been announced earlier in [25] (but without proofs). That earlier article, where examples using the square lattice and the Ammann-Beenker tiling are depicted, was intended more for experimentalists and crystallographers, while this contribution is more for mathematical crystallographers. Here, we illustrate the general results through examples involving the cubic lattices in dimension $d = 3$ and involving the hypercubic lattices in $d = 4$. The cubic lattices are certainly important lattices, and our example will also clarify the connection of our approach with colorings to the shelling argument of Grimmer *et al.* [16]. The example involving the hypercubic lattices in $d = 4$ serves to show that our approach is not only confined to periodic crystals but is also applicable for quasicrystals. Recall that the lattice \mathbb{Z}^4 can be used to generate the Ammann-Beenker tiling via the cut-and-projection scheme (*cf.* [3]). Even though both examples can be solved by means of orthogonal matrices, the most efficient way to solve them is to make use of the Hurwitz quaternions. Quaternions are so powerful and natural in this context that they have been used for CSLs since at least 1974 by Grimmer [14] (with Ranganathan's paper [32] containing them already in some disguised form), and have become a standard tool [37] in this area. The details of these calculations are contained in the appendix, to make the main results more accessible for those who are not so familiar with quaternions.

2. PRELIMINARIES

Let us briefly recall some basic notions first, for more details see [2]. A *lattice* Λ (of *rank* and *dimension* d) is a discrete subset of \mathbb{R}^d that is the \mathbb{Z} -span of d linearly independent vectors v_1, \dots, v_d over \mathbb{R} . The set $\{v_1, \dots, v_d\}$ is referred to as a *basis* of Λ . As a group, Λ is isomorphic to the free abelian group of rank d . A *sublattice* Λ' of Λ is a subset of Λ that forms a subgroup of finite index in Λ . This means that Λ' is itself a lattice and is of the same rank and dimension as Λ . Here, the group index $[\Lambda : \Lambda'] < \infty$ can be interpreted geometrically as the ratio of the volume of a fundamental domain of Λ' by the volume of a fundamental domain of Λ .

The *dual* of a lattice Λ is the lattice

$$\Lambda^* := \left\{ x \in \mathbb{R}^d : \langle x, y \rangle \in \mathbb{Z} \text{ for all } y \in \Lambda \right\},$$

where $\langle \cdot, \cdot \rangle$ denotes the standard scalar product in \mathbb{R}^d . Two lattices Λ_1 and Λ_2 are said to be *commensurate* if their intersection is a sublattice of both lattices. The *sum* of two commensurate lattices Λ_1 and Λ_2 ,

$$\Lambda_1 + \Lambda_2 := \{ \ell_1 + \ell_2 : \ell_1 \in \Lambda_1, \ell_2 \in \Lambda_2 \},$$

also forms a lattice.

An orthogonal transformation $R \in O(d) := O(d, \mathbb{R})$ is said to be a *coincidence isometry* of the lattice Λ if $\Lambda \cap R\Lambda$ is a sublattice of both Λ and $R\Lambda$. The sublattice $\Lambda(R) := \Lambda \cap R\Lambda$ is called the *coincidence site lattice* (CSL) of Λ generated by R , and

$$\Sigma_\Lambda(R) := [\Lambda : \Lambda(R)] = [R\Lambda : \Lambda(R)]$$

is called the *coincidence index of R with respect to Λ* . The set of coincidence isometries of Λ forms a group, denoted by $\text{OC}(\Lambda)$ [2, Theorem 2.1]. Note that $\text{OC}(\Lambda)$ is a countable subgroup of $O(d)$, and it contains the *point group* $P(\Lambda)$ of Λ as a subgroup. In particular, we can characterize $P(\Lambda)$ by means of the coincidence index as follows:

$$P(\Lambda) = \{R \in O(d) : R\Lambda = \Lambda\} = \{R \in \text{OC}(\Lambda) \mid \Sigma_\Lambda(R) = 1\}.$$

The subgroup of $\text{OC}(\Lambda)$ formed by all coincidence rotations of Λ is written as $\text{SOC}(\Lambda) := \text{OC}(\Lambda) \cap \text{SO}(d)$.

Coincidences of a lattice and its sublattices are closely related. In particular, we have the following result [2].

Fact 1. *If Λ_2 is a sublattice of Λ_1 , then $\text{OC}(\Lambda_1) = \text{OC}(\Lambda_2)$.*

For instance, the three cubic lattices share the same coincidence isometries. The same holds for the two four-dimensional hypercubic lattices. Using a shelling argument [16], it is known that the coincidence index for a given coincidence isometry is the same for all three cubic lattices (see Fact 3). However, this is clearly not the case for the four-dimensional hypercubic lattices because they have different point groups, and moreover, do not share the same set of coincidence indices [2, 41].

In general, even though the groups of coincidence isometries of a lattice Λ_1 and a sublattice Λ_2 are the same, the coincidence indices and corresponding multiplicities with respect to Λ_1 and Λ_2 may be different. Let $R \in \text{OC}(\Lambda_1) = \text{OC}(\Lambda_2)$, and denote by $\Sigma_1(R)$ and $\Sigma_2(R)$ the coincidence indices of R with respect to Λ_1 and Λ_2 , respectively. From the inclusions $\Lambda_2(R) \subseteq \Lambda_2 \subseteq \Lambda_1$ and $\Lambda_2(R) \subseteq \Lambda_1(R) \subseteq \Lambda_1$ we can infer the following result [2]. Here, we denote a divides b by $a \mid b$.

Fact 2. *Let Λ_2 be a sublattice of Λ_1 of index m . If $R \in \text{OC}(\Lambda_1)$, then $\Sigma_1(R) \mid m\Sigma_2(R)$.*

By considering the so-called dual lattices of Λ_1 and Λ_2 , one also obtains

$$(2.1) \quad \Sigma_2(R) \mid m\Sigma_1(R).$$

Both divisibility conditions imply the well-known bound on $\Sigma_2(R)$:

$$(2.2) \quad \frac{1}{m}\Sigma_1(R) \leq \Sigma_2(R) \leq m\Sigma_1(R).$$

In Sections 3 and 4, we characterize when $\Sigma_2(R) = \Sigma_1(R)$ and give a formula for $\Sigma_2(R)$ in terms of $\Sigma_1(R)$ by looking at certain colorings of lattices.

A *coloring* of the lattice Λ_1 by m colors is an onto mapping $c : \Lambda_1 \rightarrow C$, where C is a set of m elements, called colors [34]. If Λ_2 is a sublattice of Λ_1 of index m , then a *coloring of Λ_1 determined by Λ_2* is a coloring of Λ_1 by m colors wherein two points of Λ_1 are assigned the same color if and only if they belong to the same coset of Λ_2 . In this case, the set of colors C can be identified with the quotient group Λ_1/Λ_2 so that the color mapping c is simply the canonical projection of Λ_1 onto Λ_1/Λ_2 whose kernel is Λ_2 .

Denote by G the symmetry group of Λ_1 and fix a coloring c of Λ_1 . A symmetry h in G is said to be a *color symmetry* of c if it permutes the colors in the coloring, that is, all and only those elements of Λ_1 having the same color are mapped by h to a fixed color. We denote the set of all color symmetries of c by H_c , that is,

$$H_c = \{h \in G \mid \exists \sigma_h \in S_C, \forall \ell \in \Lambda_1, c(h(\ell)) = \sigma_h(c(\ell))\},$$

where S_C is the group of permutations on the set of colors C . The set H_c forms a group and is called the *color group* or *color symmetry group* of c [34, 17, 11]. The mapping $P : H_c \rightarrow S_C$ with $h \mapsto \sigma_h$ defines a group homomorphism, and thus the group H_c acts on C . The kernel of P ,

$$K_c = \{k \in H_c : c(k(\ell)) = c(\ell), \forall \ell \in \Lambda_1\},$$

is the subgroup of H_c whose elements fix the colors in c . In other words, K_c is the symmetry group of the colored lattice.

We shall generalize the notion of a color symmetry to that of a color coincidence. Also, we associate the property that a coincidence isometry R of Λ_1 is a color coincidence of the coloring of Λ_1 determined by a sublattice of Λ_2 with a relationship between $\Sigma_1(R)$ and $\Sigma_2(R)$.

