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### Coincidence lattices in the hyperbolic plane

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The problem of coincidences of lattices in the space  $\mathbb{R}^{p,q}$ , with p + q = 2, is analyzed using Clifford algebra. We show that, as in  $\mathbb{R}^n$ , any coincidence isometry can be decomposed as a product of at most two reflections by vectors of the lattice. Bases and coincidence indices are constructed explicitly for several interesting lattices. Our procedure is metric-independent and, in particular, the hyperbolic plane is obtained when p = q = 1. Additionally, we provide a proof of the Cartan–Dieudonné theorem for  $\mathbb{R}^{p,q}$ , with p + q = 2, that includes an algorithm to decompose an orthogonal transformation into a product of reflections.

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### 1. Introduction

Clifford or geometric 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 particular, in crystallography, Hestenes (2007) and Hitzer & Perwass (2005) have presented a geometric algebra approach to symmetry groups and Aragón *et al.* (2001) have used Clifford algebra to study the problem of facetting in quasicrystals.

In crystallography, mostly in the context of grain boundaries, one uses the so-called coincidence site lattice (CSL) theory. There are many useful references in this field, but for the purposes of this work the mathematical formulation by Baake (1997) and Reed et al. (2004) are useful. In a previous communication (Aragón et al., 2006) we showed that the CSL problem requires the use of the Cartan-Dieudonné theorem and we presented a constructive way of producing the isometries whose existence states the Cartan-Dieudonné theorem. In this way we were able to tackle the coincidence problem for lattices in Euclidean spaces  $\mathbb{R}^n$ , providing explicit expressions for bases and coincidence indices in planar lattices (Rodríguez et al., 2005). In our Clifford algebra approach to this problem, reflections are considered primitive isometries and we have found conditions under which a given reflection is a coincidence isometry. This proposal has proved to be useful as an approach to the general, n-dimensional case (Zou, 2006*a*,*b*).

The purpose of this communication is to extend the results of Rodríguez *et al.* (2005) to lattices in spaces  $\mathbb{R}^{p,q}$ , restricting our attention mostly to the case p + q = 2. In particular:

(a) a proof of the Cartan–Dieudonné theorem for  $\mathbb{R}^{p,q}$ (p+q=2) is given that includes an algorithm for the construction of the reflections that decompose a given orthogonal transformation (Proposition 1);

(b) the theory of coincidence lattices is formulated in  $\mathbb{R}^{p,q}$  (§4);

(c) it is shown that, as in  $\mathbb{R}^n$ , for p + q = 2 any coincidence isometry can be decomposed as a product of at most two reflections by hyperplanes defined by vectors of the lattice (Proposition 2); and

(d) the problem of the CSL is solved for some interesting lattices in  $\mathbb{R}^{p,q}$ , where p + q = 2, providing analytic expressions for the coincidence index and the basis of the coincidence lattice (§§5 and 6).

Concerning this last point, we should emphasize that the most interesting case is when p = q = 1, that is, the hyperbolic plane. This metric-independent approach, however, allowed us to solve the general case, including when p = 2 and q = 0,  $\mathbb{R}^2$ , already worked out in Rodríguez *et al.* (2005), and p = 0, q = 2.

In §2 the definition and most relevant properties of Clifford algebras for our purposes are presented. Finally, conclusions are presented in §7.

Our results may enrich the field of the crystallography of the hyperbolic plane, which has been useful for describing, for instance, liquid-crystalline structures (Sadoc & Charvolin, 1989). Furthermore, we believe that Clifford algebras can be the natural language for a generalized crystallography (Mackay, 2002).

### 2. Clifford algebras

Detailed accounts of Clifford algebra can be found in Riesz (1993), Porteous (1995), Chevalley (1954), Artin (1957), Hestenes & Sobczyk (1985), and Lounesto (2001), and they can be presented in various equivalent ways. However, the simplest construction of the Clifford algebra Cl is by means of generators and relations. In what follows let K be a field with char(K)  $\neq 2$ , E a vector space over K and Q a non-singular quadratic form on E over K. Thus, we can state (Ablamowicz *et al.*, 1991):

Definition 1. An associative algebra over K with identity 1 is the Clifford algebra Cl of Q on E if it contains E and  $K = K \cdot 1$ as distinct subspaces so that

- (1)  $\mathbf{x}^2 = Q(\mathbf{x})$  for any vector  $\mathbf{x}$  in E,
- (2) E generates Cl as an algebra over K and
- (3) Cl is not generated by any proper subspace of E.

One of the most significant consequences of this definition is that, for any  $\mathbf{x}, \mathbf{y} \in E$ ,

$$2\mathbf{x} \cdot \mathbf{y} = \mathbf{x}\mathbf{y} + \mathbf{y}\mathbf{x} = Q(\mathbf{x} + \mathbf{y}) - Q(\mathbf{x}) - Q(\mathbf{y}).$$
(1)

In this paper we are concerned mostly with the Clifford algebra with  $K = \mathbb{R}$ ,  $E = \mathbb{R}^{p+q}$  (which we will write simply as  $\mathbb{R}^{p,q}$ ) and Q the quadratic form given by

$$Q(\mathbf{x}) = x_1^2 + x_2^2 + \ldots + x_p^2 - x_{p+1}^2 - \ldots - x_{p+q}^2.$$
 (2)

This Clifford algebra will be denoted as  $\mathbb{R}_{p,q}$ .

In terms of the canonical orthonormal basis of  $\mathbb{R}^{p,q}$ ,  $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_{p+q}\}$  we have

$$\mathbf{e}_{i}^{2} = 1 \text{ for } 1 \leq i \leq p,$$
  

$$\mathbf{e}_{i}^{2} = -1 \text{ for } p < i \leq p + q,$$
  

$$\mathbf{e}_{i}\mathbf{e}_{i} = -\mathbf{e}_{i}\mathbf{e}_{i} \text{ for } i > j,$$
  
(3)

and, as a consequence of the last condition in Definition 1, to guarantee the universal property,

$$\mathbf{e}_1 \mathbf{e}_2 \dots \mathbf{e}_{p+q} \neq \pm 1. \tag{4}$$

Considered as a real vector space, the dimension of  $\mathbb{R}_{p,q}$  is  $2^n$  and a basis of this space consists of the identity 1 and all vector products of the form  $\mathbf{e}_1^{m_1} \dots \mathbf{e}_n^{m_n}$ , where  $m_i = 0$  or 1. The elements of length k, like  $\mathbf{e}_1 \mathbf{e}_2 \dots \mathbf{e}_k$ , are called k-vectors, and linear combinations of k-vectors are called multivectors or Clifford numbers.

The algebra Cl is a graded algebra, the elements of degree zero are the scalars (the elements of the field), the elements of degree one are the vectors in  $\mathbb{R}^n$ , the elements of degree (grade) two are linear combinations of products of two basis vectors *etc.* 

In  $\mathbb{R}_{p,q}$ , the inverse of a multivector can be defined if some conditions are satisfied (Hestenes & Sobczyk, 1985). In particular, any vector  $\mathbf{x} \in \mathbb{R}^2$ ,  $\mathbf{x} \neq 0$ , has the inverse

$$\mathbf{x}^{-1} = \frac{\mathbf{x}}{\mathbf{x}^2}.$$
 (5)

An invertible vector  $\mathbf{x} \in \mathbb{R}^{p,q}$  is called non-isotropic. Also, an orthogonal basis  $\{\mathbf{w}_1, \dots, \mathbf{w}_{p+q}\}$  of  $\mathbb{R}^{p,q}$  is called nonisotropic if each  $\mathbf{w}_i$  is invertible and  $\mathbf{w}_i \cdot \mathbf{w}_j = 0$  for  $i \neq j$  $(i, j = 1, \dots, p + q)$ .

The symmetric part of the geometric product  $\mathbf{x}\mathbf{y}$  is associated with the inner product

$$\mathbf{x} \cdot \mathbf{y} = \frac{\mathbf{x}\mathbf{y} + \mathbf{y}\mathbf{x}}{2},\tag{6}$$

and the antisymmetric part corresponds to the outer (Grassman) product

$$\mathbf{x} \wedge \mathbf{y} = \frac{\mathbf{x}\mathbf{y} - \mathbf{y}\mathbf{x}}{2}.$$
 (7)

Then, the geometric product xy can be written as

$$\mathbf{x}\mathbf{y} = \mathbf{x} \cdot \mathbf{y} + \mathbf{x} \wedge \mathbf{y}. \tag{8}$$

Many properties of the geometric, inner and outer product between general multivectors are reviewed in the textbooks already mentioned. A particularly useful fact is that the outer product of three vectors  $\mathbf{a} \wedge \mathbf{b} \wedge \mathbf{c}$  represents the oriented volume of the parallelepiped with edges  $\mathbf{a}$ ,  $\mathbf{b}$  and  $\mathbf{c}$ . *n*-dimensional oriented volumes are represented by the outer product of *n* vectors.

