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Clifford algebra approach to the coincidence problem for planar lattices

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The problem of coincidences of planar lattices is analyzed using Clifford algebra. It is shown that an arbitrary coincidence isometry can be decomposed as a product of coincidence reflections and this allows planar coincidence lattices to be characterized algebraically. The cases of square, rectangular and rhombic lattices are worked out in detail. One of the aims of this work is to show the potential usefulness of Clifford algebra in crystallography. The power of Clifford algebra for expressing geometric ideas is exploited here and the procedure presented can be generalized to higher dimensions.

1. Introduction

Coincidence site lattice (CSL) theory has provided partial answers to the complex problem that arises in the description of grain boundaries and interfaces (see, for instance, Sutton & Baluffi, 1995). Most of the existing geometric models of grain boundaries idealize the two crystals that meet at a boundary as two interpenetrating lattices and it is assumed that grain boundaries with special properties arise when there is a high degree of good fit (or matching) between the lattices. The CSL model (Ranganathan, 1966) considers points common to both lattices (the intersection lattice) as points of good fit and assumes that special boundaries arise when the density of coincidence sites is high, because many atoms would occupy sites common to both grains. The experimental support for the CSL model is based on the special properties, such as changed migration rates, observed for boundaries with certain orientational relationships. Working with this model, we have to consider two identical copies of a lattice Λ (one of the 14 Bravais lattices) brought into coincidence. Next one lattice is rotated, relative to the other, by an angle θ about an axis through a common lattice point. Then for different values of θ two possibilities will arise: no lattice sites will coincide (except the site where the rotation axis passes through) or, owing to the periodicity of Λ, an infinite number will coincide forming a lattice. Such a lattice is a CSL and the ratio of the volumes of primitive cells for the CSL and for Λ is denoted by Σ. High densities of coincident sites correspond to low values of Σ.

Since the advent of quasicrystals, it has been desirable to extend the mathematical theory of CSL to more dimensions. In general, the problem can be stated as follows. Let Λ be a lattice in $\mathbb{R}^n$ and let $R \in O(n)$ be an orthogonal transformation. R is called a *coincidence isometry* if $\Lambda \cap R\Lambda$ is a sublattice of Λ. The problem is therefore to identify and characterize the coincidence isometries of a given lattice Λ.

Several approaches have been used to tackle this problem. Fortes (1983) developed a matrix theory of CSL in arbitrary dimensions, including a method to calculate a basis for the coincidence lattice through a particular factorization of the matrix defining the relative orientation. The same matrix approach was implemented by Duneau *et al.* (1992), but they evaluated the parameters of the coincidence lattice using a method based on the Smith normal form for integer matrices. Baake (1997) used complex numbers and quaternions to solve the problem in dimensions up to 4. Finally, Aragón *et al.* (1997) proposed a weak coincidence criterion and used four-dimensional lattices to characterize coincidence lattices in the plane.

Here, we analyze the problem using Clifford algebra with a twofold purpose. First, the power of this mathematical language for expressing geometric ideas is used to solve the coincidence problem, which is merely geometric. Second, we try to show that Clifford algebra, already used as a powerful language in several fields, can also be useful in geometrical crystallography. Although nothing new emerges, the results provide new insights in this and other problems in geometrical crystallography and the approach could be valuable for extension to arbitrary dimensions. In this approach, reflections are considered as primitive transformations and Clifford algebra emerges as a natural tool for this problem, without using matrices and only a minimum of group theory. It is found that any arbitrary coincidence isometry can be decomposed as a product of coincidence reflections by vectors of the lattice Λ, and the group of coincidence isometries is characterized by providing a way to generate it from vectors of Λ.

The paper is organized as follows. In §2, we provide a brief introduction to Clifford algebra by considering the particular case of the Euclidean plane and by focusing only on results relevant to the coincidence problems. In §3 some basic mathematical definitions of the CSL problem are presented. §§4, 5 and 6 present the solution of the coincidence problem for square, rectangular and rhombic lattices, respectively. Finally, §7 is devoted to conclusions and discussion.

2. The Clifford algebra of the Euclidean plane

Clifford algebra has proved to be a useful language in many areas of physics, engineering and computer science (see, for example, Bayro-Corrochano & Sobczyk, 2001). In crystallography, Hestenes (2002) presents a new approach to symmetry groups and Aragón *et al.* (2001) use Clifford algebra to study the problem of faceting in quasicrystals and to state the basis of the CSL theory which is developed and exploited here.

In what follows, we introduce the basic elements of Clifford algebra by considering the particular case of the Euclidean plane with the standard scalar (inner) product.

Definition 1. The real associative and distributive algebra generated by the Euclidean plane and the product rules

$$\begin{aligned} \mathbf{e}_i^2 &= 1, \quad i = 1, 2, \\ \mathbf{e}_1\mathbf{e}_2 + \mathbf{e}_2\mathbf{e}_1 &= 0, \end{aligned} \tag{1}$$

where $\{\mathbf{e}_1, \mathbf{e}_2\}$ is the standard canonical basis of $\mathbb{R}^2$, is called *universal Clifford algebra* or *geometric algebra* of the plane, and is denoted by $\mathbb{R}_{2,0}$.

As a vector space, the geometric algebra $\mathbb{R}_{2,0}$ is four-dimensional, with basis $\{\mathbf{1}, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_1\mathbf{e}_2\}$, where $\mathbf{e}_1\mathbf{e}_2$ is called a *bivector*. A general element of this vector space is formed by an arbitrary linear sum over the four basis elements and is called a *multivector*. If $a_1, \ldots, a_4$ are scalars, an arbitrary multivector is then

$$A = a_1\mathbf{1} + a_2\mathbf{e}_2 + a_3\mathbf{e}_3 + a_4\mathbf{e}_1\mathbf{e}_2.$$

From Definition 1, we have that if $\mathbf{x}, \mathbf{y} \in \mathbb{R}^2$, *i.e.* $\mathbf{x} = \alpha_1\mathbf{e}_1 + \alpha_2\mathbf{e}_2$ and $\mathbf{y} = \beta_1\mathbf{e}_1 + \beta_2\mathbf{e}_2$, for real numbers α_1, α_2, β_1 and β_2, then the geometric product of $\mathbf{x}$ and $\mathbf{y}$ is

$$\mathbf{xy} = \alpha_1\beta_1 + \alpha_2\beta_2 + (\alpha_1\beta_2 - \alpha_2\beta_1)\mathbf{e}_1\mathbf{e}_2. \tag{2}$$

The multiplication rules (1) lead also to the so-called *fundamental axiom of geometric algebra*:

Proposition 1. If $\mathbf{x}, \mathbf{y} \in \mathbb{R}^2$, then $\mathbf{x}^2, \mathbf{y}^2 \geq 0$ and $\mathbf{xy} + \mathbf{yx} \in \mathbb{R}$. Further,

$$\begin{aligned} \mathbf{x}^2 &= \mathbf{x} \cdot \mathbf{x}, \\ \tfrac{1}{2}(\mathbf{xy} + \mathbf{yx}) &= \mathbf{x} \cdot \mathbf{y}, \end{aligned}$$

where $\mathbf{x} \cdot \mathbf{y}$ is the Euclidean inner product in $\mathbb{R}^2$.

Proof. Let $\mathbf{x} = \alpha_1\mathbf{e}_1 + \alpha_2\mathbf{e}_2$ and $\mathbf{y} = \beta_1\mathbf{e}_1 + \beta_2\mathbf{e}_2$ be vectors in $\mathbb{R}^2$. Then, from (2), we have that

$$\mathbf{x}^2 = (\alpha_1\mathbf{e}_1 + \alpha_2\mathbf{e}_2)^2 = \alpha_1^2 + \alpha_2^2 \geq 0$$

and

$$\mathbf{xy} + \mathbf{yx} = 2(\alpha_1\beta_1 + \alpha_2\beta_2) \in \mathbb{R}. \qquad \square$$

The scalar and bivector parts of the geometric product (2) are associated, respectively, with the inner product

$$\mathbf{x} \cdot \mathbf{y} = \alpha_1\beta_1 + \alpha_2\beta_2$$

and the outer (Grassman) product

$$\mathbf{x} \wedge \mathbf{y} = (\alpha_1\beta_2 - \alpha_2\beta_1)\mathbf{e}_1\mathbf{e}_2.$$

Consequently, the geometric product (2) can be written as

$$\mathbf{xy} = \mathbf{x} \cdot \mathbf{y} + \mathbf{x} \wedge \mathbf{y}. \tag{3}$$

From the above expressions, the inner and outer products can be defined in terms of the geometric product as

$$\mathbf{x} \wedge \mathbf{y} = \tfrac{1}{2}(\mathbf{xy} - \mathbf{yx}), \tag{4}$$

$$\mathbf{x} \cdot \mathbf{y} = \tfrac{1}{2}(\mathbf{xy} + \mathbf{yx}), \tag{5}$$

which are quite convenient coordinate-free definitions.

Notice that, since $\mathbf{x} \cdot \mathbf{y} = \mathbf{y} \cdot \mathbf{x}$ and

$$\mathbf{x} \wedge \mathbf{y} = \tfrac{1}{2}(\mathbf{xy} - \mathbf{yx}) = -\tfrac{1}{2}(\mathbf{yx} - \mathbf{xy}) = -\mathbf{y} \wedge \mathbf{x},$$

the geometric product (2) is formed by a symmetric ($\mathbf{x} \cdot \mathbf{y}$) and an antisymmetric ($\mathbf{x} \wedge \mathbf{y}$) part.

In geometric algebra, the inverse of a general multivector can be defined (Hestenes & Sobczyk, 1985). In particular, any vector $\mathbf{x} \in \mathbb{R}^2$, $\mathbf{x} \neq 0$, has the inverse

$$\mathbf{x}^{-1} = \mathbf{x}/\mathbf{x}^2. \tag{6}$$

2.1. Geometric interpretation

Bivectors have an interesting geometric interpretation. Just as a vector describes an oriented line segment, with the direction of the vector represented by the oriented line and the magnitude of the vector is equal to the length of the segment, so a bivector $\mathbf{x} \wedge \mathbf{y}$ describes an oriented plane segment, with the direction of the bivector represented by the oriented plane and the magnitude of the bivector, measuring the area of the plane segment. The same interpretation is extended to higher-order terms not discussed here: $\mathbf{x} \wedge \mathbf{y} \wedge \mathbf{z}$ represents an oriented volume, and so on.

The bivector $\mathbf{x} \wedge \mathbf{y}$ then defines an oriented parallelogram with sides $\mathbf{x}$ and $\mathbf{y}$ (Fig. 1) and area given by $|\mathbf{x} \wedge \mathbf{y}| = |\alpha_1\beta_2 - \alpha_2\beta_1|$. Notice also that $\mathbf{x} \wedge \mathbf{y}$ and $\mathbf{y} \wedge \mathbf{x}$ have the same magnitude but opposite directions, as illustrated in Fig. 1.