3. COINCIDENCE INDEX WITH RESPECT TO A SUBLATTICE

Our first goal is to give a relationship between the coincidence indices with respect to a lattice and a sublattice by means of the coloring of the lattice induced by the sublattice. Unless otherwise stated, Λ_1 is taken throughout to be a lattice having Λ_2 as a sublattice of index m , and we write $\Lambda_1 = \bigcup_{j=0}^{m-1} (c_j + \Lambda_2)$ with $c_0 := 0$. Consider the coloring of Λ_1 determined by Λ_2 , where we label the color of the coset $c_j + \Lambda_2$ by c_j .

Fix an $R \in \text{OC}(\Lambda_1) = \text{OC}(\Lambda_2)$. Consider the following subgroups of Λ_1/Λ_2 :

$$(3.1) \quad \begin{aligned} J &:= \{c_j + \Lambda_2 \in \Lambda_1/\Lambda_2 : (c_j + \Lambda_2) \cap \Lambda_1(R^{-1}) \neq \emptyset\}, \\ K &:= \{c_k + \Lambda_2 \in \Lambda_1/\Lambda_2 : (c_k + \Lambda_2) \cap \Lambda_1(R) \neq \emptyset\} \end{aligned}$$

The subgroups J and K are nonempty because both have $\Lambda_2 = c_0 + \Lambda_2$ as an element. They induce partitions of $\Lambda_1(R^{-1})$ and $\Lambda_1(R)$, respectively, given by

$$(3.2) \quad \begin{aligned} \Lambda_1(R^{-1}) &= \bigcup_{c_j + \Lambda_2 \in J} (c_j + \Lambda_2) \cap \Lambda_1(R^{-1}) \text{ and} \\ \Lambda_1(R) &= \bigcup_{c_k + \Lambda_2 \in K} (c_k + \Lambda_2) \cap \Lambda_1(R). \end{aligned}$$

The partitions in Eq. (3.2) can be thought of as colorings of $\Lambda_1(R^{-1})$ and $\Lambda_1(R)$, respectively, where the colors are inherited from the coloring of Λ_1 determined by Λ_2 . We shall refer to these colorings as the *induced colorings of $\Lambda_1(R^{-1})$ and $\Lambda_1(R)$ by c* . The set of colors in the colorings of $\Lambda_1(R^{-1})$ and $\Lambda_1(R)$ are

$$(3.3) \quad \begin{aligned} C_{R^{-1}} &:= \{c_j : c_j + \Lambda_2 \in J\} \text{ and} \\ C_R &:= \{c_k : c_k + \Lambda_2 \in K\}, \end{aligned}$$

respectively. In addition, we may assume that the coset representatives of Λ_2 in Λ_1 are chosen so that $c_j \in \Lambda_1(R^{-1})$ whenever $c_j \in C_{R^{-1}}$, and $c_k \in \Lambda_1(R)$ whenever $c_k \in C_R$.

In fact, there are two possible colorings of $\Lambda_1(R)$. On the one hand, we have the coloring of $\Lambda_1(R)$ induced by c with colors from C_R . On the other hand, a coloring of $R\Lambda_1(R^{-1}) = \Lambda_1(R)$ is obtained when R is applied to the induced coloring of $\Lambda_1(R^{-1})$ by c with colors from $C_{R^{-1}}$. We compare both colorings of $\Lambda_1(R)$ by looking at the relation σ_R from $C_{R^{-1}}$ to C_R given by

$$(3.4) \quad \sigma_R = \{(c_j, c_k) \in C_{R^{-1}} \times C_R : R[(c_j + \Lambda_2) \cap \Lambda_1(R^{-1})] \cap [(c_k + \Lambda_2) \cap \Lambda_1(R)] \neq \emptyset\}.$$

Here, $(c_j, c_k) \in \sigma_R$ means that some of the points colored c_j in the coloring of $\Lambda_1(R^{-1})$ are mapped by R onto points with color c_k in the coloring of $\Lambda_1(R)$.

Note that

$$(3.5) \quad [\Lambda_2 \cap \Lambda_1(R)] \cap R[\Lambda_2 \cap \Lambda_1(R^{-1})] = \Lambda_2(R),$$

which tells us that $(c_0, c_0) \in \sigma_R$ and so σ_R is always nonempty [25]. Moreover, $\Lambda_2(R)$ is made up of exactly those points colored c_0 in the coloring of $\Lambda_1(R)$ whose preimages under R are also points colored c_0 in the coloring of $\Lambda_1(R^{-1})$.

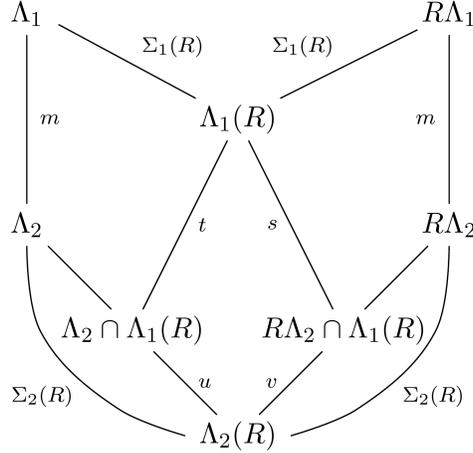


FIGURE 1. Subgroup diagram showing the relationship between $\Lambda_1, \Lambda_2(R)$ and other sublattices together with their indices

See Figure 1 for the relationships among the various lattices and the corresponding indices. In particular, we define

$$(3.6) \quad \begin{aligned} s &:= [\Lambda_1(R) : R\Lambda_2 \cap \Lambda_1(R)], \\ t &:= [\Lambda_1(R) : \Lambda_2 \cap \Lambda_1(R)], \\ u &:= [\Lambda_2 \cap \Lambda_1(R) : \Lambda_2(R)], \\ v &:= [R\Lambda_2 \cap \Lambda_1(R) : \Lambda_2(R)]. \end{aligned}$$

For further reference, we note some relationships between sublattices of a lattice Λ_1 .

Lemma 1. *Let Λ_2 and Λ'_2 be sublattices of the lattice Λ_1 . Then the following holds.*

- (i) $[\Lambda'_2 : \Lambda_2 \cap \Lambda'_2] = |\{\ell + \Lambda_2 \in \Lambda_1/\Lambda_2 : (\ell + \Lambda_2) \cap \Lambda'_2 \neq \emptyset\}|$
- (ii) $[\Lambda'_2 : \Lambda_2 \cap \Lambda'_2]$ divides $[\Lambda_1 : \Lambda_2]$
- (iii) If $(\ell + \Lambda_2) \cap \Lambda'_2 \neq \emptyset$ then $(\ell + \Lambda_2) \cap \Lambda'_2$ is a coset of $\Lambda_2 \cap \Lambda'_2$.

Proof. The second isomorphism theorem for groups implies

$$\Lambda'_2/(\Lambda_2 \cap \Lambda'_2) \cong (\Lambda_2 + \Lambda'_2)/\Lambda_2 = \{\ell + \Lambda_2 \in \Lambda_1/\Lambda_2 : (\ell + \Lambda_2) \cap \Lambda'_2 \neq \emptyset\},$$

which proves (i). Since $\Lambda_2 + \Lambda'_2$ is a sublattice of Λ_1 , $(\Lambda_2 + \Lambda'_2)/\Lambda_2$ is a subgroup of Λ_1/Λ_2 . Thus, $[\Lambda_2 + \Lambda'_2 : \Lambda_2] = [\Lambda'_2 : \Lambda_2 \cap \Lambda'_2]$ divides $[\Lambda_1 : \Lambda_2]$ by Lagrange's Theorem. The last statement is clear. \square

Using Lemma 1, we can now give restrictions on the values of $s, t, u,$ and v , as well as interpretations of these values in relation to the colorings of $\Lambda_1(R^{-1})$ and $\Lambda_1(R)$ determined by Λ_2 . These results are explicitly stated in the following theorem, which was announced in [25] without proof.