Finally, we should mention one identity that will be extensively used in the following sections:

$$\mathbf{x} \cdot (\mathbf{y} \wedge \mathbf{z}) = (\mathbf{x} \cdot \mathbf{y})\mathbf{z} - (\mathbf{x} \cdot \mathbf{z})\mathbf{y}$$
(9)

for all  $\mathbf{x}, \mathbf{y}$  and  $\mathbf{z} \in \mathbb{R}^{p,q}$ .

### **3.** Orthogonal transformations of $\mathbb{R}^{p,q}$

The algebraic properties of geometric algebra provide us with a convenient way of representing reflections with respect to hyperplanes of  $\mathbb{R}^{p,q}$ . Suppose  $\mathbf{a} \in \mathbb{R}^{p,q}$  is a non-isotropic vector and let  $H_{\mathbf{a}}$  be its orthogonal complement, *i.e.*,  $H_{\mathbf{a}} = \{\mathbf{x} \in \mathbb{R}^{p,q} \mid \mathbf{a} \cdot \mathbf{x} = 0\}$ . A reflection of  $\mathbf{a}$  with respect to  $H_{\mathbf{a}}$  is an orthogonal transformation  $\varphi_{\mathbf{a}}$  with the following properties:

$$\varphi_{\mathbf{a}}(\mathbf{a}) = -\mathbf{a},$$

$$\varphi_{\mathbf{a}}(\mathbf{w}) = \mathbf{w} \text{ if } \mathbf{w} \in H_{\mathbf{a}}.$$
(10)

This transformation  $\varphi_{\mathbf{a}}$  will be called 'simple reflection by  $\mathbf{a}$ '.

Lemma 1. The transformation  $\varphi_{\mathbf{a}} : \mathbb{R}^{p,q} \to \mathbb{R}^{p,q}$ , with **a** non-isotropic, defined by

$$\varphi_{\mathbf{a}}(\mathbf{x}) = -\mathbf{a}\mathbf{x}\mathbf{a}^{-1},\tag{11}$$

is orthogonal and corresponds to a simple reflection.

*Proof 1*. Since the Clifford algebra is distributive, we can easily see that  $\varphi_a$  is linear. Now, it remains to prove that  $\varphi_a$  has the properties (10). First, notice that

$$\varphi_{\mathbf{a}}(\mathbf{a}) = -\mathbf{a}\mathbf{a}\mathbf{a}^{-1} = -\mathbf{a}.$$
 (12)

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

$$\varphi_{\mathbf{a}}(\mathbf{w}) = -\mathbf{a}\mathbf{w}\mathbf{a}^{-1} = -(-\mathbf{w}\mathbf{a})\mathbf{a}^{-1} = \mathbf{w}, \quad \mathbf{w} \in H_{\mathbf{a}},$$
(13)

and this completes the proof.

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

$$\varphi_{\mathbf{a}}(\mathbf{x}) = -\mathbf{a}\mathbf{x}\mathbf{a}^{-1} = -\mathbf{a}^{-1}\mathbf{x}\mathbf{a} = \varphi_{\mathbf{a}^{-1}}(\mathbf{x}), \quad (14)$$

and also that

$$\varphi_{\mathbf{a}}(\mathbf{x}) = \varphi_{\lambda \mathbf{a}}(\mathbf{x}) \tag{15}$$

for  $\lambda \in \mathbb{R}$ ,  $\lambda \neq 0$ .

A useful formula, which will be used several times, is

$$\varphi_{\mathbf{v}}(\mathbf{x}) = -\mathbf{v}\mathbf{x}\mathbf{v}^{-1} = \mathbf{x} - 2\frac{\mathbf{x}\cdot\mathbf{v}}{\mathbf{v}^2}\mathbf{v},\tag{16}$$

for  $\mathbf{x}, \mathbf{v} \in \mathbb{R}^{p,q}$ ,  $\mathbf{v}$  non-isotropic. Indeed, since

v

$$\mathbf{x}\mathbf{v} = \frac{1}{2}(\mathbf{v}\mathbf{x} + \mathbf{x}\mathbf{v} + (\mathbf{v}\mathbf{x} - \mathbf{x}\mathbf{v}))\mathbf{v},$$
  
=  $\frac{1}{2}(2\mathbf{x}\cdot\mathbf{v} + (\mathbf{v}\mathbf{x} - \mathbf{x}\mathbf{v}))\mathbf{v},$   
=  $(\mathbf{x}\cdot\mathbf{v})\mathbf{v} + \frac{1}{2}\mathbf{v}\mathbf{x}\mathbf{v} - \frac{1}{2}\mathbf{x}\mathbf{v}^2,$  (17)

we have

$$-\mathbf{v}\mathbf{x}\mathbf{v}^{-1} = -(\mathbf{v}\mathbf{x}\mathbf{v})\mathbf{v}^{-1}\mathbf{v}^{-1},$$
  
=  $-((\mathbf{x}\cdot\mathbf{v})\mathbf{v} + \frac{1}{2}\mathbf{v}\mathbf{x}\mathbf{v} - \frac{1}{2}\mathbf{x}\mathbf{v}^2)\mathbf{v}^{-1}\mathbf{v}^{-1},$   
=  $-(\mathbf{x}\cdot\mathbf{v})\mathbf{v}^{-1} - \frac{1}{2}\mathbf{v}\mathbf{x}\mathbf{v}^{-1} + \frac{1}{2}\mathbf{x},$  (18)

from where equation (16) readily follows.

If p + q = 2 we have that given an arbitrary orthogonal transformation T we can always find a non-isotropic vector  $\mathbf{a} \in \mathbb{R}^2$  such that T is either a simple reflection by  $\mathbf{a}$  [equation (11)] or it is a reflection by some other basic vector followed by a reflection by the vector  $\mathbf{a}$ . In other words, the following proposition describes a method to decompose an orthogonal transformation T into a product of reflections.

Proposition 1. Let  $T : \mathbb{R}^{p,q} \to \mathbb{R}^{p,q}$  be an orthogonal transformation and  $\{\mathbf{w}_1, \mathbf{w}_2\}$  a non-isotropic orthogonal basis of  $\mathbb{R}^{p,q}$  (p+q=2). Then, there exists a non-isotropic vector  $\mathbf{a} \in \mathbb{R}^{p,q}$  such that

$$T(\mathbf{x}) = \begin{cases} \varphi_{\mathbf{a}}(\mathbf{x}) & \text{if } \det(T) = -1, \\ \varphi_{\mathbf{a}}\varphi_{\mathbf{w}_{i}}(\mathbf{x}) & \text{if } \det(T) = 1, \end{cases}$$
(19)

where *i* can be chosen as 1 or 2.

*Proof 2.* Throughout this proof, *i* and *j* can be chosen as 1 or 2 and when *i* and *j* appear in the same equation, it is assumed that  $i \neq j$ . If  $T(\mathbf{w}_j) - \mathbf{w}_j$  is non-isotropic, we will see in what follows that it is enough to take  $\mathbf{a} = T(\mathbf{w}_j) - \mathbf{w}_j$ . We start with the following result:

$$\varphi_{\mathbf{a}}(T(\mathbf{w}_i)) = \mathbf{w}_i, \tag{20}$$

which can be verified using equation (11), together with the fact that  $(T(\mathbf{w}_j))^2 = \mathbf{w}_j^2$ , or by the following geometrical argument. Consider the rhombus spanned by the vectors  $\mathbf{w}_j$ 

and  $T(\mathbf{w}_j)$ , *i.e.*, the set  $\{\alpha \mathbf{w}_j + \beta T(\mathbf{w}_j) \mid 0 \le \alpha \le 1, 0 \le \beta \le 1\}$ . The diagonals of the rhombus are  $T(\mathbf{w}_j) + \mathbf{w}_j$  and  $T(\mathbf{w}_j) - \mathbf{w}_j = \mathbf{a}$ , which are perpendicular as can be easily verified. Now,  $\varphi_{\mathbf{a}}$  is a reflection with respect to a vector perpendicular to  $\mathbf{a}$ , which is in fact  $T(\mathbf{w}_j) + \mathbf{w}_j$ . From this, we can see that  $\varphi_{\mathbf{a}}(T(\mathbf{w}_i)) = \mathbf{w}_i$  and, trivially,  $\varphi_{\mathbf{a}}(\mathbf{w}_i) = T(\mathbf{w}_i)$ .