The geometric product (2) relates algebraic operations with geometrical properties. In particular, we have the following important geometric results:

$$\begin{aligned} \mathbf{xy} = \mathbf{yx} &\Longleftrightarrow \mathbf{x} \parallel \mathbf{y} \Longleftrightarrow \mathbf{x} \wedge \mathbf{y} = 0 \Longleftrightarrow \mathbf{xy} = \mathbf{x} \cdot \mathbf{y}, \\ \mathbf{xy} = -\mathbf{yx} &\Longleftrightarrow \mathbf{x} \perp \mathbf{y} \Longleftrightarrow \mathbf{x} \cdot \mathbf{y} = 0 \Longleftrightarrow \mathbf{xy} = \mathbf{x} \wedge \mathbf{y}. \end{aligned}$$

That is, parallel vectors commute under the geometric product and perpendicular vectors anticommute.

2.2. Reflections and rotations

The algebraic properties of geometric algebra provide us with a convenient way of representing reflections and rotations. Suppose $\mathbf{a} \in \mathbb{R}^2$ is a non-zero vector and let H_a be its orthogonal complement, *i.e.* $H_a = \{\mathbf{x} \in \mathbb{R}^2 | \mathbf{a} \cdot \mathbf{x} = 0\}$. A reflection of $\mathbf{a}$ with respect to H_a is an orthogonal transformation with the following properties

$$\begin{aligned} \varphi(\mathbf{a}) &= -\mathbf{a}, \\ \varphi(\mathbf{w}) &= \mathbf{w} \quad \text{if} \quad \mathbf{w} \in H_a. \end{aligned} \tag{7}$$

The transformation φ is called reflection by the line H_a.

Lemma 1. The transformation $T_a : \mathbb{R}^2 \to \mathbb{R}^2$, defined by

$$T_a(\mathbf{x}) = -\mathbf{a}\mathbf{x}\mathbf{a}^{-1}, \tag{8}$$

is orthogonal and represents the reflection of the vector $\mathbf{x}$ by the line H_a, the orthogonal complement of $\mathbf{a}$.

Proof. Since the Clifford algebra is distributive, we can easily see that T_a is linear. Now, it remains to prove that T_a has the properties (7). First, notice that

$$T_a(\mathbf{a}) = -\mathbf{a}\mathbf{a}\mathbf{a}^{-1} = -\mathbf{a}.$$

Now, since $\mathbf{a} \cdot \mathbf{w} = 0$ for all $\mathbf{w} \in H_a$, then $\mathbf{a}\mathbf{w} = -\mathbf{w}\mathbf{a}$ and we get

$$T_a(\mathbf{w}) = -\mathbf{a}\mathbf{w}\mathbf{a}^{-1} = -(-\mathbf{w}\mathbf{a})\mathbf{a}^{-1} = \mathbf{w}, \quad \mathbf{w} \in H_a,$$

and this completes the proof.

□

Remark 1. Since the inverse of a reflection is the reflection itself, we can easily prove that

$$T_a(\mathbf{x}) = -\mathbf{a}\mathbf{x}\mathbf{a}^{-1} = -\mathbf{a}^{-1}\mathbf{x}\mathbf{a} = T_{a^{-1}}(\mathbf{x}),$$

and the following is also true

$$T_a(\mathbf{x}) = T_{\lambda a}(\mathbf{x}), \quad \text{for} \quad \lambda \in \mathbb{R}, \lambda \neq 0. \tag{9}$$

The representation of the reflection of a vector $\mathbf{x}$ given by (8) is also valid in $\mathbb{R}^n$. In this case, H_a is the hyperplane orthogonal to $\mathbf{a}$.

A rotation is the result of two successive reflections. If the transformation (8) is followed by the transformation T_b, then we have

$$T_b T_a(\mathbf{x}) = T_b(-\mathbf{a}\mathbf{x}\mathbf{a}^{-1}) = \mathbf{b}\mathbf{a}\mathbf{x}\mathbf{a}^{-1}\mathbf{b}^{-1}.$$

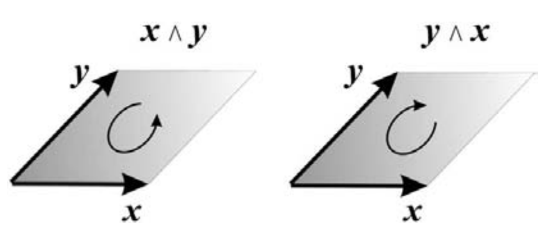

Figure 1
Geometric interpretation of the bivector $\mathbf{x} \wedge \mathbf{y}$ as a directed area.

Lemma 2. The transformation $T : \mathbb{R}^2 \to \mathbb{R}^2$, defined by

$$T(\mathbf{x}) = R\mathbf{x}R^{-1},$$

where $R = \mathbf{ab}$, is orthogonal and represents the rotation of the vector $\mathbf{x}$ through the angle 2θ, where θ is the angle formed by the vectors $\mathbf{a}$ and $\mathbf{b}$.

Now we have finally a result that will be extensively used in the following sections. It asserts that, given an arbitrary rotation T, we can always find a vector $\mathbf{a} \in \mathbb{R}^2$ such that T can be viewed as a reflection by the basis vector $\mathbf{e}_2$ followed by a reflection by the vector $\mathbf{a}$. In other words, the next proposition describes a method to decompose an arbitrary rotation T into a product of reflections.

Proposition 2. Let $T : \mathbb{R}^2 \to \mathbb{R}^2$ be a nontrivial rotation. Then, there exists $\mathbf{a} \in \mathbb{R}^2$, such that

$$T(\mathbf{x}) = \mathbf{a}\mathbf{e}_2\mathbf{x}\mathbf{e}_2\mathbf{a}^{-1} = T_a T_{e_2}(\mathbf{x}).$$

Proof. Let $T : \mathbb{R}^2 \to \mathbb{R}^2$ be a rotation through an angle θ, then

$$\begin{aligned} T(\mathbf{e}_1) &= \cos\theta\mathbf{e}_1 + \sin\theta\mathbf{e}_2, \\ T(\mathbf{e}_2) &= -\sin\theta\mathbf{e}_1 + \cos\theta\mathbf{e}_2. \end{aligned}$$

Consider $\mathbf{a} \in \mathbb{R}^2$, defined by

$$\mathbf{a} = T(\mathbf{e}_1) - \mathbf{e}_1 = (\cos\theta - 1)\mathbf{e}_1 + \sin\theta\mathbf{e}_2 \neq 0.$$

According to (6), the inverse of this vector is

$$\mathbf{a}^{-1} = \frac{\mathbf{a}}{\mathbf{a}^2} = \frac{(\cos\theta - 1)\mathbf{e}_1 + \sin\theta\mathbf{e}_2}{2(1 - \cos\theta)}.$$

Now, we define $\varphi(\mathbf{x}) = \mathbf{a}\mathbf{e}_2\mathbf{x}\mathbf{e}_2\mathbf{a}^{-1}$, and apply this map to $\mathbf{e}_1$ to get

$$\begin{aligned} \varphi(\mathbf{e}_1) &= \mathbf{a}\mathbf{e}_2\mathbf{e}_1\mathbf{e}_2\mathbf{a}^{-1} \\ &= -\mathbf{a}\mathbf{e}_1\mathbf{a}^{-1} \\ &= -\frac{\mathbf{a}\mathbf{e}_1\mathbf{a}}{2(1 - \cos\theta)} \\ &= \frac{-[(\cos\theta - 1) + \sin\theta\mathbf{e}_2\mathbf{e}_1]\mathbf{a}}{2(1 - \cos\theta)} \\ &= -\frac{[(\cos\theta - 1)^2 - \sin^2\theta]\mathbf{e}_1 + 2(\cos\theta - 1)\sin\theta\mathbf{e}_2}{2(1 - \cos\theta)}. \end{aligned}$$

Since $(\cos\theta - 1)^2 - \sin^2\theta = -2\cos\theta + 2\cos^2\theta = 2\cos\theta(\cos\theta - 1)$, we have that

$$\varphi(\mathbf{e}_1) = T(\mathbf{e}_1).$$

Now we apply φ to $\mathbf{e}_2$

$$\begin{aligned}\varphi(\mathbf{e}_2) &= \mathbf{a}\mathbf{e}_2\mathbf{e}_2\mathbf{e}_2\mathbf{a}^{-1}\\ &= \mathbf{a}\mathbf{e}_2\mathbf{a}^{-1}\\ &= \frac{\mathbf{a}\mathbf{e}_2\mathbf{a}}{2(1-\cos\theta)}\\ &= \frac{[(\cos\theta-1)\mathbf{e}_1\mathbf{e}_2+\sin\theta]\mathbf{a}}{2(1-\cos\theta)}\\ &= \frac{2(\cos\theta-1)\sin\theta\mathbf{e}_1+[\sin^2\theta-(\cos\theta-1)^2]\mathbf{e}_2}{2(1-\cos\theta)}\\ &= -\sin\theta\mathbf{e}_1+\cos\theta\mathbf{e}_2.\end{aligned}$$

We have proved that $\varphi(\mathbf{e}_i) = T(\mathbf{e}_i)$ for $i = 1, 2$, and consequently we conclude that $\varphi(\mathbf{x}) = T(\mathbf{x})$. □

3. Some mathematical definitions for the CSL problem

Here we present a brief summary of basic concepts related to coincidence lattices. For this purpose, we adopt definitions and notation given by Baake (1997), who formulated the CSL problem in more mathematical terms.

Definition 2. A discrete subset $\Lambda \subset \mathbb{R}^n$ is called a *lattice*, of dimension n, if it is spanned as $\Lambda = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2 \oplus \cdots \oplus \mathbb{Z}\mathbf{a}_n$, where $\{\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n\}$ is a set of linearly independent vectors in $\mathbb{R}^n$. These vectors form a basis of the lattice.

The lattice Λ is isomorphic to the free Abelian group of order n. It leads us to define the concept of a sublattice:

Definition 3. Let Λ be a lattice in $\mathbb{R}^n$. A subset $\Lambda' \subset \Lambda$ is called a *sublattice* of Λ if it is a subgroup of finite index, *i.e.* $[\Lambda : \Lambda'] < \infty$ (the number of right lateral classes is finite). It is also said that Λ is a superlattice of Λ'.

The following two definitions are central for the coincidence problem.

Definition 4. Two lattices Λ_1 and Λ_2 are called *commensurate*, denoted by $\Lambda_1 \sim \Lambda_2$, if and only if $\Lambda_1 \cap \Lambda_2$ is a sublattice of both Λ_1 and Λ_2.

Definition 5. Let Λ be a lattice in $\mathbb{R}^n$. An orthogonal transformation $R \in O(n)$ is called a *coincidence isometry* of Λ if and only if $R\Lambda \sim \Lambda$. The integer $\Sigma(R) := [\Lambda : \Lambda \cap R\Lambda]$ is called the *coincidence index* of R with respect to Λ. If R is not a coincidence isometry then $\Sigma(R) := \infty$. Two useful sets are also defined:

$$\begin{aligned}OC(\Lambda) &:= \{R \in O(n) \mid \Sigma(R) < \infty\},\\ SOC(\Lambda) &:= \{R \in OC(\Lambda) \mid \det(R) = 1\}.\end{aligned}$$

4. CSL from reflections for the case of the square lattice

It is well known that any isometry is the product of at most four reflections (see for instance Coxeter, 1973). In that sense, we can consider reflections as the primitive transformations[1] and, in this case, Clifford algebra is a natural tool for this problem. In Aragón *et al.* (2001), we adopted this point of view and developed some preliminary results about the CSL of the (hyper-)cubic lattice in arbitrary dimensions. The main results presented in that work can be summarized as follows.