Theorem 2. *Let Λ_2 be a sublattice of Λ_1 of index m , $R \in \text{OC}(\Lambda_1)$, and s, t, u, v be as in Eq. (3.6).*

- (i) *Then $s \mid m, t \mid m, u \mid s, v \mid t$, and*

$$(3.7) \quad \Sigma_2(R) = \frac{t \cdot u \cdot \Sigma_1(R)}{m} = \frac{s \cdot v \cdot \Sigma_1(R)}{m}.$$

- (ii) Consider the coloring of Λ_1 determined by Λ_2 where each coset $c_j + \Lambda_2$ is assigned the color c_j for $0 \leq j \leq m-1$, with $c_0 = 0$. Then
- (a) s and t are the number of colors in the coloring of $\Lambda_1(R^{-1})$ and $\Lambda_1(R)$, respectively.
 - (b) u is the number of colors c_j with the property that some points of $\Lambda_1(R^{-1})$ colored c_j are mapped by R to points colored c_0 in the coloring of $\Lambda_1(R)$.
 - (c) v is the number of colors c_k with the property that some points of $\Lambda_1(R^{-1})$ colored c_0 are mapped by R to points colored c_k in the coloring of $\Lambda_1(R)$.

Proof. Comparing indices in Figure 1 gives Eq. (3.7).

If we apply Lemma 1 to the sublattices Λ_2 and $\Lambda_1(R)$ of Λ_1 , we obtain that $t = |K| = |C_R|$ (see Eq. (3.1) and Eq. (3.3)) and $t \mid m$. Corresponding statements for s are similarly proved by looking at the sublattices $R\Lambda_2$ and $\Lambda_1(R)$ of $R\Lambda_1$.

To prove that $u \mid s$ and $v \mid t$, we characterize u and v by appropriate groups. To this end, we first mention that Lemma 1 implies that for all $c_j + \Lambda_2 \in J$ and $c_k + \Lambda_2 \in K$,

$$(3.8) \quad \begin{aligned} R[(c_j + \Lambda_2) \cap \Lambda_1(R^{-1})] &= Rc_j + [R\Lambda_2 \cap \Lambda_1(R)] \text{ and} \\ (c_k + \Lambda_2) \cap \Lambda_1(R) &= c_k + [\Lambda_2 \cap \Lambda_1(R)]. \end{aligned}$$

Let us consider the groups

$$\begin{aligned} D &:= \{c_j + \Lambda_2 \in J : (Rc_j + [R\Lambda_2 \cap \Lambda_1(R)]) \cap [\Lambda_2 \cap \Lambda_1(R)] \neq \emptyset\} \subseteq J \text{ and} \\ E &:= \{c_k + \Lambda_2 \in K : (c_k + [\Lambda_2 \cap \Lambda_1(R)]) \cap [R\Lambda_2 \cap \Lambda_1(R)] \neq \emptyset\} \subseteq K. \end{aligned}$$

Both groups are nonempty because of Eq. (3.5). Invoking Lemma 1 to the sublattices $\Lambda_2 \cap \Lambda_1(R)$ and $R\Lambda_2 \cap \Lambda_1(R)$ of $\Lambda_1(R)$ shows that $u = |D|$ and $u \mid s$. Similarly, $v = |E|$ and $v \mid t$. The interpretations of u and v via colorings follow from $|D| = |\{c_j : (c_j, c_0) \in \sigma_R\}|$ and $|E| = |\{c_k : (c_0, c_k) \in \sigma_R\}|$ (see Eq. (3.4) and Eq. (3.8)). \square

Note that Eq. (3.5) and Lemma 1 imply that

$$(Rc_j + [R\Lambda_2 \cap \Lambda_1(R)]) \cap [\Lambda_2 \cap \Lambda_1(R)] = Rc_j + \Lambda_2(R),$$

and

$$(c_k + [\Lambda_2 \cap \Lambda_1(R)]) \cap [R\Lambda_2 \cap \Lambda_1(R)] = c_k + \Lambda_2(R),$$

for all $c_j + \Lambda_2 \in D$ whenever $Rc_j \in \Lambda_2 \cap \Lambda_1(R)$, and $c_k + \Lambda_2 \in E$ whenever $c_k \in R\Lambda_2 \cap \Lambda_1(R)$.

An immediate consequence of Theorem 2 is Fact 2, (2.1), and inequality (2.2). Notice that the divisibility condition in (2.1), and hence, the inequality $\Sigma_2(R) \leq m \Sigma_1(R)$, was obtained here without going through the dual lattices of Λ_1 and Λ_2 . This means that the said divisibility condition is true not only for lattices but also for \mathbb{Z} -modules (see [2]), where (2.1) cannot be obtained by a duality argument because the notion of a dual module is in general not defined.

An explicit example involving the square lattice and the Ammann-Beenker tiling can be found in [25].

4. COLOR COINCIDENCE

We have seen from the preceding section that $\Sigma_2(R)$ can be characterized by colorings of $\Lambda_1(R^{-1})$ and $\Lambda_1(R)$. However, the corresponding groups J, K, D , and E are not explicitly known in general. Nonetheless, the problem simplifies in certain situations, which motivates the following definition.

Definition 3. Let Λ_2 be a sublattice of Λ_1 , and write $\Lambda_1 = \bigcup_{j=0}^{m-1} (c_j + \Lambda_2)$ with $c_0 = 0$. A coincidence isometry R of Λ_1 is said to be a *color coincidence* of the coloring of Λ_1 determined by Λ_2 if for any $c_j \in C_{R^{-1}}$ there exists a $c_k \in C_R$ such that

$$(4.1) \quad R[(c_j + \Lambda_2) \cap \Lambda_1(R^{-1})] = (c_k + \Lambda_2) \cap \Lambda_1(R).$$

Eq. (4.1) means that all points colored c_j in the coloring of $\Lambda_1(R^{-1})$ are mapped by R to points colored c_k in the coloring of $\Lambda_1(R)$. Thus, if $R \in \text{OC}(\Lambda_1)$ is a color coincidence, it defines an injection σ_R from $C_{R^{-1}}$ into C_R via Eq. (4.1). Whenever Eq. (4.1) is satisfied, R is said to send or map color c_j to color c_k . Furthermore, we say that R fixes the color c_j if R maps color c_j onto itself.

In fact, the injection σ_R is a bijection, which is seen as follows. By definition, R sends the color $c_0 = 0 \in C_{R^{-1}}$ to exactly one color $c_k \in C_R$, that is,

$$R[\Lambda_2 \cap \Lambda_1(R^{-1})] = R\Lambda_2 \cap \Lambda_1(R) = (c_k + \Lambda_2) \cap \Lambda_1(R).$$

Since $0 \in \Lambda_2 \cap \Lambda_1(R^{-1})$ and $R(0) = 0$, we obtain $c_k = c_0$. In other words, R fixes the color c_0 . Thus, we have $R[\Lambda_2 \cap \Lambda_1(R^{-1})] = \Lambda_2 \cap \Lambda_1(R)$, which implies that $\Lambda_2 \cap \Lambda_1(R^{-1})$ and $\Lambda_2 \cap \Lambda_1(R)$ have the same index in $\Lambda_1(R)$. It now follows from Theorem 2 that the colorings of $\Lambda_1(R^{-1})$ and $\Lambda_1(R)$ have the same number of colors, that is, $|C_{R^{-1}}| = |C_R|$. Hence σ_R is indeed a bijection. Observe that this bijection is exactly the relation σ_R defined in Eq. (3.4). This means that an $R \in \text{OC}(\Lambda_1)$ is a color coincidence if and only if the relation σ_R from $C_{R^{-1}}$ to C_R in Eq. (3.4) is a bijection. In particular, if R is a color coincidence and $C_{R^{-1}} = C_R$, then σ_R is a permutation on $C_{R^{-1}}$. Thus, a color coincidence $R \in P(\Lambda_1)$ (that is, when $\Lambda_1(R^{-1}) = \Lambda_1(R) = \Lambda_1$) is a color symmetry of the coloring of Λ_1 .

We have seen that R fixes the color c_0 if $R \in \text{OC}(\Lambda_1)$ is a color coincidence. Actually, the converse holds as well, as was mentioned in [25] without proof, and which will be proved below. This generalizes the fact that a symmetry operation R of an uncolored lattice Λ is a color symmetry of a sublattice coloring of Λ if and only if R leaves the sublattice invariant (*cf.* [11, Theorem 2(i)]).