Now, from equation (20) we have that  $\varphi_{\mathbf{a}}(T(\mathbf{w}_i))$  is either  $\mathbf{w}_i$  or  $-\mathbf{w}_i$ , because  $\varphi_{\mathbf{a}}(T(\mathbf{w}_i))$  and  $\mathbf{w}_j$  are orthogonal. If  $\varphi_{\mathbf{a}}(T(\mathbf{w}_i)) = \mathbf{w}_i$ , then, by linearity,

$$\varphi_{\mathbf{a}}T(\mathbf{x}) = I(\mathbf{x}),\tag{21}$$

so

thus

$$T(\mathbf{x}) = \varphi_{\mathbf{a}}(\mathbf{x}) \tag{22}$$

for all  $\mathbf{x} \in \mathbb{R}^{p,q}$ . Now, if  $\varphi_{\mathbf{a}}(T(\mathbf{w}_i)) = -\mathbf{w}_i$ , then

$$\varphi_{\mathbf{w}_i}\varphi_{\mathbf{a}}(T(\mathbf{w}_i)) = \mathbf{w}_i, \tag{23}$$

$$\varphi_{\mathbf{w}_{i}}\varphi_{\mathbf{a}}T(\mathbf{x}) = I(\mathbf{x}),$$

$$T(\mathbf{x}) = \varphi_{\mathbf{a}}\varphi_{\mathbf{w}_{i}}(\mathbf{x}).$$
(24)

But if  $T(\mathbf{w}_j) - \mathbf{w}_j$  is isotropic, then  $\mathbf{v} = T(\mathbf{w}_j) + \mathbf{w}_j$  is non-isotropic (Proposition 4.2 of Porteous, 1995) and

$$\varphi_{\mathbf{w}_{j}}\varphi_{\mathbf{v}}\big(T(\mathbf{w}_{j})\big) = \mathbf{w}_{j},\tag{25}$$

as  $\varphi_{\mathbf{w}_{j}}\varphi_{\mathbf{v}}(T(\mathbf{w}_{j})) = \mathbf{w}_{j}$  and  $\mathbf{w}_{i}$  are orthogonal, then  $\varphi_{\mathbf{w}_{j}}\varphi_{\mathbf{v}}(T(\mathbf{w}_{i}))$ is either  $\mathbf{w}_{i}$  or  $-\mathbf{w}_{i}$ . If  $\varphi_{\mathbf{w}_{i}}\varphi_{\mathbf{v}}(T(\mathbf{w}_{i})) = \mathbf{w}_{i}$ , by linearity

$$\varphi_{\mathbf{w}_i}\varphi_{\mathbf{v}}(T(\mathbf{x})) = I(\mathbf{x}),\tag{26}$$

so

$$T(\mathbf{x}) = \varphi_{\mathbf{v}} \varphi_{\mathbf{w}_i}(\mathbf{x}) \tag{27}$$

for all  $\mathbf{x} \in \mathbb{R}^{p,q}$ . Now, if  $\varphi_{\mathbf{w}_i}\varphi_{\mathbf{v}}(T(\mathbf{w}_i)) = -\mathbf{w}_i$ , then

$$\varphi_{\mathbf{w}_i}\varphi_{\mathbf{w}_i}\varphi_{\mathbf{v}}(T(\mathbf{x})) = I(\mathbf{x}), \tag{28}$$

so

$$T(\mathbf{x}) = \varphi_{\mathbf{v}} \varphi_{\mathbf{w}_i} \varphi_{\mathbf{w}_i}(\mathbf{x}) \tag{29}$$

for all  $\mathbf{x} \in \mathbb{R}^{p,q}$ . But, by associativity and equations (8) and (9), we have

$$\mathbf{v}(\mathbf{w}_{j}\mathbf{w}_{i}) = \mathbf{v}(\mathbf{w}_{j} \cdot \mathbf{w}_{i} + \mathbf{w}_{j} \wedge \mathbf{w}_{i})$$
  
=  $\mathbf{v}(\mathbf{w}_{j} \wedge \mathbf{w}_{i})$   
=  $\mathbf{v} \cdot (\mathbf{w}_{i} \wedge \mathbf{w}_{i}) + \mathbf{v} \wedge (\mathbf{w}_{i} \wedge \mathbf{w}_{i})$  (30)

and  $\mathbf{v} \wedge (\mathbf{w}_i \wedge \mathbf{w}_i) = 0$ , since p + q = 2. Thus, it is enough to choose  $\mathbf{a} = (\mathbf{v} \cdot \mathbf{w}_i)\mathbf{w}_i - (\mathbf{w}_i \cdot \mathbf{v})\mathbf{w}_i$  to obtain

$$T(\mathbf{x}) = \varphi_{\mathbf{a}}(\mathbf{x}) \tag{31}$$

for all  $\mathbf{x} \in \mathbb{R}^{p,q}$ .

This proof was performed without using transcendental functions as in Proposition 2 of Rodríguez *et al.* (2005) which, in fact, is now a corollary of the above Proposition 1.

In general, any orthogonal transformation can be constructed with elements of  $\mathbb{R}_{p,q}$ , since it can be obtained as a product of simple reflections by non-isotropic vectors. The formal statement is:

Theorem 1 (Cartan-Dieudonné). Any orthogonal transformation, in a non-degenerate linear orthogonal space  $\mathbb{R}^{p,q}$  with n = p + q, can be decomposed into a product of at most nsimple reflections. That is, let  $T : \mathbb{R}^{p,q} \to \mathbb{R}^{p,q}$  be an orthogonal transformation and let  $m \le p + q$ . There exist  $\mathbf{a}_1, \ldots, \mathbf{a}_m$  non-isotropic vectors such that

$$T(\mathbf{x}) = (-1)^m \left(\prod_{i=1}^m \mathbf{a}_i\right) \mathbf{x} \left(\prod_{i=1}^m \mathbf{a}_i\right)^{-1}$$
(32)

for all  $\mathbf{x} \in \mathbb{R}^{p,q}$ .

T is a rotation if m is even, and a reflection if m is odd. A demonstration of this theorem by induction can be found in Snapper & Troyer (1971).

### 4. Mathematics of the CSL problem

The CSL problem was formulated in more mathematical terms by Baake (1997). Here, however, we are considering non-Euclidean metrics and care must be taken to verify the validity of these definitions and theorems when spaces with non-zero signature are involved. Bearing this fact in mind, here we present a brief summary of basic concepts related to coincidence lattices.

Let  $\Gamma \subset \mathbb{R}^{p,q}$  be a lattice of dimension n = p + q and let  $T \in O(n)$  be an orthogonal transformation. The group

$$OC(\Gamma) = \{T \in O(n) \mid [\Gamma : \Gamma \cap T\Gamma] < \infty\}$$
(33)

is called the coincidence isometry group of  $\Gamma$ . If  $T \in OC(\Gamma)$ , then the index of the sublattice  $\Gamma \cap T\Gamma$  in  $\Gamma$ ,  $[\Gamma : \Gamma \cap T\Gamma]$  (the number of right cosets), is finite and is just the ratio of the volumes of the unit cells, *i.e.*, the coincidence index:

$$\Sigma(T) = [\Gamma : \Gamma \cap T\Gamma]. \tag{34}$$

Concerning lattices and sublattices, we will only need the following lemmas, which will be useful in the following sections:

Lemma 2. Let  $\Gamma = \bigoplus_{i=1}^{n} \mathbb{Z} \mathbf{a}_{i} \subset \mathbb{R}^{p,q}$  be a lattice, where  $\{\mathbf{a}_{1}, \ldots, \mathbf{a}_{n}\}$  is a set of linearly independent vectors in  $\mathbb{R}^{p,q}$ . If  $\Gamma'$  is a sublattice of  $\Gamma (\Gamma' < \Gamma)$ , then for each  $\mathbf{a} \in \Gamma$  there exists  $m \in \mathbb{N}$  such that  $m\mathbf{a} \in \Gamma'$ .

*Proof 3.* Since  $\Gamma'$  is a subgroup of  $\Gamma$  (which is in turn isomorphic to a finite Abelian group of order *n*), then the quotient group  $\Gamma/\Gamma' = \{\Gamma' + \mathbf{a} \mid \mathbf{a} \in \Gamma\}$  exists and its right cosets are given by

$$\Gamma' + \mathbf{a} = \{\mathbf{b} + \mathbf{a} \mid \mathbf{b} \in \Gamma'\},\tag{35}$$

which we will denote by  $\Gamma' + \mathbf{a} = [\mathbf{a}]$ . Now, as  $\Gamma/\Gamma'$  is a finite group, then for each  $[\mathbf{a}]$  there exists an  $m \in \mathbb{N}$  such that  $m[\mathbf{a}] = [m\mathbf{a}] = [0] = \Gamma'$ . Therefore  $m\mathbf{a} \in \Gamma'$ .