Proposition 3. Let $\Lambda = \mathbb{Z}^n = \mathbb{Z}\mathbf{e}_1 \oplus \mathbb{Z}\mathbf{e}_2 \oplus \cdots \oplus \mathbb{Z}\mathbf{e}_n$, with $\{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n\}$ the canonical basis of $\mathbb{R}^n$. If $\mathbf{a} \in \mathbb{Z}^n$, then the reflection defined by

$$T_a(\mathbf{x}) = -\mathbf{a}\mathbf{x}\mathbf{a}^{-1}$$

is a *coincidence reflection*, that is $T_a \in OC(\mathbb{Z}^n)$.

Proposition 4. If T is a reflection with respect to a hyperplane such that $T \in OC(\mathbb{Z}^n)$, then there exists $\mathbf{a} \in \mathbb{Z}^n$ such that

$$T(\mathbf{x}) = T_a(\mathbf{x}) = -\mathbf{a}\mathbf{x}\mathbf{a}^{-1}.$$

We then proved that, given an arbitrary coincidence reflection, we can always consider that the reflection is by a vector of the lattice. Thus coincidence reflections are identified with lattice vectors that generate the lattice $\Lambda = \mathbb{Z}^n$. We also conjectured that any orthogonal transformation $T \in OC(\mathbb{Z}^n)$ can be decomposed as a product of coincidence reflections in vectors of the lattice $\mathbb{Z}^n$. In what follows, we will prove that our conjecture is true for planar lattices, and explore some of its consequences. This result is presented in the following.

Proposition 5. Let $T : \mathbb{R}^2 \to \mathbb{R}^2$ be an orthogonal transformation, different from the identity. If $T \in OC(\mathbb{Z}^2)$, then there exists $\mathbf{a} \in \mathbb{Z}^2$ such that

$$T(\mathbf{x}) = \begin{cases} T_a(\mathbf{x}) = -\mathbf{a}\mathbf{x}\mathbf{a}^{-1} & \text{if} \quad \det(T) = -1,\\ T_a T_{e_2}(\mathbf{x}) = \mathbf{a}\mathbf{e}_2\mathbf{x}\mathbf{e}_2\mathbf{a}^{-1} & \text{if} \quad \det(T) = 1.\end{cases}$$

Proof. If $T \in OC(\mathbb{Z}^2)$ and $\det(T) = -1$ then T is a reflection by a line, say, l. Since T is different from the identity then $T(\mathbf{e}_i) \neq \mathbf{e}_i$ for any $i = 1, 2$. Now consider the vector

$$\mathbf{b} = T(\mathbf{e}_1) - \mathbf{e}_1,$$

which is orthogonal to the reflection line l and can be used to write the reflection as in Lemma 1. Since $T(\mathbf{e}_i)$ has rational components (as is readily inferred from the fact that an orthogonal matrix with only rational entries is a coincidence isometry), then $T(\mathbf{e}_1) - \mathbf{e}_1$ also has rational entries and we can find $\lambda \in \mathbb{Z}$ such that $\lambda\mathbf{b} \in \mathbb{Z}^2$. By defining $\mathbf{a} = \lambda\mathbf{b}$, from (9) we get

$$T(\mathbf{x}) = -\mathbf{a}\mathbf{x}\mathbf{a}^{-1}.$$

If $T \in OC(\mathbb{Z}^2)$, different from the identity, and $\det(T) = 1$ then T is a rotation through an angle θ. Following the previous reasoning and using Proposition 2, we have that

[1] Contrary to crystallographers' preference of considering translations, rotations and inversions as primitive transformations.

$$T(\mathbf{x}) = \mathbf{b}\mathbf{e}_2\mathbf{x}\mathbf{e}_2\mathbf{b}^{-1} = T_b T_{e_2},$$

where $\mathbf{b} = T(\mathbf{e}_1) - \mathbf{e}_1$ and there exists $\lambda \in \mathbb{Z}$ such that $\lambda\mathbf{b} \in \mathbb{Z}^2$. By defining $\mathbf{a} = \lambda\mathbf{b}$, we obtain

$$T_b T_{e_2} = T_a T_{e_2},$$
$$T(\mathbf{x}) = \mathbf{a}\mathbf{e}_2\mathbf{x}\mathbf{e}_2\mathbf{a}^{-1},$$

which proves the proposition. □

It is important to remark that, given the property (9), we can assume that in Proposition 5 the components of the vector **a** are relatively prime (they share no common positive divisors except 1). It is a consequence of the fact that if

$$\mathbf{a} = \alpha_1\mathbf{e}_1 + \alpha_2\mathbf{e}_2$$

and we define

$$\mathbf{a}' = \frac{\alpha_1}{\text{g.c.d.}(\alpha_1, \alpha_2)}\mathbf{e}_1 + \frac{\alpha_2}{\text{g.c.d.}(\alpha_1, \alpha_2)}\mathbf{e}_2 = \frac{1}{\text{g.c.d.}(\alpha_1, \alpha_2)}\mathbf{a}, \tag{10}$$

where g.c.d.(α_1, α_2) stands for the greatest common divisor of α_1 and α_2, then

$$T_a = T_{a'}.$$

Notice that with all these results we have characterized $OC(\mathbb{Z}^2)$ by providing a procedure to obtain an arbitrary element of $OC(\mathbb{Z}^2)$.

On the other hand, since $T_{e_2}(\mathbb{Z}^2) = \mathbb{Z}^2$, we have that

$$\mathbb{Z}^2 \cap (T_a T_{e_2})(\mathbb{Z}^2) = \mathbb{Z}^2 \cap T_a(\mathbb{Z}^2), \quad \mathbf{a} \in \mathbb{Z}^2,$$

and an immediate consequence is the fact that every vector $\mathbf{a} \in \mathbb{Z}^2$ defines the following two orthogonal transformations:

$$T_a(\mathbf{x}) = -\mathbf{a}\mathbf{x}\mathbf{a}^{-1},$$
$$T_a T_{e_2}(\mathbf{x}) = R_a(\mathbf{x}) = \mathbf{a}\mathbf{e}_2\mathbf{x}\mathbf{e}_2\mathbf{a}^{-1}.$$

Also, since

$$\mathbb{Z}^2 \cap T_a(\mathbb{Z}^2) = \mathbb{Z}^2 \cap R_a(\mathbb{Z}^2),$$
$$\Sigma(T_a) = \Sigma(R_a),$$

a basis of $\mathbb{Z}^2 \cap R_a(\mathbb{Z}^2)$ can be obtained if the basis of $\mathbb{Z}^2 \cap T_a(\mathbb{Z}^2)$ is known.

4.1. The coincidence index

Besides Definition 5, the coincidence index has the following interpretation. If $\Lambda' = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2 \oplus \ldots \oplus \mathbb{Z}\mathbf{a}_n$ is a coincidence lattice, which is a sublattice of $\Lambda = \mathbb{Z}\mathbf{b}_1 \oplus \mathbb{Z}\mathbf{b}_2 \oplus \ldots \oplus \mathbb{Z}\mathbf{b}_n$, then the coincidence index $[\Lambda : \Lambda']$ is the ratio of the volume of the unit cell defined by the vectors $\mathbf{a}_i$ and the volume of the unit cell defined by the vectors $\mathbf{b}_i$.

In the two-dimensional case that we are considering, the coincidence lattice $\Lambda' = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$ is a subset of $\mathbb{Z}^2$ and $[\mathbb{Z}^2 : \Lambda'] = |\mathbf{a}_1 \wedge \mathbf{a}_2|$. In what follows, we detail the procedure to find the coincidence index.

We have seen in Proposition 5 that, given an arbitrary coincidence rotation R in the plane, we can always find a vector $\mathbf{a} \in \mathbb{Z}^2$, with relatively prime components, such that the transformation can be written as $T_a T_{e_2}$. Further, at the end of the previous section we have shown that a basis for the coincidence lattice $\mathbb{Z}^2 \cap R_a(\mathbb{Z}^2)$ can be obtained from the basis of the lattice $\mathbb{Z}^2 \cap T_a(\mathbb{Z}^2)$. We will then analyze a $T_a \in OC(\mathbb{Z}^2)$, where $\mathbf{a} = \alpha_1\mathbf{e}_1 + \alpha_2\mathbf{e}_2 \in \mathbb{Z}^2$ and g.c.d.$(\alpha_1, \alpha_2) = 1$. From (6), this transformation can be written as

$$T_a(\mathbf{x}) = -\mathbf{a}\mathbf{x}\mathbf{a}^{-1} = -\frac{\mathbf{a}\mathbf{x}\mathbf{a}}{\mathbf{a}^2}.$$

Notice that $T_a(\mathbf{a}) = -\mathbf{a}$ and it can be verified that for any $\mathbf{x} \in \mathbb{Z}^2$ we have $\mathbf{a}^2 T_a(\mathbf{x}) \in \mathbb{Z}^2$.

Now consider the vector $\mathbf{b} \in \mathbb{Z}^2$ defined by

$$\mathbf{b} = \mathbf{a}\mathbf{e}_1\mathbf{e}_2 = (\alpha_1\mathbf{e}_1 + \alpha_2\mathbf{e}_2)\mathbf{e}_1\mathbf{e}_2 = -\alpha_2\mathbf{e}_1 + \alpha_1\mathbf{e}_2. \tag{11}$$

Since **b** is orthogonal to **a**, as can be easily inferred, then $\mathbf{ab} = -\mathbf{ba}$ and

$$T_a(\mathbf{b}) = -\frac{\mathbf{aba}}{\mathbf{a}^2} = \frac{\mathbf{b}\mathbf{a}^2}{\mathbf{a}^2} = \mathbf{b}.$$

It implies that the vectors $\mathbf{c} = T_a(\mathbf{a})$ and $\mathbf{d} = T_a(\mathbf{b})$ belong to $\mathbb{Z}^2 \cap T_a(\mathbb{Z}^2)$; the lattice $\Lambda_1 = \mathbb{Z}\mathbf{c} \oplus \mathbb{Z}\mathbf{d}$ is a sublattice of $\mathbb{Z}^2 \cap T_a(\mathbb{Z}^2)$ and of $\mathbb{Z}^2$. Further,

$$\Lambda_1 < \mathbb{Z}^2 \cap T_a(\mathbb{Z}^2) < \mathbb{Z}^2.$$

Now from a basic group theory result, we have that

$$[\mathbb{Z}^2 : \Lambda_1] = [\mathbb{Z}^2 \cap T_a(\mathbb{Z}^2) : \Lambda_1][\mathbb{Z}^2 : \mathbb{Z}^2 \cap T_a(\mathbb{Z}^2)],$$

and since $[\mathbb{Z}^2 : \Lambda_1] = |\mathbf{c} \wedge \mathbf{d}| = \alpha_1^2 + \alpha_2^2 = \mathbf{a}^2$, by substituting in the previous equation we conclude that

$$[\mathbb{Z}^2 : \mathbb{Z}^2 \cap T_a(\mathbb{Z}^2)] \quad \text{divides} \quad \mathbf{a}^2.$$

With this result and the definition of coincidence index, we can state the following:

Lemma 3. If $\mathbf{a} = \alpha_1\mathbf{e}_1 + \alpha_2\mathbf{e}_2 \in \mathbb{Z}^2$, where g.c.d.$(\alpha_1, \alpha_2) = 1$, then $\Sigma(T_a)$ and $\Sigma(R_a)$ divide $\mathbf{a}^2$.