Theorem 4. *Let Λ_2 be a sublattice of Λ_1 of index m , with $\Lambda_1 = \bigcup_{j=0}^{m-1} (c_j + \Lambda_2)$ where $c_0 = 0$. Then $R \in \text{OC}(\Lambda_1)$ is a color coincidence of the coloring of Λ_1 determined by Λ_2 if and only if R fixes color c_0 .*

Proof. It remains to show the “if” part. Suppose R fixes color c_0 , thus, $R[\Lambda_2 \cap \Lambda_1(R^{-1})] = \Lambda_2 \cap \Lambda_1(R)$. This implies that $R\Lambda_2 \cap \Lambda_1(R) = \Lambda_2 \cap \Lambda_1(R) = \Lambda_2(R)$ by Eq. (3.5). Hence, $u = v = 1$ and $s = t$ by Eq. (3.6). From Theorem 2, the colorings of $\Lambda_1(R)$ and $\Lambda_1(R^{-1})$ determined by Λ_2 must have equal number of colors. Under the assumption that $c_j \in \Lambda_1(R^{-1})$ for each $c_j + \Lambda_2 \in J$, it then follows from Eq. (3.8) that

$$\begin{aligned} R[(c_j + \Lambda_2) \cap \Lambda_1(R^{-1})] &= Rc_j + [R\Lambda_2 \cap \Lambda_1(R)] \\ &= Rc_j + [\Lambda_2 \cap \Lambda_1(R)] \\ &= (Rc_j + \Lambda_2) \cap \Lambda_1(R). \end{aligned}$$

This means that $Rc_j + \Lambda_2$ must be one of the cosets $c_k + \Lambda_2 \in K$. Therefore, R is a color coincidence of the coloring of Λ_1 . \square

By Theorem 4, it is then sufficient to check whether $R[\Lambda_2 \cap \Lambda_1(R^{-1})] = \Lambda_2 \cap \Lambda_1(R)$ is satisfied to identify if $R \in \text{OC}(\Lambda_1)$ is a color coincidence.

Let R be a color coincidence. Equations (3.8), (3.2), (3.5), and Theorem 4, yield the following coset decompositions of $\Lambda_1(R)$ with respect to $\Lambda_2(R)$:

$$\Lambda_1(R) = \bigcup_{c_k + \Lambda_2 \in K} [c_k + \Lambda_2(R)] = \bigcup_{c_j + \Lambda_2 \in J} [Rc_j + \Lambda_2(R)]$$

In the language of colorings, this means that a color coincidence R determines a permutation on the set of cosets of $\Lambda_2(R)$ in $\Lambda_1(R)$. Here, $Rc_j + \Lambda_2(R) = c_k + \Lambda_2(R)$ if and only if R sends color c_j to c_k .

Theorem 2 is simpler for color coincidences since $u = v = 1$. In particular, we have the following result.

Corollary 5. *If R is a color coincidence of the coloring of the lattice Λ_1 determined by the sublattice Λ_2 , then $\Sigma_2(R) \mid \Sigma_1(R)$.*

If the colorings of $\Lambda_1(R)$ and $\Lambda_1(R^{-1})$ contain all m colors, that is, if $s = t = m$, then we get the following criterion for color coincidences.

Corollary 6. *Let Λ_1 be a lattice having Λ_2 as a sublattice of index m . If $s = t = m$ in Eq. (3.6), then $R \in \text{OC}(\Lambda_1)$ is a color coincidence of the coloring of Λ_1 induced by Λ_2 if and only if $\Sigma_2(R) = \Sigma_1(R)$.*

Denote by H_{Λ_1, Λ_2} the set of all color coincidences of the coloring of a lattice Λ_1 determined by a sublattice Λ_2 . Clearly, the identity isometry is in H_{Λ_1, Λ_2} . In addition, it follows from the definition of a color coincidence that if $R \in H_{\Lambda_1, \Lambda_2}$, then so is R^{-1} . The question of whether the product of two color coincidences is again a color coincidence, and in effect, whether H_{Λ_1, Λ_2} forms a group, is yet to be resolved. A step in answering this question is the following proposition.

Proposition 7. *Let Λ_2 be a sublattice of Λ_1 of index m , and $R_1, R_2 \in H_{\Lambda_1, \Lambda_2}$. If $\Sigma_1(R_1)$ is relatively prime to $\Sigma_1(R_2)$, then $R_2R_1 \in H_{\Lambda_1, \Lambda_2}$.*

Proof. Since $\Sigma_1(R_1)$ and $\Sigma_1(R_2)$ are relatively prime, $\Lambda_1(R_2R_1) = \Lambda_1 \cap R_2\Lambda_1 \cap R_2R_1\Lambda_1$ by [42, Corollary 3]. Applying Theorem 4 and Eq. (3.5) to R_1 , one obtains

$$R_1\Lambda_2 \cap \Lambda_1 = R_1\Lambda_2 \cap \Lambda_1(R_1) = \Lambda_2 \cap \Lambda_1(R_1) = \Lambda_2 \cap R_1\Lambda_1.$$

Similarly, $R_2\Lambda_2 \cap \Lambda_1 = \Lambda_2 \cap R_2\Lambda_1$. These three equalities yield

$$R_2R_1\Lambda_2 \cap \Lambda_1(R_2R_1) = \Lambda_2 \cap \Lambda_1(R_2R_1).$$

Thus, R_2R_1 fixes color c_0 , which means that $R_2R_1 \in H_{\Lambda_1, \Lambda_2}$ by Theorem 4. \square

5. SPECIAL CASES

We now apply the theory developed in the previous two sections to some special cases. First, assume that $\Lambda_1(R) \subseteq \Lambda_2$. Then all points of $\Lambda_1(R)$ have the same color, or in other words, $t = 1$. Hence, $\Sigma_2(R) \mid \Sigma_1(R)$. More generally, we have the following result.

Lemma 8. *Let Λ_2 be a sublattice of Λ_1 with $[\Lambda_1 : \Lambda_2] = m$, and $R \in \text{OC}(\Lambda_1)$. If $\Lambda_1(R)$ or $\Lambda_1(R^{-1})$ is a sublattice of Λ_2 , then $\Sigma_2(R) \mid \Sigma_1(R)$. In particular, both $\Lambda_1(R)$ and $\Lambda_1(R^{-1})$ are sublattices of Λ_2 if and only if $\Sigma_2(R) = (1/m)\Sigma_1(R)$.*

Proof. Both $\Lambda_1(R)$ and $\Lambda_1(R^{-1})$ are sublattices of Λ_2 if and only if $s = t = u = v = 1$. Applying Eq. (3.7) completes the proof. \square

The possibilities are quite limited when the sublattice Λ_2 is of prime index in Λ_1 , as can be seen in the next proposition.

Proposition 9. *Suppose Λ_2 is a sublattice of Λ_1 of prime index p and $R \in \text{OC}(\Lambda_1)$.*

- (i) *If both $\Lambda_1(R)$ and $\Lambda_1(R^{-1})$ are sublattices of Λ_2 then $\Sigma_2(R) = (1/p)\Sigma_1(R)$.*
- (ii) *If exactly one of $\Lambda_1(R)$ and $\Lambda_1(R^{-1})$ is a sublattice of Λ_2 then $\Sigma_2(R) = \Sigma_1(R)$.*
- (iii) *If neither $\Lambda_1(R)$ nor $\Lambda_1(R^{-1})$ is a sublattice of Λ_2 , then $\Sigma_2(R) = \Sigma_1(R)$ whenever R is a color coincidence of the coloring of Λ_1 induced by Λ_2 , and $\Sigma_2(R) = p\Sigma_1(R)$ otherwise.*

Proof. Statements (i) and (ii) are immediate from Lemma 8. If neither $\Lambda_1(R)$ nor $\Lambda_1(R^{-1})$ is contained in Λ_2 , then $s, t > 1$ (see Eq. (3.6)). We have $s = t = p$ by Theorem 2. Recall that R is a color coincidence of the coloring of Λ_1 if and only if $u = v = 1$ by Theorem 4 and Eq. (3.5). Thus, $\Sigma_2(R) = \Sigma_1(R)$ whenever R is a color coincidence of the coloring of Λ_1 by Eq. (3.7). Otherwise, $u = v = p$ by Theorem 2, and it follows from Eq. (3.7) that $\Sigma_2(R) = p\Sigma_1(R)$. \square

We can say more if $\Sigma_1(R)$ and m are relatively prime.