This lemma also holds for each element of the basis.

Lemma 3. Let  $\Gamma = \bigoplus_{i=1}^{n} \mathbb{Z}\mathbf{a}_{i}$  and  $\Gamma' = \bigoplus_{i=1}^{n} \mathbb{Z}\mathbf{b}_{i}$  be lattices in  $\mathbb{R}^{p,q}$ . If for each  $\mathbf{a}_{i}$  there exists  $m_{i} \in \mathbb{N}$  such that  $m_{i}\mathbf{a}_{i} \in \Gamma'$ , then  $\Gamma' < \Gamma$ .

*Proof 4.* We have to show that  $\Gamma/\Gamma'$  is of finite order, that is,  $\Gamma/\Gamma'$  has a finite number of elements. Let  $k_i = \min\{m \in \mathbb{N} \mid m\mathbf{a}_i \in \Gamma'\}$ . Then  $k_i\mathbf{a}_i \in \Gamma'$  or, equivalently  $[k_i\mathbf{a}_i] = [0]$ , and if  $0 < r < k_i$  then  $[r\mathbf{a}_i] \neq [0]$  is obtained.

Let  $\mathbf{a} = z_1 \mathbf{a}_1 + \ldots + z_n \mathbf{a}_n \in \Gamma$ . For each  $z_i$  there are integers  $q_i, r_i$  such that  $z_i = q_i k_i + r_i$ , with  $0 \le r_i < k_i$ . Thus

$$[z_i \mathbf{a}_i] = [r_i \mathbf{a}_i], \tag{36}$$

from which we get

$$[\mathbf{a}] = [z_1\mathbf{a}_1 + \ldots + z_n\mathbf{a}_n] = \sum_{i=1}^n [z_i\mathbf{a}_i] = \sum_{i=1}^n [r_i\mathbf{a}_i].$$
 (37)

Therefore the group  $\Gamma/\Gamma'$  has at most  $\prod_{i=1}^{n} k_i$  elements.

Concerning coincidence isometries, the following will be useful:

Theorem 2. Let  $\Gamma = \bigoplus_{i=1}^{n} \mathbb{Z}\mathbf{a}_{i}$  be a lattice and T be an orthogonal transformation.  $T \in OC(\Gamma)$  if and only if there are  $m_{i} \in \mathbb{N}$  such that  $m_{i}T(\mathbf{a}_{i}) \in \Gamma$ .

*Proof* 5.  $\Longrightarrow$ ) As  $T(\Gamma) \cap \Gamma < \Gamma$  is of finite index, there exists  $n_i \in \mathbb{N}$  such that  $n_i \mathbf{a}_i \in T(\Gamma) \cap \Gamma$ . Thus  $n_i \mathbf{a}_i \in T(\Gamma)$ . Now,  $\mathbf{a}_i$  can be expressed as

$$\mathbf{a}_{i} = \sum_{i=1}^{n} \alpha_{ij} T(\mathbf{a}_{j}), \qquad (38)$$

where  $A = [\alpha_{ij}]$  is the inverse of the matrix associated with *T* (with respect to the basis  $\{\mathbf{a}_1, \ldots, \mathbf{a}_n\}$ ), with rational entries. Then

$$T(\mathbf{a}_i) = \sum_{i=1}^n \beta_{ij} \mathbf{a}_j, \tag{39}$$

where  $B = [\beta_{ij}] = A^{-1}$  has rational entries too. Therefore, there exists  $m_i \in \mathbb{N}$  such that  $m_i T(\mathbf{a}_i) \in \Gamma$ .

⇐=) As  $m_i T(\mathbf{a}_i) \in \Gamma$ , then  $T(\Gamma) \cap \Gamma < \Gamma$  and from Lemma 3 it follows that  $T \in OC(\Gamma)$ .

Given the importance of simple reflections to the study of coincidence lattices (Rodríguez *et al.*, 2005; Zou, 2006*a*), we state the following theorems and lemma:

Theorem 3. Let  $\Gamma \subset \mathbb{R}^{p,q}$  be a lattice and  $\varphi_{\mathbf{u}} : \mathbb{R}^{p,q} \to \mathbb{R}^{p,q}$  be a simple reflection. If  $\varphi_{\mathbf{u}} \in OC(\Gamma)$  then there exists a non-zero  $\lambda \in \mathbb{R}$  such that

$$\lambda \mathbf{u} \in \Gamma. \tag{40}$$

*Proof 6.* If  $T \in OC(\Gamma)$  then  $T\Gamma \cap \Gamma < \Gamma$ . Now, by Lemma 2, for each  $\mathbf{a} \in \Gamma$  there exists  $m \in \mathbb{Z}$  such that  $m\mathbf{a} \in T\Gamma \cap \Gamma$ , that is  $mT(\mathbf{a}) = T(m\mathbf{a}) \in \Gamma$ , which is equivalent to claiming that there are  $\mathbf{x}, \mathbf{y} \in \Gamma$  such that

$$\mathbf{y} = T(\mathbf{x}). \tag{41}$$

In particular, this is satisfied for  $\varphi_{\mathbf{u}} \in OC(\Gamma)$ . Thus

$$\mathbf{y} = -\mathbf{u}\mathbf{x}\mathbf{u}^{-1},\tag{42}$$

$$\mathbf{y}\mathbf{u} = -\mathbf{u}\mathbf{x},\tag{43}$$

and this implies that

$$\mathbf{y} \cdot \mathbf{u} = -\mathbf{u} \cdot \mathbf{x},\tag{44}$$

$$\mathbf{y} \wedge \mathbf{u} = -\mathbf{u} \wedge \mathbf{x} = \mathbf{x} \wedge \mathbf{u},\tag{45}$$

so

$$(\mathbf{y} - \mathbf{x}) \wedge \mathbf{u} = 0. \tag{46}$$

Then  $(\mathbf{y} - \mathbf{x})$  and  $\mathbf{u}$  are parallel. Therefore, there exists a non-zero  $\lambda \in \mathbb{R}$  such that  $\lambda \mathbf{u} = \mathbf{y} - \mathbf{x} \in \Gamma$ .

Theorem 4. Let  $\Gamma = \bigoplus_{i=1}^{n} \mathbb{Z} \mathbf{a}_{i}$  be a lattice of  $\mathbb{R}^{p,q}$  and  $\mathbf{u} \in \Gamma$ . If the simple reflection  $\varphi_{\mathbf{u}} : \mathbb{R}^{p,q} \to \mathbb{R}^{p,q} \in OC(\Gamma)$ , then

$$\frac{\mathbf{u} \cdot \mathbf{a}_i}{\mathbf{u}^2} \in \mathbb{Q} \tag{47}$$

for i = 1, ..., p + q.

*Proof* 7. Since  $\varphi_{\mathbf{u}} \in OC(\Gamma)$ , then  $\varphi_{\mathbf{u}}(\Gamma) \cap \Gamma < \Gamma$ . Thus  $\varphi_{\mathbf{u}}(\mathbf{a}_i) \in \Gamma$  and also  $m_i \varphi_{\mathbf{u}}(\mathbf{a}_i) \in \Gamma$  for  $m_i \in \mathbb{Z}$ ,  $i = 1, \ldots, p + q$ . But, from equation (16),

$$m_i \varphi_{\mathbf{u}}(\mathbf{a}_i) = m_i \mathbf{a}_i - m_i \frac{2(\mathbf{u} \cdot \mathbf{a}_i)}{\mathbf{u}^2} \mathbf{u}, \qquad (48)$$

$$m_i \frac{2(\mathbf{u} \cdot \mathbf{a}_i)}{\mathbf{u}^2} \mathbf{u} = m_i \mathbf{a}_i - m_i \varphi_{\mathbf{u}}(\mathbf{a}_i) \in \Gamma.$$
(49)

As  $\mathbf{u} = \sum_{i=1}^{p+q} \alpha_i \mathbf{a}_i$ , where  $\alpha_i \in \mathbb{Z}$   $(i = 1, \dots, p+q)$ , then

$$m_i \frac{2(\mathbf{u} \cdot \mathbf{a}_i)}{\mathbf{u}^2} \alpha_i \in \mathbb{Z}$$
(50)

and thus

$$\frac{(\mathbf{u} \cdot \mathbf{a}_i)}{\mathbf{u}^2} \in \mathbb{Q}.$$
 (51)

*Lemma 4.* Let  $\Gamma = \bigoplus_{i=1}^{n} \mathbb{Z} \mathbf{a}_{i}$  be a lattice of  $\mathbb{R}^{p,q}$ . If  $\mathbf{a}_{i}^{2}$ ,  $\mathbf{a}_{i} \cdot \mathbf{a}_{i} \in \mathbb{Q}$ , then for each non-isotropic  $\mathbf{u} \in \Gamma$ 

$$\varphi_{\mathbf{u}} \in OC(\Gamma) \tag{52}$$

holds.