More can be said about the coincidence index. By considering $\mathbf{a} = \alpha_1\mathbf{e}_1 + \alpha_2\mathbf{e}_2 \in \mathbb{Z}^2$, where g.c.d.$(\alpha_1, \alpha_2) = 1$, we have that

$$\begin{aligned}
T_a(\mathbf{e}_1) &= \frac{(\alpha_2^2 - \alpha_1^2)\mathbf{e}_1 - 2\alpha_1\alpha_2\mathbf{e}_2}{\alpha_1^2 + \alpha_2^2} \\
&= \frac{-2\alpha_1}{\alpha_1^2 + \alpha_2^2}\mathbf{a} + \mathbf{e}_1, \\
T_a(\mathbf{e}_2) &= \frac{-2\alpha_1\alpha_2\mathbf{e}_1 - (\alpha_2^2 - \alpha_1^2)\alpha_2\mathbf{e}_2}{\alpha_1^2 + \alpha_2^2} \\
&= \frac{-2\alpha_2}{\alpha_1^2 + \alpha_2^2}\mathbf{a} + \mathbf{e}_2.
\end{aligned}$$

If both α_1 and α_2 are odd numbers, then $\alpha_1^2 + \alpha_2^2$ is even and, consequently,

$$\frac{\mathbf{a}^2}{2} T_a(\mathbf{e}_i) \in \mathbb{Z}^2, \quad i = 1, 2.$$

It can be proved that $\mathbf{a}^2/2$ is the least positive integer such that $(\mathbf{a}^2/2)T_a(\mathbf{e}_i) \in \mathbb{Z}^2$ and therefore $\mathbf{a}^2/2$ divides $\Sigma(T_a)$.

Now let us consider the vectors $\mathbf{c}' = (\mathbf{a}^2/2)T_a(\mathbf{e}_1)$ and $\mathbf{d}' = (\mathbf{a}^2/2)T_a(\mathbf{e}_2)$. The lattice spanned by these vectors is a sublattice of $T_a(\mathbb{Z}^2) \cap \mathbb{Z}^2$ and, by the above reasoning, we can see that $\Sigma(T_a)$ divides $(\mathbf{a}^2/2)^2$.

All the above results can be summarized as follows:

$$\frac{\mathbf{a}^2}{2} \mid \Sigma(T_a), \tag{12}$$

$$\Sigma(T_a) \mid \mathbf{a}^2, \tag{13}$$

$$\Sigma(T_a) \mid \left(\frac{\mathbf{a}^2}{2}\right)^2. \tag{14}$$

From (12) and (13), we get

$$\mathbf{a}^2 = \Sigma(T_a)q = \frac{\mathbf{a}^2}{2}pq, \quad 2 = pq.$$

Since p and q are integers, we have two possibilities:

1. $p = 2$ and $q = 1$. In this case, we can conclude that $\mathbf{a}^2 = \Sigma(T_a)$, but from (14) we have

$$\left(\frac{\mathbf{a}^2}{2}\right)^2 = \mathbf{a}^2 k, \quad k \in \mathbb{Z}, \quad \mathbf{a}^2 = 4k,$$

which cannot be fulfilled since $\mathbf{a}^2/4$ has a remainder of 2.

2. $p = 1$ and $q = 2$. In this case, we obtain a valid condition:

$$\mathbf{a}^2 = \Sigma(T_a)2, \quad \frac{\mathbf{a}^2}{2} = \Sigma(T_a).$$

Finally, let us consider that α_1 and α_2 are relatively prime and one of them is an even number. It can be proved that in this case $\mathbf{a}^2$ is the least positive integer such that $\mathbf{a}^2 T(\mathbf{e}_1) \in \mathbb{Z}^2$. It implies that $\mathbf{a}^2 \mid \Sigma(T_a)$ and, from the above results, $\mathbf{a}^2 = \Sigma(T_a)$.

We have now all the ingredients to state the following

Proposition 6. If $\mathbf{a} = \alpha_1\mathbf{e}_1 + \alpha_2\mathbf{e}_2 \in \mathbb{Z}^2$ and g.c.d.$(\alpha_1, \alpha_2) = 1$, then

1. If α_1 and α_2 are both odd numbers, then

$$\Sigma(T_a) = \Sigma(R_a) = \frac{\mathbf{a}^2}{2}.$$

2. If either α_1 or α_2 is even, then

$$\Sigma(T_a) = \Sigma(R_a) = \mathbf{a}^2.$$

4.2. Basis for the CSL

The following theorem states that the CSL of $\mathbb{Z}^2$ is a square lattice and the basis vectors are obtained during the proof.

Theorem 1. Let $\mathbf{a} = \alpha_1\mathbf{e}_1 + \alpha_2\mathbf{e}_2 \in \mathbb{Z}^2$ be a vector such that g.c.d.$(\alpha_1, \alpha_2) = 1$, then $\mathbb{Z}^2 \cap T_a(\mathbb{Z}^2)$ and $\mathbb{Z}^2 \cap R_a(\mathbb{Z}^2)$ are square lattices.

Proof. If either α_1 or α_2 is even, then $\mathbf{a}^2$ is odd and

$$[\mathbb{Z}^2 : \mathbb{Z}^2 \cap T_a(\mathbb{Z}^2)] = \mathbf{a}^2, \quad \mathbf{a}^2 \text{ odd}.$$

If both α_1 and α_2 are odd, then $\mathbf{a}^2$ is even and

$$[\mathbb{Z}^2 : \mathbb{Z}^2 \cap T_a(\mathbb{Z}^2)] = \frac{\mathbf{a}^2}{2}, \quad \mathbf{a}^2 \text{ even}.$$

Both cases are now considered in detail.

1. $\mathbf{a}^2$ is odd.

Consider the vector defined in (11):

$$\mathbf{b} = -\alpha_2\mathbf{e}_1 + \alpha_1\mathbf{e}_2.$$

From the previous section, we know that $T_a(\mathbf{a}) = -\mathbf{a}$, $T_b(\mathbf{b}) = \mathbf{b}$ and that the lattice spanned by $\mathbf{a}$ and $\mathbf{b}$ is a sublattice of $\mathbb{Z}^2 \cap T_a(\mathbb{Z}^2)$. Since $|\mathbf{a} \wedge \mathbf{b}| = \mathbf{a}^2$, as can be easily verified, then

$$\mathbb{Z}\mathbf{a} \oplus \mathbb{Z}\mathbf{b} = \mathbb{Z}^2 \cap T_a(\mathbb{Z}^2).$$

2. $\mathbf{a}^2$ is even.

In this case, there exist vectors $\mathbf{c}, \mathbf{d} \in \mathbb{Z}^2 \cap T_a(\mathbb{Z}^2)$ such that

$$\mathbf{d}^2 = \mathbf{c}^2, \quad \mathbf{dc} = -\mathbf{cd}.$$

It turns out that $\{\mathbf{c}, \mathbf{d}\}$ is a square basis of $\mathbb{Z}^2 \cap T_a(\mathbb{Z}^2)$, as we will prove in what follows.

Consider the following vectors in $\mathbb{Z}^2$:

$$\begin{aligned} \mathbf{c} &= \tfrac{1}{2}(\mathbf{a} - \mathbf{b}) = T_a(\mathbf{c}'), \\ \mathbf{d} &= \tfrac{1}{2}(\mathbf{a} + \mathbf{b}) = T_a(\mathbf{d}'), \end{aligned} \tag{15}$$

where $\mathbf{b}$ is given in (11) and

$$\mathbf{c}' = -\tfrac{1}{2}(\mathbf{a} + \mathbf{b}), \quad \mathbf{d}' = \tfrac{1}{2}(\mathbf{b} - \mathbf{a}).$$

The vectors defined in (15) fulfill

$$\mathbf{c} + \mathbf{d} = \mathbf{a},$$

$$\mathbf{c}^2 = \mathbf{d}^2 = \frac{\mathbf{a}^2}{2},$$

$$|\mathbf{c} \wedge \mathbf{d}| = \frac{\mathbf{a}^2}{2} = [\mathbb{Z}^2 : \mathbb{Z}^2 \cap T_a(\mathbb{Z}^2)],$$

so we can conclude that $\{\mathbf{c}, \mathbf{d}\}$ is a square basis of $\mathbb{Z}^2 \cap T_a(\mathbb{Z}^2)$. □

From the previous theorem, we have in summary that, if $\mathbf{a}^2$ is odd, a basis for the CSL is $\{\mathbf{a}, \mathbf{b}\}$, where $\mathbf{b}$ is given by (11). Otherwise, if $\mathbf{a}^2$ is even, a basis of the CSL is $\{\mathbf{c}, \mathbf{d}\}$, where $\mathbf{c}$ and $\mathbf{d}$ are defined in (15).

Corollary 1. If $T : \mathbb{R}^2 \to \mathbb{R}^2$ is a transformation such that $T \in OC(\mathbb{Z}^2)$, then $\mathbb{Z}^2 \cap T(\mathbb{Z}^2)$ is a square lattice.

Proof. From Proposition 5, T can be written as either $T(\mathbf{x}) = -\mathbf{axa}^{-1}$ or $T(\mathbf{x}) = \mathbf{ae}_2\mathbf{xe}_2\mathbf{a}^{-1}$, where $\mathbf{a} = \alpha_1\mathbf{e}_1 + \alpha_2\mathbf{e}_2 \in \mathbb{Z}^2$ and g.c.d.$(\alpha_1, \alpha_2) = 1$. Thus, Theorem 1 applies. □

4.3. Examples

1. As a simple example consider the problem of determining a basis of the CSL corresponding to $\Sigma = 17$. We know (see

Table 1
Elements of the set Σ_5, where $\mathbf{a} = \alpha_1\mathbf{e}_1 + \alpha_2\mathbf{e}_2$ and $\mathbf{b}$ is a vector orthogonal to $\mathbf{a}$.

Only rotations are tabulated, with the rotation angle given in the last column. To each coincidence rotation there corresponds a coincidence reflection defined by the vector $\mathbf{a}$.