Proposition 10. *Let Λ_2 be a sublattice of Λ_1 with $[\Lambda_1 : \Lambda_2] = m$, and $R \in \text{OC}(\Lambda_1)$. If $\Sigma_1(R)$ and m are relatively prime, then all colors in the coloring of Λ_1 determined by Λ_2 appear in both colorings of $\Lambda_1(R)$ and $\Lambda_1(R^{-1})$, and $\Sigma_2(R) \mid \Sigma_1(R)$.*

Proof. From (3.7), $(t/m)\Sigma_1(R) = (1/u)\Sigma_2(R) \in \mathbb{N}$ because $u \mid \Sigma_2(R)$ (see Figure 1). Since $\Sigma_1(R)$ is relatively prime to m , then $m \mid t$. However, $t \mid m$ as well by Theorem 2 and so $t = m$. Similar arguments yield $s = m$. Finally, $\Sigma_2(R) \mid \Sigma_1(R)$ follows from Eq. (3.7). \square

6. EXAMPLES

We now give examples involving the cubic and hypercubic lattices. For this, we parametrize linear isometries in three and four dimensions by quaternions. Before we proceed, we recall several properties of the quaternion algebra $\mathbb{H}(\mathbb{R})$.

Let $\{\mathbf{e}, \mathbf{i}, \mathbf{j}, \mathbf{k}\}$ be the standard basis of \mathbb{R}^4 where $\mathbf{e} = (1, 0, 0, 0)^T$, $\mathbf{i} = (0, 1, 0, 0)^T$, $\mathbf{j} = (0, 0, 1, 0)^T$, and $\mathbf{k} = (0, 0, 0, 1)^T$. The *quaternion algebra* is the algebra $\mathbb{H} := \mathbb{H}(\mathbb{R}) = \mathbb{R}\mathbf{e} + \mathbb{R}\mathbf{i} + \mathbb{R}\mathbf{j} + \mathbb{R}\mathbf{k} \cong \mathbb{R}^4$, whose elements are called *quaternions* and are written as either $q = q_0\mathbf{e} + q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k}$ or $q = (q_0, q_1, q_2, q_3)$. The product of two quaternions $q = (q_0, q_1, q_2, q_3)$ and $p = (p_0, p_1, p_2, p_3)$ is given by

$$\begin{aligned} qp = & (q_0p_0 - q_1p_1 - q_2p_2 - q_3p_3)\mathbf{e} + \\ & (q_0p_1 + q_1p_0 + q_2p_3 - q_3p_2)\mathbf{i} + (q_0p_2 - q_1p_3 + q_2p_0 + q_3p_1)\mathbf{j} \\ & + (q_0p_3 + q_1p_2 - q_2p_1 + q_3p_0)\mathbf{k}. \end{aligned}$$

The *conjugate* of a quaternion $q = (q_0, q_1, q_2, q_3)$ is $\bar{q} = (q_0, -q_1, -q_2, -q_3)$, and its *norm* is

$$|q|^2 = q\bar{q} = q_0^2 + q_1^2 + q_2^2 + q_3^2 \in \mathbb{R}.$$

The *real part* and *imaginary part* of q are defined as $\text{Re}(q) = q_0$ and $\text{Im}(q) = q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k}$, respectively. In addition, we define $\text{Im}(\mathbb{H}) := \{\text{Im}(q) : q \in \mathbb{H}\}$. Every nonzero quaternion q has a multiplicative inverse given by $q^{-1} = \bar{q}/|q|^2$, which makes \mathbb{H} an associative division algebra.

A quaternion whose components are all integers is called a *Lipschitz quaternion* or *Lipschitz integer*. The set of Lipschitz quaternions shall be denoted by

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

A *primitive quaternion* $q = (q_0, q_1, q_2, q_3)$ is a quaternion in \mathbb{L} whose components are relatively prime, that is, $\text{gcd}(q_0, q_1, q_2, q_3) = 1$. On the other hand, a *Hurwitz quaternion* or *Hurwitz integer* is a quaternion whose components are all integers or all half-integers. The set \mathbb{J} of Hurwitz quaternions can be written as

$$\mathbb{J} = \mathbb{L} \cup [(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}) + \mathbb{L}].$$

For an extensive treatment on quaternions, we refer to [22, 9, 21, 18].

It suffices to look at the primitive cubic lattice when studying the coincidences of the three-dimensional cubic lattices because of the following well-known result [16, 2].

Fact 3. *Let $\Lambda_P = \mathbb{Z}^3$, $\Lambda_B = \Lambda_P \cup [(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) + \Lambda_P]$, and $\Lambda_F = \Lambda_B^*$ denote the primitive cubic, body-centered cubic, and face-centered cubic lattice, respectively. Then $\text{OC}(\Lambda_P) = \text{OC}(\Lambda_F) = \text{OC}(\Lambda_B) = \text{O}(3, \mathbb{Q})$. Moreover, if $R \in \text{O}(3, \mathbb{Q})$, then $\Sigma_{\Lambda_P}(R) = \Sigma_{\Lambda_F}(R) = \Sigma_{\Lambda_B}(R)$.*

We now embed the cubic lattices in the Hurwitz ring \mathbb{J} of integer quaternions and we employ *Cayley's parametrization* of $\text{SO}(3)$ (cf. [22]). That is, for every $R \in \text{SOC}(\Lambda) = \text{SO}(3, \mathbb{Q})$, there exists a primitive quaternion q (which is unique up to a sign) so that for all $x \in \text{Im}(\mathbb{H})$, $R(x) = qxq^{-1} = qx\bar{q}/|q|^2$. In such a case, we denote R by R_q . In fact, the coincidence index of $R_q \in \text{SOC}(\Lambda)$ is given by $\Sigma(R_q) = |q|^2/2^\ell$, where ℓ is the largest power of 2 that divides $|q|^2$ (called the odd part of $|q|^2$) [16, 15, 2]. Also, $T \in \text{OC}(\Lambda) \setminus \text{SO}(\Lambda)$ can be written as $T_q = -R_q$, where $R_q \in \text{SOC}(\Lambda)$.

Example 1. Let Λ_1 be the body-centered cubic lattice $\Lambda_1 = \text{Im}(\mathbb{J})$ and Λ_2 its maximal primitive cubic sublattice $\Lambda_2 = \text{Im}(\mathbb{L})$. Here, $[\Lambda_1 : \Lambda_2] = 2$ and so the coloring of Λ_1 determined by Λ_2 consists of two colors. For each $R \in \text{OC}(\Lambda_1) = \text{OC}(\Lambda_2)$, one has $\Sigma_2(R) = \Sigma_1(R)$ (see Fact 3).

Since all the coincidence indices of Λ_1 are odd numbers, both colorings of $\Lambda_1(R)$ and $\Lambda_1(R^{-1})$ induced by Λ_2 include two colors by Proposition 10. It follows then from Corollary 6 that H_{Λ_1, Λ_2} is the entire group $\text{OC}(\Lambda_1)$ with all coincidence isometries fixing both colors. \square

Example 2. This time, take the primitive cubic lattice $\Lambda_1 = \text{Im}(\mathbb{L})$ to be the parent lattice and the body-centered cubic lattice $\Lambda_2 = 2\text{Im}(\mathbb{J})$ to be the sublattice of index 4 in Λ_1 . Write $\Lambda_1 = \cup_{j=0}^3 (c_j + \Lambda_2)$ where $c_0 = 0$.

Arguments analogous to Example 1 yield that all four colors in the coloring of Λ_1 determined by Λ_2 show up in the coloring of $\Lambda_1(R)$ and $\Lambda_1(R^{-1})$, and $H_{\Lambda_1, \Lambda_2} = \text{OC}(\Lambda_1)$. Indeed, the result that $H_{\Lambda_1, \Lambda_2} = \text{OC}(\Lambda_1)$ in Examples 1 and 2 also follows from a shelling argument [16]. That is, since all the points of Λ_1 that lie on the same shell about the origin are either from Λ_2 or from $\Lambda_1 \setminus \Lambda_2$, then every coincidence isometry of Λ_1 must be a color coincidence by Theorem 4.

We also identify the color permutation induced by each coincidence isometry of Λ_1 . If a coincidence isometry $R \in \text{OC}(\Lambda_1)$ is parametrized by the primitive quaternion q , then

- (i) R fixes all the colors if and only if $|q|^2 \equiv 1 \pmod{4}$,
- (ii) R fixes two of the colors (one of the fixed colors is c_0) if and only if $|q|^2 \equiv 2 \pmod{4}$, and
- (iii) R fixes only color c_0 if and only if $|q|^2 \equiv 0 \pmod{4}$.