*Proof 8.* We have that for i = 1, 2,

$$\varphi_{\mathbf{u}}(\mathbf{a}_i) = \mathbf{a}_i - 2\frac{\mathbf{u} \cdot \mathbf{a}_i}{\mathbf{u}^2}\mathbf{u}$$
(53)

and, given the hypotheses, we can see that

$$\frac{\mathbf{u} \cdot \mathbf{a}_i}{\mathbf{u}^2} \in \mathbb{Q}.$$
 (54)

Thus, for each *i* there exists a non-zero  $m_i \in \mathbb{Q}$  such that  $m_i \varphi_{\mathbf{u}}(\mathbf{a}_i) \in \Gamma$  and by Theorem 2 we conclude that  $\varphi_{\mathbf{u}} \in OC(\Gamma)$ .

Finally, it is worth mentioning that  $[\Gamma : \Gamma \cap T\Gamma]$ , the coincidence index, can be calculated using determinants (see for instance Rotman, 1995, Exercise 10.17), which in turn can be evaluated in a metric-independent way by using the outer product: in fact given the geometrical interpretation of the outer product we have

Lemma 5. Let  $\Gamma = \bigoplus_{i=1}^{n} \mathbb{Z}\mathbf{a}_{i}$  and  $\Gamma' = \bigoplus_{i=1}^{n} \mathbb{Z}\mathbf{b}_{i}$  be lattices in  $\mathbb{R}^{p,q}$ , and  $\Gamma' < \Gamma$ . Then

$$[\Gamma:\Gamma'] = \left| \frac{\mathbf{b}_1 \wedge \ldots \wedge \mathbf{b}_n}{\mathbf{a}_1 \wedge \ldots \wedge \mathbf{a}_n} \right|.$$
(55)

### 5. CSL problem for $\mathbb{Z}^{p,q}$ (*p* + *q* = 2)

The particular cases of lattices spanned by the canonical basis of  $\mathbb{R}^{p,q}$  will be denoted as  $\mathbb{Z}^{p,q}$ , that is,  $\mathbb{Z}^{p,q} = \mathbb{Z}\mathbf{e}_1 \oplus \mathbb{Z}\mathbf{e}_2 \oplus \ldots \oplus \mathbb{Z}\mathbf{e}_n$ , where  $\{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n\}$  is the canonical basis of  $\mathbb{R}^{p,q}$ .

An interesting result is that given a lattice  $\Gamma \subset \mathbb{R}^n$ , any coincidence isometry of  $\Gamma$  can be decomposed as a product of at most *n* reflections by hyperplanes defined by vectors of  $\Gamma$  (for a proof, see Zou, 2006*a*, Th. 3.1; Aragón-González *et al.*, 2006, Th. 21). In Rodríguez *et al.* (2005) we studied in detail the case of lattices in the plane  $\mathbb{R}^2$  (p = 2, q = 0) by providing coincidence indexes and bases of the coincidence lattices. In what follows we analyze the general case of lattices in  $\mathbb{R}^{p,q}$  where p + q = 2, but, as already mentioned, the most interesting case is when p = q = 1, that is, the hyperbolic plane. In order to unify the treatment, this case requires special attention because isotropic vectors may appear, so first of all we show, in Lemmas 6 and 7, how to handle these vectors.

If a lattice  $\Gamma \subset \mathbb{R}^{1,1}$  is generated by isotropic basis vectors, we can always find a non-isotropic basis. To see how this is possible, consider the vectors

$$\mathbf{v}_1 = \mathbf{e}_1 + \mathbf{e}_2$$
 and  $\mathbf{v}_2 = \mathbf{e}_1 - \mathbf{e}_2$ , (56)

where  $\{\mathbf{e}_1, \mathbf{e}_2\}$  is the canonical basis of  $\mathbb{Z}^{1,1}$  (thus  $\mathbf{e}_1^2 = 1$  and  $\mathbf{e}_2^2 = -1$ ). It is easy to verify that if  $\mathbf{x} \in \mathbb{R}^{1,1}$ , we have  $\mathbf{x}^2 = 0$  if and only if  $\mathbf{x} = \lambda \mathbf{v}_1$  or  $\mathbf{x} = \lambda \mathbf{v}_2$ , where  $\lambda \in \mathbb{R}$ . Also, notice that the orthogonal complement of  $\mathbf{v}_1$  is the set spanned by  $\mathbf{v}_1$  itself and the same occurs with  $\mathbf{v}_2$ . Bearing all this in mind, we propose the following two lemmas:

Lemma 6. Let  $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2 \subset \mathbb{R}^{1,1}$  be a lattice. If it turns out that  $\mathbf{a}_1^2 = \mathbf{a}_2^2 = 0$ , we can always find a basis  $\{\mathbf{b}_1, \mathbf{b}_2\}$  for  $\Gamma$  such that  $\mathbf{b}_1^2 \neq 0$  and  $\mathbf{b}_2^2 \neq 0$ .

*Proof 9.* As  $\mathbf{a}_1$  and  $\mathbf{a}_2$  are both linearly independent and isotropic, without loss of generality we can assume that

$$\mathbf{a}_1 = \lambda_1 \mathbf{v}_1$$
 and  $\mathbf{a}_2 = \lambda_2 \mathbf{v}_2$ , (57)

where  $\lambda_i \neq 0$ , for i = 1, 2,  $\mathbf{v}_1 = \mathbf{e}_1 + \mathbf{e}_2$  and  $\mathbf{v}_2 = \mathbf{e}_1 - \mathbf{e}_2$ . It is straightforward to verify that the vectors

$$\mathbf{b}_1 = \mathbf{a}_1 + \mathbf{a}_2$$
 and  $\mathbf{b}_2 = -2\mathbf{a}_1 - \mathbf{a}_2$  (58)

have the desired properties.

From this lemma, we can always assume that given a lattice  $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2 \subset \mathbb{R}^{1,1}$  at least one of the basis vectors  $\mathbf{a}_i$  is non-isotropic. Henceforth, when referred to the case p = q = 1, we shall consider lattices with this property.

The following lemma will be used to demonstrate Proposition 2:

Lemma 7. Let  $T : \mathbb{R}^{1,1} \to \mathbb{R}^{1,1}$  be an orthogonal transformation such that

$$T(\mathbf{x}) - \mathbf{x} \neq 0$$
 and  $(T(\mathbf{x}) - \mathbf{x})^2 = 0$ , (59)

then both vectors,  $\mathbf{x}$  and  $T(\mathbf{x})$ , are isotropic and linearly dependent.

*Proof 10.* Taking into account that *T* is an orthogonal transformation, *i.e.*,  $(T(\mathbf{x}))^2 = \mathbf{x}^2$ , we have

$$(T(\mathbf{x}) - \mathbf{x})^2 = 0,$$
  

$$(T(\mathbf{x}))^2 - 2T(\mathbf{x}) \cdot \mathbf{x} + \mathbf{x}^2 = 0,$$
  

$$\mathbf{x}^2 - T(\mathbf{x}) \cdot \mathbf{x} = 0,$$
  

$$\mathbf{x} \cdot (\mathbf{x} - T(\mathbf{x})) = 0,$$
 (60)

since  $\mathbf{x} - T(\mathbf{x})$  is a non-zero isotropic vector, then  $\mathbf{x} - T(\mathbf{x}) = \lambda \mathbf{v}_1$  or  $\mathbf{x} - T(\mathbf{x}) = \lambda \mathbf{v}_2$ , where  $\mathbf{v}_1$  and  $\mathbf{v}_2$  are given in equation (56). In both cases, it turns out that the orthogonal complement of  $\mathbf{x} - T(\mathbf{x})$  is the space spanned by  $\mathbf{x} - T(\mathbf{x})$  itself and thus from equation (60) we have that  $\mathbf{x}$  belongs to the space spanned by  $\mathbf{x} - T(\mathbf{x})$ . Consequently,  $\mathbf{x}$  is isotropic and linearly dependent on  $T(\mathbf{x})$ . In an analogous manner, it can be shown that

$$T(\mathbf{x}) \cdot (\mathbf{x} - T(\mathbf{x})) = 0, \tag{61}$$

from where it is inferred that  $T(\mathbf{x})$  is isotropic and linearly dependent on  $\mathbf{x}$ .

Proposition 2. Let  $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$  be a lattice of  $\mathbb{R}^{p,q}$ , where p + q = 2. If  $T \in OC(\Gamma)$ , there exist  $\mathbf{c}_1, \mathbf{c}_2 \in \Gamma$  such that

$$T = \varphi_{\mathbf{c}_1} \tag{62}$$

or

$$T = \varphi_{\mathbf{c}_1} \varphi_{\mathbf{c}_2}. \tag{63}$$

*Proof 11.* Assume that T is different from the identity. We can also assume, without loss of generality, that  $\mathbf{a}_1^2 \neq 0$ .