α_1	α_2	$\mathbf{a}$	$\mathbf{b}$	Basis of the CSL	Rotation angle (°)
1	2	$\mathbf{e}_1+2\mathbf{e}_2$	$2\mathbf{e}_1-\mathbf{e}_2$	$\{\mathbf{e}_1+2\mathbf{e}_2, 2\mathbf{e}_1-\mathbf{e}_2\}$	−53.13
2	1	$2\mathbf{e}_1+\mathbf{e}_2$	$\mathbf{e}_1-2\mathbf{e}_2$	$\{2\mathbf{e}_1+\mathbf{e}_2, \mathbf{e}_1-2\mathbf{e}_2\}$	233.13
1	−2	$\mathbf{e}_1-\mathbf{e}_2$	$2\mathbf{e}_1+\mathbf{e}_2$	$\{2\mathbf{e}_1+\mathbf{e}_2, \mathbf{e}_1-2\mathbf{e}_2\}$	53.13
2	−1	$2\mathbf{e}_1-\mathbf{e}_2$	$\mathbf{e}_1+2\mathbf{e}_2$	$\{2\mathbf{e}_1-\mathbf{e}_2, \mathbf{e}_1+2\mathbf{e}_2\}$	126.87
1	3	$\mathbf{e}_1+3\mathbf{e}_2$	$3\mathbf{e}_1-\mathbf{e}_2$	$\{2\mathbf{e}_1+\mathbf{e}_2, \mathbf{e}_1-2\mathbf{e}_2\}$	−36.87
3	1	$3\mathbf{e}_1+\mathbf{e}_2$	$\mathbf{e}_1-3\mathbf{e}_2$	$\{2\mathbf{e}_1-\mathbf{e}_2, \mathbf{e}_1+2\mathbf{e}_2\}$	216.87
1	−3	$\mathbf{e}_1-3\mathbf{e}_2$	$3\mathbf{e}_1+\mathbf{e}_2$	$\{2\mathbf{e}_1-\mathbf{e}_2, \mathbf{e}_1+2\mathbf{e}_2\}$	36.87
3	−1	$3\mathbf{e}_1-\mathbf{e}_2$	$\mathbf{e}_1+3\mathbf{e}_2$	$\{2\mathbf{e}_1+\mathbf{e}_2, \mathbf{e}_1-\mathbf{e}_2\}$	143.13

Ranganathan, 1966) that $\Sigma = 17 = 1^2 + 4^2$ and $\tan(\theta/2) = 1/4$, which gives a rotation angle $\theta = 28.0724°$. With respect to the canonical basis, the matrix associated with this orthogonal transformation is

$$T = \begin{pmatrix} \frac{15}{17} & -\frac{8}{17} \\ \frac{8}{17} & \frac{5}{17} \end{pmatrix}.$$

Thus $T(\mathbf{e}_1) - \mathbf{e}_1 = (-2/17, 8/17)$ and we can consider $\mathbf{a} = (-1, 4) \in \mathbb{Z}^2$. By using the geometric product, this transformation is written as

$$T_a(\mathbf{x}) = -(-\mathbf{e}_1 + 4\mathbf{e}_2)\mathbf{e}_2\mathbf{x}\mathbf{e}_2(-\mathbf{e}_1 + 4\mathbf{e}_2)^{-1}.$$

From Proposition 6, we obtain the expected coincidence index

$$\Sigma(T_a) = \mathbf{a}^2 = 17.$$

A basis for CSL is deduced from Theorem 1 (case $\mathbf{a}^2$ odd). We have $\mathbf{b} = -4\mathbf{e}_1 - \mathbf{e}_2$ and therefore a basis for $\mathbb{Z}^2 \cap T_a\mathbb{Z}^2$ is

$$\{-\mathbf{e}_1 + 4\mathbf{e}_2, -4\mathbf{e}_1 - \mathbf{e}_2\}.$$

2. Consider the set of orthogonal transformations in $\mathbb{R}^2$ that when applied to $\mathbb{Z}^2$ produce coincident lattices with coincidence index equal to 5, that is

$$\Sigma_5 = \{T \in OC(\mathbb{Z}^2) \mid \Sigma(T) = 5\}.$$

With the procedure discussed in this section, we can easily find the elements of Σ_5 and the basis for the coincidence lattice in each case. From the simple facts that $1^2 + 2^2 = 5$ and $1^2 + 3^2 = 10$, the orthogonal transformations belonging to Σ_5 are tabulated in Table 1. As explained above, $\mathbf{a} = \alpha_1\mathbf{e}_1 + \alpha_2\mathbf{e}_2$ and in this case $\mathbf{b}$ is a vector orthogonal to $\mathbf{a}$. Notice that the set is composed of 16 transformations: eight reflections and eight rotations.

5. The rectangular lattice

Let Γ be a rectangular lattice in $\mathbb{R}^2$, *i.e.* $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$ and $\mathbf{a}_1 \cdot \mathbf{a}_2 = 0$. In this section, we study and characterize the group $OC(\Gamma)$.

Here we can also associate coincidence reflections with reflections by vectors in Γ. This is stated in the following proposition, which is valid for arbitrary lattices in $\mathbb{R}^2$ (see Proposition 4).

Proposition 7. Let $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$ be a lattice in $\mathbb{R}^2$. If $T \in OC(\Gamma)$ is a reflection such that $T(\mathbf{x}) = T_b(\mathbf{x}) = -\mathbf{b}\mathbf{x}\mathbf{b}^{-1}$, $\mathbf{b} \in \mathbb{R}^2$, then we can always find $\mathbf{c} \in \Gamma$ such that $T(\mathbf{x}) = -\mathbf{b}\mathbf{x}\mathbf{b}^{-1} = -\mathbf{c}\mathbf{x}\mathbf{c}^{-1}$.

Proof. Since $T \in OC(\Gamma)$, for a given $\mathbf{a} \in \Gamma$ we can always find $m \in \mathbb{Z}$ such that $mT(\mathbf{a}) = T(m\mathbf{a}) \in \Gamma$. It is equivalent to say that there exists $\mathbf{x} \in \Gamma$ such that $\mathbf{y} = T(\mathbf{x}) \in \Gamma$, that is $\mathbf{y} = -\mathbf{b}\mathbf{x}\mathbf{b}^{-1} \in \Gamma$. Thus $\mathbf{y}\mathbf{b} = -\mathbf{b}\mathbf{x}$ and, consequently,

$$\mathbf{y} \cdot \mathbf{b} = -\mathbf{b} \cdot \mathbf{x},$$
$$\mathbf{y} \wedge \mathbf{b} = -\mathbf{b} \wedge \mathbf{x} = \mathbf{x} \wedge \mathbf{b}.$$

The last equation implies that $(\mathbf{y} - \mathbf{x}) \wedge \mathbf{b} = 0$ and, since $\mathbf{x}, \mathbf{y} \in \Gamma$, there exists $\lambda \in \mathbb{R}$ such that $\mathbf{y} - \mathbf{x} = \lambda\mathbf{b} \in \Gamma$. By taking $\mathbf{c} = \lambda\mathbf{b} \in \Gamma$, we get $T(\mathbf{x}) = -\mathbf{b}\mathbf{x}\mathbf{b}^{-1} = -\mathbf{c}\mathbf{x}\mathbf{c}^{-1}$. □

The generalization to rectangular basis of Proposition 2, to decompose an arbitrary orthogonal transformation T into a product of reflections, reads as follows.

Proposition 8. Let $T : \mathbb{R}^2 \to \mathbb{R}^2$ be a nontrivial orthogonal transformation. If $\mathbf{a}_1, \mathbf{a}_2 \in \mathbb{R}^2$ are vectors such that $\mathbf{a}_1 \cdot \mathbf{a}_2 = 0$, then there exists $\mathbf{b} \in \mathbb{R}^2$ such that

$$T(\mathbf{x}) = \begin{cases} T_b(\mathbf{x}) = -\mathbf{b}\mathbf{x}\mathbf{b}^{-1} & \text{if } \det(T) = -1, \\ T_bT_{a_2}(\mathbf{x}) = \mathbf{b}\mathbf{a}_2\mathbf{x}\mathbf{a}_2^{-1}\mathbf{b}^{-1} & \text{if } \det(T) = 1. \end{cases}$$

Proof. Assume $T : \mathbb{R}^2 \to \mathbb{R}^2$, different from the identity, and $\det(T) = -1$. In this case, T is a reflection by a line, say, l. Since T is different from the identity and $\{\mathbf{a}_1, \mathbf{a}_2\}$ is an orthogonal basis of $\mathbb{R}^2$, then $T(\mathbf{a}_i) \neq \mathbf{a}_i$ for some $i = 1, 2$. Now consider the vector

$$\mathbf{b} = T(\mathbf{a}_1) - \mathbf{a}_1, \tag{16}$$

which is orthogonal to the reflection line l and can be used to write the reflection as in Lemma 1: $T(\mathbf{x}) = T_b(\mathbf{x}) = -\mathbf{b}\mathbf{x}\mathbf{b}^{-1}$.

Now assume $\det(T) = 1$. In this case, T is a rotation through an angle θ and also $T(\mathbf{a}_i) \neq \mathbf{a}_i$ for $i = 1, 2$. Considering the vector $\mathbf{b}$ defined in (16) and since $T_b(\mathbf{a}_1) = T(\mathbf{a}_1)$, we have that

$$T_b[T(\mathbf{a}_1)] = T_b(\mathbf{b} + \mathbf{a}_1) = -\mathbf{b} + T_b(\mathbf{a}_1) = \mathbf{a}_1.$$

Since $\det(T_bT) = -1$, it readily follows that $T_b[T(\mathbf{a}_2)] = -\mathbf{a}_2$ and that $T_{a_2}T_b[T(\mathbf{a}_2)] = \mathbf{a}_2$. Therefore, $T = T_bT_{a_2}$. □

As in the square lattice, here also any orthogonal transformation $T \in OC(\Gamma)$ can be decomposed as a product of coincidence reflections by vectors of the lattice Γ, as follows from the following.

Proposition 9. Let $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$ be a lattice in $\mathbb{R}^2$, where $\mathbf{a}_1$ and $\mathbf{a}_2$ are orthogonal vectors. If $T : \mathbb{R}^2 \to \mathbb{R}^2$, is a nontrivial coincidence transformation, *i.e.* $T \in OC(\Gamma)$, then there exists $\mathbf{c} \in \Gamma$ such that

$$T(\mathbf{x}) = \begin{cases} T_c(\mathbf{x}) = -\mathbf{cxc}^{-1} & \text{if } \det(T) = -1, \\ T_c T_{a_2}(\mathbf{x}) = \mathbf{ca}_2\mathbf{xa}_2^{-1}\mathbf{c}^{-1} & \text{if } \det(T) = 1. \end{cases}$$

Proof. Consider $\det(T) = -1$. Then T is a reflection and, by Proposition 8, there exists $\mathbf{b} \in \mathbb{R}^2$ such that $T(\mathbf{x}) = T_b(\mathbf{x}) = -\mathbf{bxb}^{-1}$. Since $T \in OC(\Gamma)$, $T(\mathbf{a}_1)$ has rational components with respect to the basis $\{\mathbf{a}_1, \mathbf{a}_2\}$ and, consequently, $\mathbf{b}$ also has rational components. Thus, we can find $\lambda \in \mathbb{Z}$ such that $\lambda\mathbf{b} \in \Gamma$. By defining $\mathbf{c} = \lambda\mathbf{b}$ and using (9), we have $T(\mathbf{x}) = -\mathbf{cxc}^{-1}$.