This result is justified in the Appendix. Furthermore, the set of color permutations generated by the color coincidences of the coloring of Λ_1 forms a group that is isomorphic to S_3 . \square

We now look at an example involving lattices in \mathbb{R}^4 . There are only two distinct types of hypercubic lattices in four dimensions, namely the primitive hypercubic lattice \mathbb{Z}^4 and the centered hypercubic lattice D_4 (cf. [8, 6]). We identify D_4 and \mathbb{Z}^4 with the set of Hurwitz quaternions \mathbb{J} and the set of Lipschitz quaternions \mathbb{L} , respectively. Even though $\text{OC}(\mathbb{Z}^4) = \text{OC}(D_4) = \text{O}(4, \mathbb{Q})$, the coincidence indices of a coincidence isometry with respect to the two lattices are not necessarily equal [2, 41, 4].

Elements of $\text{O}(4)$ can be parametrized by pairs of quaternions. For any $R \in \text{SO}(4)$, there exists a pair of quaternions (q, p) such that $R(x) = qx\bar{p}/|qp|$. In this case we write $R = R_{q,p}$. Whenever $R_{q,p} \in \text{SO}(4, \mathbb{Q})$, then q and p can be chosen to be primitive quaternions in \mathbb{L} . However, not every pair (q, p) of primitive quaternions defines an $R \in \text{SO}(4, \mathbb{Q})$. In fact, a primitive pair (q, p) defines an $R \in \text{SO}(4, \mathbb{Q})$ if and only if (q, p) is *admissible*, that is, if $|qp| \in \mathbb{N}$.

The coincidence index of $R_{q,p} \in \text{SOC}(D_4)$ is given by $\Sigma_{D_4}(R_{q,p}) = \text{lcm}(|q|^2/2^k, |p|^2/2^\ell)$, where k and ℓ are the highest powers such that 2^k and 2^ℓ divide $|q|^2$ and $|p|^2$, respectively. On the other hand,

$$(6.1) \quad \Sigma_{\mathbb{Z}^4}(R_{q,p}) = \text{lcm}(\Sigma_{D_4}(R_{q,p}), \text{den}(R_{q,p})),$$

where $\text{den}(R_{q,p})$ is the denominator of $R_{q,p}$, that is, the least common denominator of all entries of $R_{q,p}$ in its canonical matrix representation [2].

Every rotoreflection T in $\text{O}(4, \mathbb{Q})$ can also be parametrized by an admissible pair of quaternions, namely via $T(x) = T_{q,p}(x) = q\bar{x}p/|qp|$. In particular, $T_{1,1}(x) = \bar{x}$ and $T_{q,p} = R_{q,p} \cdot T_{1,1}$. Moreover, we have $\Sigma_{D_4}(T_{q,p}) = \Sigma_{D_4}(R_{q,p})$ and $\Sigma_{\mathbb{Z}^4}(T_{q,p}) = \Sigma_{\mathbb{Z}^4}(R_{q,p})$.

The following example examines the set of color coincidences of the coloring of D_4 determined by \mathbb{Z}^4 which forms a proper subgroup of $\text{OC}(D_4)$.

Example 3. Take Λ_1 to be the centered hypercubic lattice $\Lambda_1 = \mathbb{J}$ and Λ_2 to be the primitive hypercubic lattice $\Lambda_2 = \mathbb{L}$ of index 2 in Λ_1 . Let $R = R_{q,p} \in \text{SOC}(\Lambda_1)$ be parametrized by the admissible pair (q, p) of primitive quaternions.

Since $[\Lambda_1 : \Lambda_2] = 2$ and $\Sigma_1(R)$ is always odd, $s = t = 2$ by Proposition 10. It follows from Theorem 2 that $\Sigma_2(R) = u \Sigma_1(R)$ with $u = 1$ or $u = 2$. In particular, $\Sigma_2(R) = \Sigma_1(R)$ if and only if $R \in H_{\Lambda_1, \Lambda_2}$ by Corollary 6. Hence, $H_{\Lambda_1, \Lambda_2} = \{R \in \text{OC}(\Lambda_1) : \Sigma_2(R) = \Sigma_1(R)\}$.

The set H_{Λ_1, Λ_2} in this instance still forms a group. To see this, write

$$H_{\Lambda_1, \Lambda_2} = \{R \in \text{OC}(\Lambda_1) : \Sigma_2(R) \text{ is odd}\}.$$

Now, if $R_1, R_2 \in H_{\Lambda_1, \Lambda_2}$ then $\Sigma_2(R_2 R_1) \mid \Sigma_2(R_2) \cdot \Sigma_2(R_1)$ by [42, Lemma 1]. This implies that $\Sigma_2(R_2 R_1)$ must also be odd, and hence $R_2 R_1 \in H_{\Lambda_1, \Lambda_2}$. This proves that the product of two color coincidences of the coloring of Λ_1 is again in H_{Λ_1, Λ_2} , and hence, H_{Λ_1, Λ_2} is a subgroup of $\text{OC}(\Lambda_1)$.

We identify the conditions that the quaternion pair (q, p) should satisfy so that $R \in H_{\Lambda_1, \Lambda_2}$ in the Appendix. This yields the following result about the coincidence index of a coincidence isometry of \mathbb{Z}^4 (compare with Eq. (6.1)).

Proposition 11. *Let $R_{q,p} \in \text{SOC}(\mathbb{Z}^4)$ where (q, p) is an admissible pair of primitive quaternions. Then either*

$$\begin{aligned} \Sigma_{\mathbb{Z}^4}(R_{q,p}) &= \Sigma_{D_4}(R_{q,p}) = \text{lcm}\left(\frac{|q|^2}{2^k}, \frac{|p|^2}{2^\ell}\right) \quad \text{or} \\ \Sigma_{\mathbb{Z}^4}(R_{q,p}) &= 2\Sigma_{D_4}(R_{q,p}), \end{aligned}$$

where k and ℓ are the highest powers such that 2^k and 2^ℓ divide $|q|^2$ and $|p|^2$, respectively. In particular, $\Sigma_{\mathbb{Z}^4}(R_{q,p}) = \Sigma_{D_4}(R_{q,p})$ holds if and only if one of the following conditions are satisfied:

- (i) $|q|^2$ and $|p|^2$ are odd,
- (ii) $|q|^2 \equiv |p|^2 \equiv 2 \pmod{4}$ with $\langle q, p \rangle$ even,
- (iii) $|q|^2 \equiv |p|^2 \equiv 0 \pmod{4}$ with $4 \mid \langle q, p \rangle$.

The same holds for $T_{q,p} \in \text{OC}(\mathbb{Z}^4) \setminus \text{SOC}(\mathbb{Z}^4)$.

Note that Proposition 11 is consistent and similar to the conditions set forth in [41] on how to identify which of the 576 pure symmetry rotations of D_4 are also pure symmetry rotations of \mathbb{Z}^4 .

7. CONCLUSION AND OUTLOOK

Let Λ_1 be a lattice and $R \in \text{OC}(\Lambda_1)$. A method to compute for the coincidence index of R with respect to a sublattice Λ_2 of Λ_1 was formulated in Theorem 2 via properties of the coloring of Λ_1 determined by Λ_2 . This led to the extension of color symmetries to color coincidences of sublattice colorings of Λ_1 . Theorem 4 shows that the color coincidences of a coloring of Λ_1 induced by Λ_2 are precisely those coincidence isometries of Λ_1 that leave Λ_2 invariant.

The authors suspect that the set of color coincidences of a sublattice coloring of Λ_1 does not form a group. A counterexample will not only confirm this suspicion, but should also shed more light on the coincidence index of a product of two coincidence isometries. The generalization of a color symmetry to color coincidences is not only interesting in its own right, but it also provides a further connection between the relationship of the coincidence indices of a lattice and sublattice. It would also be helpful if a comparable connection between similar isometries (*cf.* [13]) and colorings of lattices can be set up. This would give a unified perspective among similar sublattices (SSLs), CSLs, and colorings of lattices.

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APPENDIX

Here, we give the promised justifications and proofs in Examples 2 and 3.

Example 2. Recall that $\Lambda_1 = \cup_{j=0}^3 (c_j + \Lambda_2)$, where $\Lambda_1 = \text{Im}(\mathbb{L})$, $\Lambda_2 = 2\text{Im}(\mathbb{J})$, and $c_0 = 0$. Let $R = R_q \in \text{SOC}(\Lambda_1)$, where $q = (q_0, q_1, q_2, q_3)$ is a primitive quaternion. For sure, R is a color coincidence that fixes color c_0 because of Theorem 4. We shall now determine how R acts on the other colors c_1, c_2, c_3 , and thus, the color permutation that R generates.