Let us first consider that  $T(\mathbf{a}_1) - \mathbf{a}_1 = 0$ . In this case  $T = \varphi_{\mathbf{c}_1}$ , where  $\mathbf{c}_1 \in \Gamma$ . Indeed, since  $\mathbf{a}_1$  is non-isotropic there exists  $\mathbf{b}_1$  such that  $\{\mathbf{a}_1, \mathbf{b}_1\}$  is a non-isotropic orthogonal basis of  $\mathbb{R}^{p,q}$ . Since  $T(\mathbf{a}_1) = \mathbf{a}_1$ , then  $T(\mathbf{b}_1) = \alpha \mathbf{b}_1$  for some  $\alpha \in \mathbb{R}$ , but as T is an orthogonal transformation different from the identity, necessarily  $T(\mathbf{b}_1) = -\mathbf{b}_1$  and thus  $T = \varphi_{\mathbf{b}_1}$ . Since  $T \in OC(\Gamma)$ , from Theorem 3 we have that there exists  $\lambda \in \mathbb{R}$  such that  $\mathbf{c}_1 = \lambda \mathbf{b}_1 \in \Gamma$  and therefore  $T = \varphi_{\mathbf{c}_1}$ .

Now suppose that  $T(\mathbf{a}_1) - \mathbf{a}_1 \neq 0$  and  $(\dot{T}(\mathbf{a}_1) - \mathbf{a}_1)^2 = 0$ . From Lemma 7 it turns out that  $T(\mathbf{a}_1)$  and  $\mathbf{a}_1$  are isotropic, which is a contradiction. Therefore, there must be  $\mathbf{a}_i$  such that  $T(\mathbf{a}_i) - \mathbf{a}_i$  is non-isotropic. By Lemma 2, there exists  $m_i \in \mathbb{Z}$  such that  $m_i(T(\mathbf{a}_i) - \mathbf{a}_i) \in \Gamma$ . If  $\mathbf{c}_1 = m_i(T(\mathbf{a}_i) - \mathbf{a}_i)$ , then

$$\varphi_{\mathbf{c}_1} T(\mathbf{a}_i) = \mathbf{a}_i. \tag{64}$$

Thus, we have two possibilities: (a) if  $\det(T) = -1$ , then  $T = \varphi_{\mathbf{c}_1}$  and (b) if  $\det(T) = 1$ , then  $\varphi_{\mathbf{c}_1}T \in OC(\Gamma)$  is a simple reflection, say  $\varphi_{\mathbf{c}_1}T = \varphi_{\mathbf{u}} \in OC(\Gamma)$ . According to Theorem 3, there exists  $\mathbf{c}_2 = \lambda \mathbf{u} \in \Gamma$ , therefore

$$\varphi_{\mathbf{e}_1} T = \varphi_{\mathbf{e}_2},$$

$$T = \varphi_{\mathbf{e}_1} \varphi_{\mathbf{e}_2}.$$
(65)

Finally, we should mention that Proposition 2 is the necessary condition; for the sufficiency condition we have:

Theorem 5. Let  $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$  be a lattice of  $\mathbb{R}^{p,q}$ , where p + q = 2 and  $\mathbf{a}_i \cdot \mathbf{a}_j \in \mathbb{Q}$ , (i, j = 1, 2). Then  $T \in OC(\Gamma)$  if and only if there exist  $\mathbf{c}_1, \mathbf{c}_2 \in \Gamma$  such that

$$T(\mathbf{x}) = \varphi_{\mathbf{c}_1} \varphi_{\mathbf{c}_2}(\mathbf{x}) = \mathbf{c}_1 \mathbf{c}_2 \mathbf{x} \mathbf{c}_2^{-1} \mathbf{c}_1^{-1}.$$
 (66)

In what follows, we will assume that the hypotheses of Theorem 5 are fulfilled.

Given any  $\mathbf{u} \in \Gamma$ , there exists  $\lambda \in \mathbb{Z}$  such that  $\mathbf{v} = \lambda(\mathbf{u} \cdot (\mathbf{a}_1 \wedge \mathbf{a}_2)) \in \Gamma$ , and moreover  $\mathbf{v} \cdot \mathbf{u} = 0$ . Indeed, by the identity (9) we have

$$\mathbf{u} \cdot (\mathbf{a}_1 \wedge \mathbf{a}_2) = (\mathbf{u} \cdot \mathbf{a}_1)\mathbf{a}_2 - (\mathbf{u} \cdot \mathbf{a}_2)\mathbf{a}_1 \tag{67}$$

and, as  $(\mathbf{u} \cdot \mathbf{a}_i) \in \mathbb{Q}$ , we can find a positive integer such that  $\lambda(\mathbf{u} \cdot \mathbf{a}_i) \in \mathbb{Z}$  for i = 1, 2. Obviously, **v** is orthogonal to **u**.

Let any  $\mathbf{u} = \alpha_1 \mathbf{a}_1 + \alpha_2 \mathbf{a}_2 \in \Gamma$  and if we consider the simple reflection  $\varphi_{\mathbf{u}}$ , it is evident that

$$\varphi_{\mathbf{u}}(\mathbf{u}) = -\mathbf{u},\tag{68}$$

$$\varphi_{\mathbf{u}}(\mathbf{v}) = \mathbf{v}.\tag{69}$$

Therefore, the lattice  $\Lambda = \mathbb{Z}\mathbf{u} \oplus \mathbb{Z}\mathbf{v}$  must satisfy the following relations:

$$\Lambda < \Gamma \cap \varphi_{\mathbf{u}}(\Gamma) > \Gamma, \tag{70}$$

$$[\Gamma : \Lambda] = [\Gamma \cap \varphi_{\mathbf{u}}(\Gamma) : \Lambda][\Gamma : \Gamma \cap \varphi_{\mathbf{u}}(\Gamma)]$$
(71)

$$[\Gamma : \Lambda] = [\Gamma \cap \varphi_{\mathbf{u}}(\Gamma) : \Lambda] \Sigma(\varphi_{\mathbf{u}}).$$
(72)

Since it is known that given two lattices  $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$  and  $\Gamma' = \mathbb{Z}\mathbf{b}_1 \oplus \mathbb{Z}\mathbf{b}_2$  such that  $\Gamma' < \Gamma$ , then  $[\Gamma : \Gamma']$  is equal to the ratio of the volume of the unit cell defined by the vectors  $\{\mathbf{b}_1, \mathbf{b}_2\}$  to the volume of the unit cell defined by the vectors  $\{\mathbf{a}_1, \mathbf{a}_2\}$ . As a consequence, we have that the ratio  $[\Gamma : \Lambda]/\Sigma(\varphi_{\mathbf{u}})$  is an integer and it is said that  $\Sigma(\varphi_{\mathbf{u}})$  divides  $[\Gamma : \Lambda]$  and is denoted as

$$\Sigma(\varphi_{\mathbf{u}}) \mid [\Gamma : \Lambda]. \tag{73}$$

Here  $[\Gamma : \Lambda] = |(\mathbf{u} \wedge \mathbf{v})/(\mathbf{a}_1 \wedge \mathbf{a}_2)|$ . Computation leads to

$$\mathbf{u} \wedge \mathbf{v} = \lambda \mathbf{u}^2 (\mathbf{a}_1 \wedge \mathbf{a}_2). \tag{74}$$

Thus, we have proved the following:

Proposition 3. Let  $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$  be a lattice of  $\mathbb{R}^{p,q}$ , where p + q = 2. If  $\mathbf{a}_i \cdot \mathbf{a}_j \in \mathbb{Q}$ , i, j = 1, 2, then for any non-isotropic  $\mathbf{u} \in \Gamma$  the following holds:

(1) There exists  $\lambda \in \mathbb{Z}$  such that  $\mathbf{v} = \lambda \mathbf{u} \cdot (\mathbf{a}_1 \wedge \mathbf{a}_2) \in \Gamma$ , where  $\mathbf{v}$  is orthogonal to  $\mathbf{u}$ .

(2)  $\Sigma(\varphi_{\mathbf{u}})$  divides  $\lambda(\mathbf{u}^2)$ , where  $\lambda \in \mathbb{Z}$  is the same as in (1).