Now assume $\det(T) = 1$. In this case, T is a rotation through an angle θ and, by Proposition 8, there exists $\mathbf{b} \in \mathbb{R}^2$ such that $T(\mathbf{x}) = \mathbf{ba}_2\mathbf{xa}_2^{-1}\mathbf{b}^{-1}$. By the above arguments, we can find $\lambda \in \mathbb{Z}$ such that $\lambda\mathbf{b} \in \Gamma$. By defining $\mathbf{c} = \lambda\mathbf{b}$, we have $T(\mathbf{x}) = \mathbf{ca}_2\mathbf{xa}_2^{-1}\mathbf{c}^{-1}$. □

Notice that, contrary to the case of the square lattice, given a vector $\mathbf{c} \in \Gamma$, the reflection $T_c(\mathbf{x}) = \mathbf{cxc}^{-1}$ is not necessarily a coincidence reflection, that is, it may occur that $T_c \notin OC(\Gamma)$. In §5.2, we provide conditions under which a reflection T_c is a coincidence reflection.

As in the case of square lattices, we can consider that in Proposition 9 the components of the vector $\mathbf{c}$, with respect to the basis $\{\mathbf{a}_1, \mathbf{a}_2\}$, are relatively prime [see equation (10)]. Also, since $T_{a_2}(\Gamma) = \Gamma$, we have that

$$\Gamma \cap (T_c T_{a_2})(\Gamma) = \Gamma \cap T_c(\Gamma), \quad \mathbf{c} \in \Gamma,$$

and, consequently, every vector $\mathbf{c} \in \Gamma$ defines the following two orthogonal transformations:

$$T_c(\mathbf{x}) = -\mathbf{cxc}^{-1},$$
$$T_c T_{a_2}(\mathbf{x}) = R_c(\mathbf{x}) = \mathbf{ca}_2\mathbf{xa}_2\mathbf{c}^{-1}.$$

In particular, if $T_c(\mathbf{x}) \in OC(\Gamma)$, then

$$\Gamma \cap T_c(\Gamma) = \Gamma \cap R_c(\Gamma),$$
$$\Sigma(T_c) = \Sigma(R_c)$$

and a basis of $\Gamma \cap R_c(\Gamma)$ can be obtained if the basis of $\Gamma \cap T_c(\Gamma)$ is known.

5.1. Coincidence index and basis of the CSL

Let $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$ be a lattice in $\mathbb{R}^2$, where $\mathbf{a}_1 \cdot \mathbf{a}_2 = 0$. From the previous results, we know that there exists $\mathbf{c} = \alpha_1\mathbf{a}_1 + \alpha_2\mathbf{a}_2 \in \Gamma$, where $\text{g.c.d.}(\alpha_1, \alpha_2) = 1$, such that $T_c \in OC(\Gamma)$. Given that α_1 and α_2 are relatively prime, there exist integers β_1 and β_2 such that

$$\alpha_1\beta_1 + \alpha_2\beta_2 = 1.$$

It guarantees the existence of a vector $\mathbf{d} \in \Gamma$ such that

$$\Gamma = \mathbb{Z}\mathbf{c} \oplus \mathbb{Z}\mathbf{d}. \tag{17}$$

To see this, define

$$\mathbf{d} = \beta_2\mathbf{a}_1 - \beta_1\mathbf{a}_2,$$

and the previous statement follows from

$$\begin{aligned} \mathbf{c} \wedge \mathbf{d} &= (\alpha_1\mathbf{a}_1 + \alpha_2\mathbf{a}_2) \wedge (\beta_2\mathbf{a}_1 - \beta_1\mathbf{a}_2) \\ &= (\alpha_1\beta_1 + \alpha_2\beta_2)\mathbf{a}_1 \wedge \mathbf{a}_2 \\ &= \mathbf{a}_1 \wedge \mathbf{a}_2. \end{aligned} \tag{18}$$

Now, since $T_c(\mathbf{c}) = -\mathbf{c}$, then

$$T_c(\mathbf{c}) \in \Gamma \cap T_c(\Gamma).$$

By considering the least natural number m such that

$$mT_c(\mathbf{d}) \in \Gamma \cap T_c(\Gamma),$$

we claim that $\{\mathbf{c}, mT_c(\mathbf{d})\}$ is a basis of $\Gamma \cap T_c(\Gamma)$.

It can be proved by noticing that, if $\mathbf{y} \in \Gamma \cap T_c(\Gamma)$, then there exists $\mathbf{x} \in \Gamma$ such that $\mathbf{y} = T_c(\mathbf{x})$. From (17), we have

$$\mathbf{y} = T_c(\alpha\mathbf{c} + \beta\mathbf{d}) = \alpha T_c(\mathbf{c}) + \beta T_c(\mathbf{d}) = -\alpha\mathbf{c} + \beta T_c(\mathbf{d}),$$

which leads to $\mathbf{y} + \alpha\mathbf{c} = \beta T_c(\mathbf{d})$. Since m is the least natural number such that $mT_c(\mathbf{d}) \in \Gamma \cap T_c(\Gamma)$, then

$$\beta = km, \quad k \in \mathbb{Z},$$

which proves our claim.

The importance of the number m becomes evident if we evaluate the quantity $\mathbf{c} \wedge mT_c(\mathbf{d}) = -m(\mathbf{c} \wedge \mathbf{cdc}^{-1})$. By using (4) and (18), we have

$$\begin{aligned} -m(\mathbf{c} \wedge \mathbf{cdc}^{-1}) &= -\frac{m}{2}(\mathbf{ccdc}^{-1} - \mathbf{cdc}^{-1}\mathbf{c}) \\ &= -\frac{m}{2}(\mathbf{dc} - \mathbf{cd}) \\ &= m(\mathbf{c} \wedge \mathbf{d}) \\ &= m(\mathbf{a}_1 \wedge \mathbf{a}_2). \end{aligned}$$

With this result, the coincidence index $\Sigma(T_c)$ turns out to be

$$\Sigma(T_c) = \frac{|\mathbf{c} \wedge mT_c(\mathbf{d})|}{|\mathbf{a}_1 \wedge \mathbf{a}_2|} = \frac{m|\mathbf{a}_1 \wedge \mathbf{a}_2|}{|\mathbf{a}_1 \wedge \mathbf{a}_2|} = m.$$

The value of m is obtained by noticing that the components of the vector $T_c(\mathbf{d})$, with respect to the basis $\{\mathbf{a}_1, \mathbf{a}_2\}$, are rational numbers. Let us assume that

$$T_c(\mathbf{d}) = \frac{p_1}{q_1}\mathbf{a}_1 + \frac{p_2}{q_2}\mathbf{a}_2,$$

then

$$\Sigma(T_c) = m = \text{l.c.m.}(q_1, q_2),$$

where l.c.m. stands for the least common multiple function.

5.2. Characterization of $OC(\Gamma)$

We mentioned above that, in the case under study, it may occur that, given a vector $\mathbf{c} \in \Gamma$, $T_c \notin OC(\Gamma)$. Here we provide conditions under which a reflection T_c is a coincidence reflection.

As a general result, first notice that, for any non-zero vectors $\mathbf{x}$ and $\mathbf{v}$, we have that

$$-\mathbf{vxv}^{-1} = -2\frac{\mathbf{x} \cdot \mathbf{v}}{\mathbf{v}^2}\mathbf{v} + \mathbf{x},$$

which readily follows from

$$\begin{aligned}\mathbf{vxv} &= \mathbf{v}(\mathbf{x}\cdot\mathbf{v}+\mathbf{x}\wedge\mathbf{v})\\ &= (\mathbf{x}\cdot\mathbf{v})\mathbf{v}+\mathbf{v}(\mathbf{x}\wedge\mathbf{v})\\ &= (\mathbf{x}\cdot\mathbf{v})\mathbf{v}+\tfrac{1}{2}\mathbf{v}(\mathbf{xv}-\mathbf{vx})\\ &= (\mathbf{x}\cdot\mathbf{v})\mathbf{v}+\tfrac{1}{2}\mathbf{vxv}-\tfrac{1}{2}\mathbf{v}^2\mathbf{x}.\end{aligned}$$

Now let $\Gamma=\mathbb{Z}\mathbf{a}_1\oplus\mathbb{Z}\mathbf{a}_2$ be a lattice in $\mathbb{R}^2$ (not necessarily rectangular). If $\mathbf{c}\in\Gamma$, then $T_c(\mathbf{x})=-\mathbf{cxc}^{-1}\in OC(\Gamma)$ provided that there exist $m_i\in\mathbb{Z}$ such that $m_iT_c(\mathbf{a}_i)=m_i(-\mathbf{ca}_i\mathbf{c}^{-1})\in\Gamma$, for each $i=1,2$. That is,

$$m_i(-\mathbf{ca}_i\mathbf{c}^{-1})=-m_i\frac{2(\mathbf{c}\cdot\mathbf{a}_i)}{\mathbf{c}^2}\mathbf{c}+m_i\mathbf{a}_i\in\Gamma,\quad i=1,2.$$

It is then enough that $-m_i[2(\mathbf{c}\cdot\mathbf{a}_i)/\mathbf{c}^2]\mathbf{c}\in\Gamma$ or, equivalently,

$$\frac{(\mathbf{c}\cdot\mathbf{a}_i)}{\mathbf{c}^2}\in\mathbb{Q},\quad i=1,2. \tag{19}$$

Consider the rectangular lattice $\Gamma=\mathbb{Z}\mathbf{a}_1\oplus\mathbb{Z}\mathbf{a}_2$, $\mathbf{a}_1\cdot\mathbf{a}_2=0$. Without loss of generality, suppose that $\mathbf{a}_1^2=1$ and $\mathbf{a}_2^2=\lambda$. If $\mathbf{c}=\alpha_1\mathbf{a}_1+\alpha_2\mathbf{a}_2\in\Gamma$, where g.c.d.$(\alpha_1,\alpha_2)=1$, then

$$\begin{aligned}\mathbf{c}\cdot\mathbf{a}_1&=\alpha_1\\ \mathbf{c}\cdot\mathbf{a}_2&=\lambda\alpha_2\\ \mathbf{c}^2&=\alpha_1^2+\lambda\alpha_2^2.\end{aligned}$$

Consequently, $T_c\in OC(\Gamma)$ provided that $\lambda\in\mathbb{Q}$.

Now suppose $\lambda\notin\mathbb{Q}$. It follows that

$$\frac{\alpha_1}{\alpha_1^2+\lambda\alpha_2^2}=\frac{p}{q},\quad \frac{\lambda\alpha_2}{\alpha_1^2+\lambda\alpha_2^2}=\frac{r}{s},$$

where $p,q,r,s\in\mathbb{Z}$ and g.c.d.$(p,q)=$ g.c.d.$(r,s)=1$. From the above expressions, we obtain

$$p\alpha_2^2\lambda=\alpha_1(q-\alpha_1p),\quad \alpha_2\lambda(s-\alpha_2r)=r\alpha_1^2.$$

Since $\lambda\notin\mathbb{Q}$, then necessarily $\alpha_1=0$ or $\alpha_2=0$, that is, $\mathbf{c}=\mathbf{a}$ or $\mathbf{c}=\mathbf{b}$. Consequently, if $\lambda=\mathbf{a}_2^2\notin\mathbb{Q}$, then $OC(\Gamma)=\{I,T_{a_1},T_{a_2},T_{a_2}T_{a_1}\}$.