Since R is a color coincidence, it is enough to consider a representative from each coset of Λ_2 in Λ_1 that is in $\Lambda_1(R^{-1})$, and afterwards identify to which coset of Λ_2 the representative is sent by R . Take $c_1 = \Sigma_1(R)\mathbf{i}$, $c_2 = \Sigma_1(R)\mathbf{j}$, and $c_3 = \Sigma_1(R)\mathbf{k}$. Indeed, for $j \in \{1, 2, 3\}$, $c_j \notin \Lambda_2$ since $\Sigma_1(R)$ is odd, and $c_j \in \Lambda_1(R^{-1})$ because $\Sigma_1(R) = \text{den}(R) = \text{gcd}\{k \in \mathbb{N} : kR \text{ is an integral matrix}\}$ (see [2]). One obtains

$$\begin{aligned} R(c_1) &= \frac{\Sigma_1(R)}{|q|^2} q\mathbf{i}\bar{q}, \\ R(c_2) &= \frac{\Sigma_1(R)}{|q|^2} q\mathbf{j}\bar{q}, \\ R(c_3) &= \frac{\Sigma_1(R)}{|q|^2} q\mathbf{k}\bar{q}, \end{aligned}$$

where $\Sigma_1(R)/|q|^2 = 1/2^\ell$ with $\ell \in \{0, 1, 2\}$. This gives rise to three different cases.

Before we proceed, we take note of the following facts that will be used in the computations thereafter.

Fact 4. For every $q \in \mathbb{H}$ and $x \in \text{Im}(\mathbb{H})$, we have $qx\bar{q} \in \text{Im}(\mathbb{H})$.

If $q \in \mathbb{J}$ and j is the highest power of 2 such that 2^j divides $|q|^2$, then $q = (1 + \mathbf{i})^j p$ for some $p \in \mathbb{J}$ of odd norm [21, page 37]. The next statement follows from this result.

Fact 5. The set $(1 + \mathbf{i})^r \mathbb{J} = \{q \in \mathbb{J} : 2^r \mid |q|^2\}$ is a two-sided ideal of \mathbb{J} for all $r \in \mathbb{N}$.

Fact 6. Let $\Lambda_2 = 2\text{Im}(\mathbb{J}) = 2\text{Im}(\mathbb{L}) \cup [(0, 1, 1, 1) + 2\text{Im}(\mathbb{L})]$. Then the following hold:

- (i) $2\mathbb{J} \cap \text{Im}(\mathbb{H}) = 2\text{Im}(\mathbb{L}) \subseteq \Lambda_2$
- (ii) If $q \in \mathbb{J}$ then $q - \bar{q} \in \Lambda_2$.

Proof. Statement (i) is clear. If $q \in \mathbb{L}$ then $q - \bar{q} \in \Lambda_2$ by (i). On the other hand, if $q \in \mathbb{J} \setminus \mathbb{L}$ then $q - \bar{q} \in (0, 1, 1, 1) + 2\text{Im}(\mathbb{L}) \subseteq \Lambda_2$. This proves (ii). \square

The three possible ratios of $\Sigma_1(R)/|q|^2$ are investigated below.

CASE I: $\Sigma_1(R)/|q|^2 = 1$, that is, $|q|^2 \equiv 1 \pmod{4}$ and either one or three among the components of q is/are odd.

For instance, suppose q_0 is odd while q_1, q_2, q_3 are even, or q_0 is even while q_1, q_2, q_3 are odd. In both instances, one can write $q = r + s$, where $r \in 2\mathbb{J}$ and $s = \mathbf{e}$. One obtains

$$R(c_j) = qx_j\bar{q} = rx_j\bar{r} + rx_j\bar{s} + sx_j\bar{r} + sx_j\bar{s}$$

where $x_j = \mathbf{i}, \mathbf{j}, \mathbf{k}$ if $j = 1, 2, 3$, respectively. Facts 4, 5, and 6(i) imply that $rx_j\bar{r} \in \Lambda_2$, and $rx_j\bar{s} + sx_j\bar{r} = rx_j\bar{s} - \overline{rx_j\bar{s}} \in \Lambda_2$ by Fact 6(ii). Hence, $R(c_j) \in sx_j\bar{s} + \Lambda_2 = x_j + \Lambda_2 = c_j + \Lambda_2$ for $j \in \{1, 2, 3\}$. Similarly, for the other three possibilities, $R(c_j) \in c_j + \Lambda_2$ for $j \in \{1, 2, 3\}$. Therefore, in all instances, R fixes all colors.

CASE II: $\Sigma_1(R)/|q|^2 = \frac{1}{2}$, that is, $|q|^2 \equiv 2 \pmod{4}$ and exactly two components of q are odd.

Consider the instance when both q_0 and q_1 are odd, or when both q_2 and q_3 are odd. Either way, one can express q as $q = r + s$ where $r \in 2\mathbb{J}$ and $s = (1, 1, 0, 0)$. One has in this case

$$R(c_j) = \frac{1}{2}(rx_j\bar{r} + rx_j\bar{s} + sx_j\bar{r} + sx_j\bar{s})$$

where $x_j = \mathbf{i}, \mathbf{j}, \mathbf{k}$ if $j = 1, 2, 3$, respectively. Now, $\frac{1}{2}rx_j\bar{r} \in 2\mathbb{J}$ because 4 divides $|\frac{1}{2}rx_j\bar{r}|^2$. This, with Facts 4 and 6(i), implies that $\frac{1}{2}rx_j\bar{r} \in \Lambda_2$. Since $\frac{1}{2}rx_j\bar{s} \in \mathbb{J}$, one obtains that $\frac{1}{2}rx_j\bar{s} + \frac{1}{2}sx_j\bar{r} \in \Lambda_2$

by Fact 6(ii). Therefore,

$$R(c_j) \in \frac{1}{2}sx_j\bar{s} + \Lambda_2 = \begin{cases} c_1 + \Lambda_2, & \text{if } j = 1 \\ c_3 + \Lambda_2, & \text{if } j = 2 \\ c_2 + \Lambda_2, & \text{if } j = 3. \end{cases}$$

Thus, R induces the permutation (c_2c_3) of colors. Similar computations for the other two possibilities yield that if q_0 and q_j are of the same parity, where $j \in \{1, 2, 3\}$, then R fixes both colors c_0 and c_j and swaps the other two colors.

CASE III: $\Sigma_1(R)/|q|^2 = \frac{1}{4}$, that is, $|q|^2 \equiv 0 \pmod{4}$ and all components of q are odd.

Suppose an even number of components of q are congruent to 1 modulo 4. Then, one can write $q = r + s$, where $r \in (1, 1, 0, 0)2\mathbb{J}$ and $s = (1, 1, 1, 1)$. Thus,

$$R(c_j) = \frac{1}{4}(rx_j\bar{r} + rx_j\bar{s} + sx_j\bar{r} + sx_j\bar{s})$$

where $x_j = \mathbf{i}, \mathbf{j}, \mathbf{k}$ if $j = 1, 2, 3$, respectively. Since 4 divides $|\frac{1}{4}rx_j\bar{r}|^2$, one has $\frac{1}{4}rx_j\bar{r} \in 2\mathbb{J}$ and together with Facts 4 and 6(i), $\frac{1}{4}rx_j\bar{r} \in \Lambda_2$. Also, by Fact 6(ii) one concludes that $\frac{1}{4}rx_j\bar{s} + \frac{1}{4}sx_j\bar{r} \in \Lambda_2$ because $\frac{1}{4}rx_j\bar{s} \in \mathbb{J}$. Finally,

$$R(c_j) \in \frac{1}{4}sx_j\bar{s} + \Lambda_2 = \begin{cases} c_2 + \Lambda_2, & \text{if } j = 1 \\ c_3 + \Lambda_2, & \text{if } j = 2 \\ c_1 + \Lambda_2, & \text{if } j = 3. \end{cases}$$

Hence, R generates the permutation $(c_1c_2c_3)$ of colors. On the other hand, if an odd number of components of q are congruent to 1 modulo 4, then similar arguments show that R induces the permutation $(c_1c_3c_2)$ of colors.

Given a coincidence reflection $T_q \in \text{OC}(\Lambda_1)$, the color permutation that it effects is the same as that of the coincidence rotation R_q .