Proposition 3 and the next one (Proposition 4) will be useful for finding a basis and the coincidence index for twodimensional lattices and will be used in the next section. The following reasoning corresponds to a demonstration of Proposition 4:

A basis of  $\varphi_{\mathbf{u}}(\Gamma) \cap \Gamma$ , where  $\varphi_{\mathbf{u}}$  is a simple reflection, can be found as follows. First, the simple reflections  $\varphi_{\mathbf{u}}$  and  $\varphi_{\alpha \mathbf{u}}$  are the same for all non-zero  $\alpha \in \mathbb{R}$  (or, better,  $\mathbb{Z}$ ). Then, we can consider, without loss of generality, that  $\varphi_{\mathbf{u}}$ , where  $\mathbf{u} = \alpha_1 \mathbf{a}_1 + \alpha_2 \mathbf{a}_2$ , satisfies  $gcd(\alpha_1, \alpha_2) = 1$ , where gcd stands for the greatest common divisor. Thus, there is a  $\mathbf{w} \in \Gamma$  such that

$$\Gamma = \mathbb{Z}\mathbf{u} \oplus \mathbb{Z}\mathbf{w}.$$
 (75)

Indeed, as  $gcd(\alpha_1, \alpha_2) = 1$ , then there exist  $\beta_1, \beta_2 \in \mathbb{Z}$  satisfying

$$\alpha_1 \beta_1 + \alpha_2 \beta_2 = 1 \tag{76}$$

and it is enough to choose  $\mathbf{w} = -\beta_2 \mathbf{a}_1 + \beta_1 \mathbf{a}_2$ , since

$$\mathbf{u} \wedge \mathbf{w} = (\alpha_1 \beta_1 + \alpha_2 \beta_2) \mathbf{a}_1 \wedge \mathbf{a}_2 = \mathbf{a}_1 \wedge \mathbf{a}_2.$$
(77)

Now,

$$\varphi_{\mathbf{u}}(\mathbf{u}) = -\mathbf{u} \in \Gamma \cap \varphi_{\mathbf{u}}(\Gamma) \tag{78}$$

and we can choose the least  $m \in \mathbb{N}$  such that

$$m\varphi_{\mathbf{u}}(\mathbf{w}) \in \Gamma \cap \varphi_{\mathbf{u}}(\Gamma). \tag{79}$$

Finally, we claim that a basis for the coincidence lattice  $\Gamma \cap \varphi_{\mathbf{u}}(\Gamma)$  is given by

$$\{\mathbf{u}, m\varphi_{\mathbf{u}}(\mathbf{w})\}.$$
 (80)

Indeed, let  $\mathbf{y} \in \Gamma \cap \varphi_{\mathbf{u}}(\Gamma)$ , then there exists  $\mathbf{x} = \alpha \mathbf{u} + \beta \mathbf{w} \in \Gamma$ , where  $\alpha, \beta \in \mathbb{Z}$ , such that

$$\begin{aligned} \mathbf{y} &= \varphi_{\mathbf{u}}(\mathbf{x}) \\ &= \alpha \varphi_{\mathbf{u}}(\mathbf{u}) + \beta \varphi_{\mathbf{u}}(\mathbf{w}) \\ &= -\alpha \mathbf{u} + \beta \varphi_{\mathbf{u}}(\mathbf{w}), \end{aligned} \tag{81}$$

thus

$$\mathbf{y} + \alpha \mathbf{u} = \beta \varphi_{\mathbf{u}}(\mathbf{w}), \tag{82}$$

and since  $m \in \mathbb{N}$  is the least number that satisfies  $m\varphi_{\mathbf{u}}(\mathbf{w}) \in \Gamma \cap \varphi_{\mathbf{u}}(\Gamma)$ , then

$$\beta = km, \tag{83}$$

where k is an integer. An important consequence is that the coincidence index is exactly m because

$$\left|\frac{\varphi_{\mathbf{u}}(\mathbf{u}) \wedge (m\varphi_{\mathbf{u}}(\mathbf{w}))}{\mathbf{a}_1 \wedge \mathbf{a}_2}\right| = m.$$
(84)

Thus, we have the following proposition:

Proposition 4. Let  $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$  be a lattice of  $\mathbb{R}^{p,q}$  where p + q = 2 and  $\mathbf{a}_i \cdot \mathbf{a}_j \in \mathbb{Q}$  (i, j = 1, 2). Then, for non-isotropic  $\mathbf{u} = \alpha_1 \mathbf{a}_1 + \alpha_2 \mathbf{a}_2 \in \Gamma$ , where  $gcd(\alpha_1, \alpha_2) = 1$ , we have:

(1) There exists  $\mathbf{w} \in \Gamma$ , such that  $\{\mathbf{u}, \mathbf{w}\}$  is a basis of  $\Gamma$ .

(2) If *m* is the least natural number such that  $m\varphi_{\mathbf{u}}(\mathbf{w}) \in \Gamma \cap \varphi_{\mathbf{u}}(\Gamma)$ , then  $\Sigma(\varphi_{\mathbf{u}}) = m$ .

A basis for the coincidence lattice  $\Gamma \cap \varphi_{\mathbf{u}}(\Gamma)$  is given by equation (80).

## 6. Bases and coincidence index for two-dimensional lattices

In this section, coincidence lattices in  $\mathbb{R}^{p,q}$  with p + q = 2 will be studied. A particularly interesting case is when p = q = 1, that is, lattices in the hyperbolic plane. Analytic expressions for the coincidence index and bases for the coincidence lattices are provided. Unless otherwise explicitly stated, throughout this section we work in  $\mathbb{R}^{p,q}$  where p + q = 2.

It should be pointed out that the factorization of an orthogonal transformation as a product of simple reflections by hyperplanes is not unique. This fact, however, can be used to find an adequate factorization as follows. Assume that  $T \in OC(\Gamma)$ , where  $\Gamma \subset \mathbb{R}^{p,q}$  and  $\det(T) = 1$ . If we can find vectors  $\mathbf{c}_1, \mathbf{c}_2 \in \Gamma$  such that

$$T = \varphi_{\mathbf{c}_1} \varphi_{\mathbf{c}_2} \quad \text{and} \quad \varphi_{\mathbf{c}_2}(\Gamma) = \Gamma, \tag{85}$$

then  $T(\Gamma) = \varphi_{\mathbf{e}_1}(\Gamma)$  and the problem of finding the coincidence index and a basis for  $T(\Gamma) \cap \Gamma$  is reduced to the problem of finding the coincidence index and a basis for  $\varphi_{\mathbf{e}_1}(\Gamma) \cap \Gamma$ . We can use Proposition 4 for this purpose. In the next section we analyze some interesting cases where it was possible to apply this strategy.

### 6.1. Pseudo-square lattices

We will explore the properties of the pseudo-square lattices in order to find the coincidence index and a basis for  $\Gamma = \mathbb{Z}^{p.q}$ . Applying Propositions 1 and 4 we obtain the following corollary:

Corollary 1. Let  $\Gamma = \mathbb{Z}^{p,q}$  and let  $\{\mathbf{e}_1, \mathbf{e}_2\}$  be the canonical basis of  $\mathbb{R}^{p,q}$ . If  $T \in OC(\Gamma)$  then there exists  $\mathbf{u} \in \mathbb{Z}^{p,q}$  such that

$$T(\mathbf{x}) = \begin{cases} \varphi_{\mathbf{u}}(\mathbf{x}) & \text{if } \det(T) = -1, \\ \varphi_{\mathbf{u}}\varphi_{\mathbf{e}_i}(\mathbf{x}) & \text{if } \det(T) = 1, \end{cases}$$
(86)

for i = 1, 2. Furthermore,  $\Sigma(T)$  divides  $\mathbf{u}^2$ .

*Remark* 2. The previous corollary extends Proposition 5 of Rodríguez *et al.* (2005) to any p, q such that p + q = 2. Furthermore, the group  $OC(\mathbb{Z}^{p,q})$  has been characterized and we can obtain any element of  $OC(\mathbb{Z}^{p,q})$ , since our theorems contain implicitly the required procedures.

**6.1.1. Coincidence index and a basis of the CSL**. In what follows, we shall obtain the coincidence index for  $OC(\mathbb{Z}^{p,q})$ . Since  $\varphi_{\mathbf{e}_i}(\mathbb{Z}^{p,q}) = \mathbb{Z}^{p,q}$ , we can apply the strategy discussed at the beginning of this section, since

$$(\varphi_{\mathbf{u}}\varphi_{\mathbf{e}_i})(\mathbb{Z}^{p,q}) \cap \mathbb{Z}^{p,q} = \varphi_{\mathbf{u}}(\mathbb{Z}^{p,q}) \cap \mathbb{Z}^{p,q}, \tag{87}$$

where  $\mathbf{u} \in \mathbb{Z}^{p,q}$ .