The above results can be summarized in the following theorem, which characterizes $OC(\Gamma)$ by providing a way to generate it from vectors of Γ:

Theorem 2. Let $\Gamma=\mathbb{Z}\mathbf{a}_1\oplus\mathbb{Z}\mathbf{a}_2$ be a lattice in $\mathbb{R}^2$, where $\mathbf{a}_1\cdot\mathbf{a}_2=0$ and $\mathbf{a}_1^2=1$. Let $\mathbf{c}=\alpha_1\mathbf{a}_1+\alpha_2\mathbf{a}_2$ be a vector in Γ, where g.c.d.$(\alpha_1,\alpha_2)=1$, and $T_c(\mathbf{x})=-\mathbf{cxc}^{-1}$ be a reflection by the vector $\mathbf{c}$. We have the following possibilities.

1. If $\mathbf{a}_2^2\in\mathbb{Q}$ then $T_c\in OC(\Gamma)$.
2. If $\mathbf{a}_2^2\notin\mathbb{Q}$ then $OC(\Gamma)=\{I,T_{a_1},T_{a_2},T_{a_2}T_{a_1}\}$.

5.3. Example

Let Γ be a rectangular lattice spanned by the vectors $\mathbf{a}_1=\frac{3}{5}\mathbf{e}_1+\frac{4}{5}\mathbf{e}_2$ and $\mathbf{a}_2=-\frac{8}{15}\mathbf{e}_1+\frac{2}{5}\mathbf{e}_2$. Now consider the orthogonal transformation T with matrix representation, with respect to the canonical basis, given by

$$T=\begin{pmatrix}-\frac{7}{25} & -\frac{24}{25}\\ \frac{24}{25} & -\frac{7}{25}\end{pmatrix},$$

which corresponds to a rotation through an angle $\theta=106.2602^\circ$, that belongs to $OC(\Gamma)$. The vector $\mathbf{b}$, defined in (16), is $\mathbf{b}=T(\mathbf{a}_1)-\mathbf{a}_1=-\frac{32}{25}\mathbf{a}_1+\frac{36}{25}\mathbf{a}_2$. Thus, $\mathbf{c}$, defined in Proposition 9, can be

$$\mathbf{c}=\tfrac{25}{4}[T(\mathbf{a}_1)-\mathbf{a}_1]=-8\mathbf{a}_1+9\mathbf{a}_2,$$

which belongs to Γ. We now follow the procedure described in §5.1 to obtain the coincidence index and a basis of the CSL. Since $-8(1)+9(1)=1$, we define $\mathbf{d}=\mathbf{a}_1-\mathbf{a}_2$ to get

$$\Gamma=\mathbb{Z}\mathbf{c}\oplus\mathbb{Z}\mathbf{d},\quad T(\mathbf{x})=\mathbf{ca}_2\mathbf{xa}_2\mathbf{c}^{-1}.$$

Then after some calculation we have that

$$T_c(\mathbf{d})=-\mathbf{cdc}^{-1}=\tfrac{23}{25}\mathbf{a}_1-\tfrac{29}{25}\mathbf{a}_2,$$

and the least natural number m such that $mT_c(\mathbf{d})\in\Gamma\cap T_c(\Gamma)$ is $m=25$. With this result, we obtain the coincidence index $\Sigma(T_c)=m=25$ and a basis of the CSL, $\Gamma\cap T(\Gamma)$:

$$\{\mathbf{c},25T_c(\mathbf{d})\}=\{-8\mathbf{a}_1+9\mathbf{a}_2,23\mathbf{a}_1-29\mathbf{a}_2\}.$$

6. The rhombic lattice

Let Γ be a rhombic lattice in $\mathbb{R}^2$, *i.e.* $\Gamma=\mathbb{Z}\mathbf{a}_1\oplus\mathbb{Z}\mathbf{a}_2$, where $\mathbf{a}_1$ and $\mathbf{a}_2$ are two linearly independent vectors such that $\mathbf{a}_1^2=\mathbf{a}_2^2$. In this section, we study and characterize the group $OC(\Gamma)$.

First, notice that Proposition 7 is valid for arbitrary lattices in $\mathbb{R}^2$, so it remains to show that an arbitrary orthogonal transformation T can be decomposed into a product of reflections by using the basis vectors of a rhombic lattice.

Proposition 10. Let $T:\mathbb{R}^2\to\mathbb{R}^2$ be a nontrivial orthogonal transformation. If $\mathbf{a}_1$ and $\mathbf{a}_2$ are linearly independent vectors such that $\mathbf{a}_1^2=\mathbf{a}_2^2$, then there exists $\mathbf{b}\in\mathbb{R}^2$ such that

$$T(\mathbf{x})=\begin{cases}T_b(\mathbf{x})=-\mathbf{bxb}^{-1} & \text{if } \det(T)=-1,\\ T_bT_{a_1-a_2}(\mathbf{x})=\mathbf{b}(\mathbf{a}_1-\mathbf{a}_2)\mathbf{x}(\mathbf{a}_1-\mathbf{a}_2)^{-1}\mathbf{b}^{-1} & \text{if } \det(T)=1.\end{cases}$$

Proof. Let us first prove that $\mathbf{a}_1-\mathbf{a}_2$ and $\mathbf{a}_1+\mathbf{a}_2$ are orthogonal:

$$\begin{aligned}2(\mathbf{a}_1-\mathbf{a}_2)\cdot(\mathbf{a}_1+\mathbf{a}_2)&=(\mathbf{a}_1-\mathbf{a}_2)(\mathbf{a}_1+\mathbf{a}_2)\\ &\quad+(\mathbf{a}_2+\mathbf{a}_1)(\mathbf{a}_1-\mathbf{a}_2)\\ &=(\mathbf{a}_1^2-\mathbf{a}_2\mathbf{a}_1+\mathbf{a}_1\mathbf{a}_2-\mathbf{a}_2^2)\\ &\quad+(\mathbf{a}_2\mathbf{a}_1+\mathbf{a}_1^2-\mathbf{a}_1\mathbf{a}_2-\mathbf{a}_2^2)\\ &=0.\end{aligned}$$

Therefore, $\{\mathbf{a}_1+\mathbf{a}_2,\mathbf{a}_1-\mathbf{a}_2\}$ is an orthogonal basis of $\mathbb{R}^2$. Let us define

$$\begin{aligned}\mathbf{d}_1&=\mathbf{a}_1+\mathbf{a}_2,\\ \mathbf{d}_2&=\mathbf{a}_1-\mathbf{a}_2.\end{aligned} \tag{20}$$

Assume $T:\mathbb{R}^2\to\mathbb{R}^2$, different from the identity, and $\det(T)=-1$. In this case, T is a reflection by a line, say l. Since

T is different from the identity and $\{\mathbf{d}_1, \mathbf{d}_2\}$ is an orthogonal basis of $\mathbb{R}^2$, then $T(\mathbf{d}_i) \neq \mathbf{d}_i$ for some $i = 1, 2$. Now consider the vector

$$\mathbf{b} = T(\mathbf{d}_1) - \mathbf{d}_1, \tag{21}$$

which is orthogonal to the reflection line l and can be used to write the reflection as in Lemma 1: $T(\mathbf{x}) = T_b(\mathbf{x}) = -\mathbf{bxb}^{-1}$.

Now assume $\det(T) = 1$. In this case, T is a rotation through an angle θ and also $T(\mathbf{d}_i) \neq \mathbf{d}_i$ for some $i = 1, 2$. By considering the vector $\mathbf{b}$ defined in (21), we have that

$$T_b[T(\mathbf{d}_1)] = T_b(\mathbf{b} + \mathbf{d}_1) = -\mathbf{b} + T(\mathbf{d}_1) = \mathbf{d}_1.$$

Since $\det(T_bT) = -1$, it readily follows that $T_b[T(\mathbf{d}_2)] = -\mathbf{d}_2$ and that $T_{d_2}T_b[T(\mathbf{d}_2)] = \mathbf{d}_2$. Therefore, $T = T_bT_{d_2}$. □

Now we will see that any orthogonal transformation $T \in OC(\Gamma)$ can be decomposed as a product of coincidence reflections in vectors of the lattice Γ.

Proposition 11. Let $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$ be a lattice in $\mathbb{R}^2$, where $\mathbf{a}_1^2 = \mathbf{a}_2^2$. If $T : \mathbb{R}^2 \to \mathbb{R}^2$ is a nontrivial coincidence transformation, *i.e.* $T \in OC(\Gamma)$, then there exists $\mathbf{c} \in \Gamma$ such that

$$T(\mathbf{x}) = \begin{cases} T_c(\mathbf{x}) = -\mathbf{cxc}^{-1} & \text{if } \det(T) = -1, \\ T_cT_{d_2}(\mathbf{x}) = -\mathbf{cd}_2\mathbf{xd}_2^{-1}\mathbf{c}^{-1} & \text{if } \det(T) = 1, \end{cases}$$

where $\mathbf{d}_2 = \mathbf{a}_1 - \mathbf{a}_2$.

Proof. Consider $\det(T) = -1$. Then T is a reflection and, by Proposition 10, there exists $\mathbf{b} \in \mathbb{R}^2$ such that $T(\mathbf{x}) = T_b(\mathbf{x}) = -\mathbf{bxb}^{-1}$. Since $T \in OC(\Gamma)$, $T(\mathbf{d}_1)$ has rational components with respect to the basis $\{\mathbf{d}_1, \mathbf{d}_2\}$ and, consequently, $\mathbf{b}$ also has rational components. Thus, we can find $\lambda \in \mathbb{Z}$ such that $\lambda\mathbf{b} \in \Gamma$. By defining $\mathbf{c} = \lambda\mathbf{b}$, and using (9), we have $T(\mathbf{x}) = -\mathbf{cxc}^{-1}$.

Now assume $\det(T) = 1$. In this case, T is a rotation through an angle θ and, by Proposition 10, there exists $\mathbf{b} \in \mathbb{R}^2$ such that $T(\mathbf{x}) = \mathbf{bd}_2\mathbf{xd}_2^{-1}\mathbf{b}^{-1}$. By the above arguments, we can find $\lambda \in \mathbb{Z}$ such that $\lambda\mathbf{b} \in \Gamma$. By defining $\mathbf{c} = \lambda\mathbf{b}$, we have $T(\mathbf{x}) = \mathbf{cd}_2\mathbf{xd}_2^{-1}\mathbf{c}^{-1}$. □

As in the case of the rectangular lattice, given a vector $\mathbf{c} \in \Gamma$, it may occur that $T_c \notin OC(\Gamma)$. In §6.2, we provide conditions under which a reflection T_c is a coincidence reflection.

By following the same ideas applied to the case of the rectangular lattice, we have that every vector $\mathbf{c} \in \Gamma$ defines the following two orthogonal transformations:

$$T_c(\mathbf{x}) = -\mathbf{cxc}^{-1},$$
$$T_cT_{d_2}(\mathbf{x}) = R_c(\mathbf{x}) = \mathbf{cd}_2\mathbf{xd}_2\mathbf{c}^{-1}.$$

In particular, if $T_c(x) \in OC(\Gamma)$, since $T_{d_2}(\Gamma) = \Gamma$, then

$$\Gamma \cap T_c(\Gamma) = \Gamma \cap R_c(\Gamma), \quad \Sigma(T_c) = \Sigma(R_c),$$

and a basis of $\Gamma \cap R_c(\Gamma)$ can be obtained if the basis of $\Gamma \cap T_c(\Gamma)$ is known.