Example 3. Recall that $\Lambda_1 = \mathbb{J}$, $\Lambda_2 = \mathbb{L}$, and $R = R_{q,p} \in \text{SOC}(\Lambda_1)$ is parametrized by the admissible pair (q, p) of primitive quaternions. The following looks at the conditions that the quaternion pair (q, p) should satisfy so that $R \in H_{\Lambda_1, \Lambda_2}$.

Going through the different possible admissible quaternion pairs (q, p) results in the following cases. In each case, the sets $R\Lambda_2 \cap \Lambda_1(R)$ and $\Lambda_2 \cap \Lambda_1(R)$ are compared in order to ascertain whether $R \in H_{\Lambda_1, \Lambda_2}$ or not (see Theorem 4).

CASE I: $|q|^2$ and $|p|^2$ are odd

Suppose $v \in \Lambda_2 \cap \Lambda_1(R)$ and write $v = qw\bar{p}/|q\bar{p}|$ for some $w \in \mathbb{J}$. This means that $|q\bar{p}|v = qw\bar{p} \in \mathbb{L}$. Since $|q|^2$ and $|p|^2$ are odd, one can express $q = r_1 + s_1$ and $p = r_2 + s_2$, where $r_1, r_2 \in 2\mathbb{J}$, and $s_1, s_2 \in \{\mathbf{e}, \mathbf{i}, \mathbf{j}, \mathbf{k}\}$. With this, one obtains

$$qw\bar{p} = r_1w\bar{r}_2 + r_1w\bar{s}_2 + s_1w\bar{r}_2 + s_1w\bar{s}_2 \in \mathbb{L}.$$

By Fact 5, $r_1w\bar{r}_2 + r_1w\bar{s}_2 + s_1w\bar{r}_2 \in 2\mathbb{J} \subseteq \mathbb{L}$, which implies that $s_1w\bar{s}_2 \in \mathbb{L}$. Thus, $v = Rw \in R\Lambda_2$ and $\Lambda_2 \cap \Lambda_1(R) \subseteq R\Lambda_2 \cap \Lambda_1(R)$. It follows then that $R\Lambda_2 \cap \Lambda_1(R) = \Lambda_2 \cap \Lambda_1(R)$, and so $R \in H_{\Lambda_1, \Lambda_2}$.

CASE II: $|q|^2$ is odd and $|p|^2 \equiv 0 \pmod{4}$, or $|q|^2 \equiv 0 \pmod{4}$ and $|p|^2$ is odd

Consider $x = \frac{1}{2}|q\bar{p}| \in \mathbb{L}$. One has $R(x) = qx\bar{p}/|q\bar{p}| = \frac{1}{2}q\bar{p} \in \mathbb{J}$. Thus, $R(x) \in R\Lambda_2 \cap \Lambda_1(R)$. However, the first component of $q\bar{p}$, which is equal to the inner product $\langle q, p \rangle$ of q and p (or the standard scalar product of q and p as vectors in \mathbb{R}^4), is odd. This implies that $\frac{1}{2}q\bar{p} \notin \mathbb{L}$ and $R(x) \notin \Lambda_2 \cap \Lambda_1(R)$. Hence, $R\Lambda_2 \cap \Lambda_1(R) \neq \Lambda_2 \cap \Lambda_1(R)$ and $R \notin H_{\Lambda_1, \Lambda_2}$.

CASE III: $|q|^2 \equiv |p|^2 \equiv 2 \pmod{4}$

Write $q = r_1 + s_1$ and $p = r_2 + s_2$ where $r_1, r_2 \in 2\mathbb{J}$ and

$$s_1, s_2 \in \{(1, 1, 0, 0), (1, 0, 1, 0), (1, 0, 0, 1)\}.$$

Note that $\langle q, p \rangle$ is even if and only if $s_1 = s_2$.

Consider again $x = \frac{1}{2}|q\bar{p}| \in \mathbb{L}$ so that $R(x) = \frac{1}{2}q\bar{p} \in R\Lambda_2 \cap \Lambda_1(R)$. Now, $\frac{1}{2}q\bar{p} \notin \mathbb{L}$ if and only if $\langle q, p \rangle$ is odd. Since $\frac{1}{2}q\bar{p} \notin \mathbb{L}$ implies that $R\Lambda_2 \cap \Lambda_1(R) \neq \Lambda_2 \cap \Lambda_1(R)$, $R \notin H_{\Lambda_1, \Lambda_2}$ whenever $\langle q, p \rangle$ is odd.

It remains to check the case $s_1 = s_2$. Take $v \in \Lambda_2 \cap \Lambda_1(R)$. Write $v = qw\bar{p}/|q\bar{p}|$ for some $w \in \mathbb{J}$. One has

$$\frac{1}{2}|q\bar{p}|v = \frac{1}{2}(r_1w\bar{r}_2 + r_1w\bar{s}_1 + s_1w\bar{r}_2 + s_1w\bar{s}_1) \in \mathbb{L}.$$

Now, $\frac{1}{2}r_1w\bar{r}_2 \in 2\mathbb{J} \subseteq \mathbb{L}$ and $\frac{1}{2}r_1w\bar{s}_1, \frac{1}{2}s_1w\bar{r}_2 \in (1, 1, 0, 0)\mathbb{J} \subseteq \mathbb{L}$ by Fact 5. Hence, $\frac{1}{2}s_1w\bar{s}_1 = s_1ws_1^{-1} \in \mathbb{L}$ meaning $w \in s_1^{-1}\mathbb{L}s_1 = \mathbb{L}$ for all three possible values of s_1 . It follows then that $v \in R\Lambda_2$ and $R\Lambda_2 \cap \Lambda_1(R) = \Lambda_2 \cap \Lambda_1(R)$. Thus, $R \in H_{\Lambda_1, \Lambda_2}$ if $\langle q, p \rangle$ is even.

CASE IV: $|q|^2 \equiv |p|^2 \equiv 0 \pmod{4}$

Write $q = r_1 + s_1$ and $p = r_2 + s_2$ where $r_1, r_2 \in (1, 1, 0, 0)2\mathbb{J}$ and

$$s_1, s_2 \in \{(1, 1, 1, 1), (1, 1, 1, -1)\}.$$

Note that $4 \mid \langle q, p \rangle$ if and only if $s_1 = s_2$.

Take $x = \frac{1}{4}|q\bar{p}| \in \mathbb{L}$. One obtains $R(x) = (\frac{1}{2}q)(\frac{1}{2}\bar{p}) \in \mathbb{J}$. Hence, $Rx \in R\Lambda_2 \cap \Lambda_1(R)$. Observe however that $\frac{1}{4}q\bar{p} \notin \mathbb{L}$ if and only if $4 \nmid \langle q, p \rangle$. Since $\frac{1}{4}q\bar{p} \notin \mathbb{L}$ means that $R\Lambda_2 \cap \Lambda_1(R) \neq \Lambda_2 \cap \Lambda_1(R)$, $4 \nmid \langle q, p \rangle$ implies $R \notin H_{\Lambda_1, \Lambda_2}$.

Again, it remains to check the instance when $s_1 = s_2$. Let $v \in \Lambda_2 \cap \Lambda_1(R)$. If one writes $v = qw\bar{p}/|q\bar{p}|$ for some $w \in \mathbb{J}$, one gets

$$\frac{1}{4}|q\bar{p}|v = \frac{1}{4}(r_1w\bar{r}_2 + r_1w\bar{s}_1 + s_1w\bar{r}_2 + s_1w\bar{s}_1) \in \mathbb{L}.$$

By Fact 5, $\frac{1}{4}r_1w\bar{r}_2, \frac{1}{4}r_1w\bar{s}_1$, and $\frac{1}{4}s_1w\bar{r}_2 \in (1, 1, 0, 0)\mathbb{J} \subseteq \mathbb{L}$. Therefore, $w \in \mathbb{L}$ for both possible values of s_1 . Hence, $v \in R\Lambda_2$ which implies that $R\Lambda_2 \cap \Lambda_1(R) = \Lambda_2 \cap \Lambda_1(R)$. Therefore, $R \in H_{\Lambda_1, \Lambda_2}$ whenever $\langle q, p \rangle$ is divisible by 4.

The results above also hold for coincidence reflections $T_{q,p} = R_{q,p} \cdot T_{1,1} \in \text{OC}(\Lambda_1)$.

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