6.1. Coincidence index and basis of the CSL

The procedure to determine the coincidence index $\Sigma(T_c)$ and a basis of the CSL, $\Gamma \cap T_c(\Gamma)$, follows the same lines as in the case of the rectangular lattice. For that reason, here we only summarize the results without further details.

Let $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$ be a lattice in $\mathbb{R}^2$, such that $\mathbf{a}_1^2 = \mathbf{a}_2^2$. From the previous results, we know that there exists $\mathbf{c} = \alpha_1\mathbf{a}_1 + \alpha_2\mathbf{a}_2 \in \Gamma$, where $\text{g.c.d.}(\alpha_1, \alpha_2) = 1$, such that $T_c \in OC(\Gamma)$. Given that α_1 and α_2 are relatively prime, there exist integers β_1 and β_2 such that

$$\alpha_1\beta_1 + \alpha_2\beta_2 = 1.$$

It guarantees the existence of a vector $\mathbf{d} \in \Gamma$ such that

$$\Gamma = \mathbb{Z}\mathbf{c} \oplus \mathbb{Z}\mathbf{d},$$

where

$$\mathbf{d} = \beta_2\mathbf{a}_1 - \beta_1\mathbf{a}_2.$$

A basis of $\Gamma \cap T_c(\Gamma)$ is $\{\mathbf{c}, mT_c(\mathbf{d})\}$, where m is the least natural number such that

$$mT_c(\mathbf{d}) \in \Gamma \cap T_c(\Gamma).$$

The natural number m is also the coincidence index $\Sigma(T_c)$, and its value can be obtained by assuming that

$$T_c(\mathbf{d}) = \frac{p_1}{q_1}\mathbf{a}_1 + \frac{p_2}{q_2}\mathbf{a}_2,$$

then

$$\Sigma(T_c) = m = \text{l.c.m.}(q_1, q_2).$$

6.2. Characterization of $OC(\Gamma)$

In this section, the conditions under which a reflection T_c is a coincidence reflection are deduced. We start from the condition (19), which is valid for arbitrary lattices.

Let $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$, $\mathbf{a}_1^2 = \mathbf{a}_2^2$, be a rhombic lattice. If $\mathbf{c} \in \Gamma$, our purpose is to find conditions under which $T_c(\mathbf{x}) = -\mathbf{cxc}^{-1} \in \Gamma$. Without loss of generality, suppose that $\mathbf{a}_1^2 = \mathbf{a}_2^2 = 1$. If $\mathbf{c} = \alpha_1\mathbf{a}_1 + \alpha_2\mathbf{a}_2 \in \Gamma$, where $\text{g.c.d.}(\alpha_1, \alpha_2) = 1$, then from (19) we have

$$\begin{aligned} \mathbf{c} \cdot \mathbf{a}_1 &= \alpha_1 + \alpha_2\mathbf{a}_1 \cdot \mathbf{a}_2, \\ \mathbf{c} \cdot \mathbf{a}_2 &= \alpha_2 + \alpha_1\mathbf{a}_1 \cdot \mathbf{a}_2, \\ \mathbf{c}^2 &= \alpha_1^2 + \alpha_2^2 + 2\alpha_1\alpha_2\mathbf{a}_1 \cdot \mathbf{a}_2. \end{aligned}$$

Consequently, $T_c \in OC(\Gamma)$ provided that $\mathbf{a}_1 \cdot \mathbf{a}_2 \in \mathbb{Q}$.

Now suppose that $\mathbf{a}_1 \cdot \mathbf{a}_2 \notin \mathbb{Q}$. It follows that

$$\frac{\alpha_1 + \alpha_2\mathbf{a}_1 \cdot \mathbf{a}_2}{\alpha_1^2 + \alpha_2^2 + 2\alpha_1\alpha_2\mathbf{a}_1 \cdot \mathbf{a}_2} = \frac{p}{q},$$
$$\frac{\alpha_2 + \alpha_1\mathbf{a}_1 \cdot \mathbf{a}_2}{\alpha_1^2 + \alpha_2^2 + 2\alpha_1\alpha_2\mathbf{a}_1 \cdot \mathbf{a}_2} = \frac{r}{s},$$

where $p, q, r, s \in \mathbb{Z}$ and $\text{g.c.d.}(p, q) = \text{g.c.d.}(r, s) = 1$. From the above expressions, we obtain:

$$\alpha_2(q - 2\alpha_1 p)\mathbf{a}_1 \cdot \mathbf{a}_2 = p(\alpha_1^2 + \alpha_2^2) - q\alpha_1,$$
$$\alpha_1(s - 2\alpha_2 r)\mathbf{a}_1 \cdot \mathbf{a}_2 = r(\alpha_1^2 + \alpha_2^2) - s\alpha_2.$$

Since $\mathbf{a}_1 \cdot \mathbf{a}_2 \notin \mathbb{Q}$, then necessarily the coefficients of $\mathbf{a}_1 \cdot \mathbf{a}_2$ must vanish, that is

$$\begin{aligned} \alpha_2(q - 2\alpha_1 p) &= 0, \\ \alpha_1(s - 2\alpha_2 r) &= 0, \\ p(\alpha_1^2 + \alpha_2^2) - q\alpha_1 &= 0, \\ r(\alpha_1^2 + \alpha_2^2) - s\alpha_2 &= 0, \end{aligned} \tag{22}$$

for some $\alpha_i \neq 0$, $i = 1, 2$.

Suppose that $\alpha_1 \neq 0$. In this case, the following equation must be fulfilled:

$$\frac{r}{s} = \frac{1}{2\alpha_2},$$

thus $r = 1$, $s = 2\alpha_2$ and (22) becomes

$$\begin{aligned} r(\alpha_1^2 + \alpha_2^2) - s\alpha_2 &= 0, \\ (\alpha_1^2 + \alpha_2^2) - 2\alpha_2^2 &= 0, \\ \alpha_1^2 - \alpha_2^2 &= 0, \\ (\alpha_1 + \alpha_2)(\alpha_1 - \alpha_2) &= 0. \end{aligned}$$

These equations lead to $\mathbf{c} = \mathbf{a}_1 + \mathbf{a}_2$ or $\mathbf{c} = \mathbf{a}_1 - \mathbf{a}_2$. The same conclusion is obtained if $\alpha_2 \neq 0$. Consequently, if $\mathbf{a}_1 \cdot \mathbf{a}_2 \notin \mathbb{Q}$, then $OC(\Gamma) = \{I, T_{d_1}, T_{d_2}, T_{d_2}T_{d_1}\}$, where $\mathbf{d}_1$ and $\mathbf{d}_2$ are given by (20).

The above results can be summarized in the following theorem, which characterizes $OC(\Gamma)$ by providing a way to generate it from vectors of Γ:

Theorem 3. Let $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$ be a lattice in $\mathbb{R}^2$, where $\mathbf{a}_1^2 = \mathbf{a}_2^2$. Let $\mathbf{c} = \alpha_1\mathbf{a}_1 + \alpha_2\mathbf{a}_2$ be a vector in Γ, where g.c.d.$(\alpha_1, \alpha_2) = 1$ and $T_c(\mathbf{x}) = -\mathbf{cxc}^{-1}$ is a reflection by the vector $\mathbf{c}$. We have the following possibilities.

1. If $\mathbf{a}_1 \cdot \mathbf{a}_2 \in \mathbb{Q}$, then $T_c \in OC(\Gamma)$.
2. If $\mathbf{a}_1 \cdot \mathbf{a}_2 \notin \mathbb{Q}$, then $OC(\Gamma) = \{I, T_{d_1}, T_{d_2}, T_{d_2}T_{d_1}\}$, where $\mathbf{d}_1 = \mathbf{a}_1 + \mathbf{a}_2$ and $\mathbf{d}_2 = \mathbf{a}_1 - \mathbf{a}_2$.

6.3. Example

Consider the hexagonal lattice $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$, where $\mathbf{a}_1 = (1, 0)$ and $\mathbf{a}_2 = (1/2, \sqrt{3}/2)$. The diagonals (20) are then given by $\mathbf{d}_1 = (3/2, \sqrt{3}/2)$ and $\mathbf{d}_2 = (1/2, -\sqrt{3}/2)$.

Now let $T : \mathbb{R}^2 \to \mathbb{R}^2$ be an orthogonal transformation with matrix representation, with respect to the canonical basis, given by

$$\begin{pmatrix} -\frac{13}{14} & -\frac{3\sqrt{3}}{14} \\ \frac{3\sqrt{3}}{14} & -\frac{13}{14} \end{pmatrix}.$$

With respect to the basis $\{\mathbf{a}_1, \mathbf{a}_2\}$, the matrix is

$$\begin{pmatrix} -\frac{8}{7} & -\frac{3}{7} \\ \frac{3}{7} & -\frac{5}{7} \end{pmatrix}.$$

Therefore, (21) yields $\mathbf{b} = T(\mathbf{d}_1) - \mathbf{d}_1 = -(45/14)\mathbf{e}_1 - (9\sqrt{3}/14)\mathbf{e}_2 = -(18/7)\mathbf{a}_1 - (9/7)\mathbf{a}_2$ and the vector $\mathbf{c}$ $(= \lambda\mathbf{b})$ can be

$$\mathbf{c} = 2\mathbf{a}_1 + \mathbf{a}_2.$$

Since the determinant of the matrix representation is 1, the transformation is a rotation given by $T(\mathbf{x}) = T_c T_{d_2}(\mathbf{x})$.

Now, since $\alpha_1 = 2$ and $\alpha_2 = 1$ then Γ is spanned by $\{\mathbf{c}, \mathbf{d}\}$, where $\mathbf{d} = \mathbf{a}_1 + \mathbf{a}_2$. As described at the end of §6.1, a basis of $\Gamma \cap T_a(\Gamma)$ is $\{\mathbf{c}, mT_c(\mathbf{d})\}$ and the value of m is obtained from $T_c(\mathbf{d}) = -\mathbf{cdc}^{-1}$. By substituting the values of $\mathbf{c}$ and $\mathbf{d}$, after some calculation we get

$$T_c(\mathbf{d}) = -\tfrac{11}{7}\mathbf{a}_1 - \tfrac{2}{7}\mathbf{a}_2.$$

Thus, $m = \Sigma(T) = 7$ and a basis of the coincidence lattice is $\{2\mathbf{a}_1 + \mathbf{a}_2, -11\mathbf{a}_1 - 2\mathbf{a}_2\}$.

7. Conclusions

In this work, we solve the coincidence problem for planar lattices by using Clifford algebra. It allows us to algebraically characterize the group of coincidence isometries in terms of the lattice vectors (objects on which the group operates), and to provide explicit expressions for both the coincidence index and the basis of the coincidence lattices.

Clifford algebra has proved to be a useful language in many areas of physics, engineering and computer science and we hope that its power for expressing geometric ideas, used here to solve the coincidence problem in planar lattices, would motivate its use in other fields of geometric crystallography. The present approach can be extended to higher dimensions and this work is under way.

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