Now, it follows from Corollary 1 that for any  $T \in OC(\mathbb{Z}^{p,q})$ we can find a non-isotropic vector  $\mathbf{u} \in \mathbb{Z}^{p,q}$  such that

$$T(\mathbf{x}) = -\mathbf{u}\mathbf{x}\mathbf{u}^{-1} \quad \text{or} \quad T(\mathbf{x}) = \mathbf{u}\mathbf{e}_i\mathbf{x}\mathbf{e}_i^{-1}\mathbf{u}^{-1}, \qquad (88)$$

where *i* can be chosen as 1 or 2. Then to analyze the group  $OC(\mathbb{Z}^{p,q})$  it is enough to consider the isometries

$$\varphi_{\mathbf{u}}(\mathbf{x}) = -\mathbf{u}\mathbf{x}\mathbf{u}^{-1} \quad \text{or} \quad R_{\mathbf{u}}(\mathbf{x}) = \mathbf{u}\mathbf{e}_i\mathbf{x}\mathbf{e}_i^{-1}\mathbf{u}^{-1}, \qquad (89)$$

where *i* can be chosen as 1 or 2 and it is clear that there are two rotations  $R_{\mu}$ , one with  $e_1$  and another with  $e_2$ . Besides,

$$\varphi_{\mathbf{u}}(\mathbb{Z}^{p,q}) \cap \mathbb{Z}^{p,q} = R_{\mathbf{u}}(\mathbb{Z}^{p,q}) \cap \mathbb{Z}^{p,q}, \tag{90}$$

$$\Sigma(\varphi_{\mathbf{u}}) = \Sigma(R_{\mathbf{u}}). \tag{91}$$

That is, if we want to obtain a basis of  $R_{\mathbf{u}}(\mathbb{Z}^{p,q}) \cap \mathbb{Z}^{p,q}$  it is enough to calculate a basis of  $\varphi_{\mathbf{u}}(\mathbb{Z}^{p,q}) \cap \mathbb{Z}^{p,q}$ .

With these last results, we can also extend Proposition 6 of Rodríguez *et al.* (2005) to the following:

*Proposition 5.* If  $\mathbf{u} = \alpha_1 \mathbf{e}_1 + \alpha_2 \mathbf{e}_2 \in \mathbb{Z}^{p,q}$  and  $gcd(\alpha_1, \alpha_2) = 1$ , then

$$\Sigma(\varphi_{\mathbf{u}}) = \Sigma(R_{\mathbf{u}}) = \begin{cases} |\mathbf{u}^2|/2 & \text{if } \alpha_1 \text{ and } \alpha_2 \text{ are both odd,} \\ |\mathbf{u}^2| & \text{if either } \alpha_1 \text{ or } \alpha_2 \text{ is even.} \end{cases}$$
(92)

*Proof 12.* The proof is similar to that given in Rodríguez *et al.* (2005) with some changes. Here we only focus on these changes. Let  $\varphi_{\mathbf{u}} \in OC(\mathbb{Z}^{p,q})$ , where  $\mathbf{u} = \alpha_1 \mathbf{e}_1 + \alpha_2 \mathbf{e}_2 \in \mathbb{Z}^{p,q}$  and  $gcd(\alpha_1, \alpha_2) = 1$ . Since

$$\varphi_{\mathbf{u}}(\mathbf{x}) = -\mathbf{u}\mathbf{x}\mathbf{u}^{-1} = -\frac{\mathbf{u}\mathbf{x}\mathbf{u}}{\mathbf{u}^2},\tag{93}$$

then

$$\varphi_{\mathbf{u}}(\mathbf{e}_1) = -\frac{(\alpha_2^2 + \alpha_1^2)\mathbf{e}_1 + 2\alpha_1\alpha_2\mathbf{e}_2}{\alpha_1^2 - \alpha_2^2},$$
(94)

$$\varphi_{\mathbf{u}}(\mathbf{e}_2) = \frac{2\alpha_1\alpha_2\mathbf{e}_1 + (\alpha_1^2 + \alpha_2^2)\mathbf{e}_2}{\alpha_1^2 - \alpha_2^2}.$$
 (95)

Thus we obtain that

$$\mathbf{u}^2 \varphi_{\mathbf{u}}(\mathbf{e}_i) \in \mathbb{Z}^{p,q},\tag{96}$$

and we have to consider two cases:

(1)  $\alpha_1, \alpha_2$  are odd numbers. In this case  $\alpha_1^2 + \alpha_2^2, 2\alpha_1\alpha_2$  and  $\alpha_1^2 - \alpha_2^2$  are even numbers.

Therefore

$$\frac{\mathbf{u}^2}{2}\varphi_{\mathbf{u}}(\mathbf{e}_i) \in \mathbb{Z}^{p,q}$$
(97)

for i = 1, 2. It only remains to show that  $|\mathbf{u}^2|/2$  is the least positive integer such that  $(|\mathbf{u}^2|/2)\varphi_{\mathbf{u}}(\mathbf{e}_i) \in \mathbb{Z}^{p,q}$ , because in that case  $|\mathbf{u}^2|/2$  divides  $\Sigma(\varphi_{\mathbf{u}})$ . Indeed, it is clear that  $|\mathbf{u}^2|/2$  is a positive integer such that

$$\frac{|\mathbf{u}^2|}{2}\varphi_{\mathbf{u}}(\mathbf{e}_1) \in \mathbb{Z}^{p,q}.$$
(98)

Let *m* be the order of  $[\varphi_{\mathbf{u}}(\mathbf{e}_1)] \subset \mathbb{Z}^{p,q} / (\mathbb{Z}^{p,q} \cap \varphi_{\mathbf{u}}(\mathbb{Z}^{p,q}))$ . We have that  $m \mid |\mathbf{u}^2|/2$  and  $m \leq |\mathbf{u}^2|/2$ , thus there exists an integer  $\lambda$  such that

$$\frac{|\mathbf{u}^2|}{2} = m\lambda \tag{99}$$

(100)

and also

$$m\varphi_{\mathbf{u}}(\mathbf{e}_1) \in \mathbb{Z}^{p,q}.$$

Since

### Table 1

Basis and coincidence index for a rotation  $R \in OC(\mathbb{Z}^{p,q})$ , p + q = 2.

	Basis of $\mathbb{Z}^{p,q} \cap R(\mathbb{Z}^{p,q})$	Coincidence index
$\mathbf{u}^2$ odd $\mathbf{u}^2$ even	$\begin{array}{l} \{\mathbf{u},\mathbf{v}\}\\ \{\frac{1}{2}(\mathbf{u}-\mathbf{v}),\frac{1}{2}(\mathbf{u}+\mathbf{v})\} \end{array}$	$\begin{vmatrix} \mathbf{u}^2 \\ \mathbf{u}^2 \end{vmatrix} / 2$

$$\varphi_{\mathbf{u}}(\mathbf{e}_1) = -\frac{\alpha_1^2 + \alpha_2^2}{\mathbf{u}^2} \mathbf{e}_1 + \frac{2\alpha_1\alpha_2}{\mathbf{u}^2} \mathbf{e}_2, \qquad (101)$$

then

$$\frac{2m|\alpha_1||\alpha_2|}{|\mathbf{u}^2|} \quad \text{and} \quad \frac{2m|\alpha_1||\alpha_2|}{2m\lambda} \tag{102}$$

are integers. Thus

$$\lambda \mid |\alpha_1| |\alpha_2| \quad \text{and} \quad \lambda \mid |\mathbf{u}^2|. \tag{103}$$

As  $gcd(\alpha_1, \alpha_2) = 1$ , we can propose

$$gcd(\alpha_1, \alpha_2, \mathbf{u}^2) = 1, \qquad (104)$$

which yields  $\lambda = 1$  and the order of  $\varphi_{\mathbf{u}}(\mathbf{e}_1)$  turns out to be  $|\mathbf{u}^2|/2$ .

A similar argument is used to prove that the order of  $\varphi_{\mathbf{u}}(\mathbf{e}_2)$  is  $|\mathbf{u}^2|/2$ .

(2) Either  $\alpha_1$  or  $\alpha_2$  is even. In this case, following the above procedure, it can also be proved that  $|\mathbf{u}^2|$  is the least positive integer such that  $|\mathbf{u}^2|\varphi_{\mathbf{u}}(\mathbf{e}_i) \in \mathbb{Z}^{p,q}$ .

With these results, formulae for  $\Sigma(\varphi_{\mathbf{u}})$  are obtained as in the proof of Lemma 3 in Rodríguez *et al.* (2005).

We can also characterize the CSL of  $\mathbb{Z}^{p,q}$  and the demonstration leads to an explicit construction of the basic vectors.

Theorem 6. Let  $\mathbf{u} = \alpha_1 \mathbf{e}_1 + \alpha_2 \mathbf{e}_2 \in \mathbb{Z}^{p,q}$  and  $gcd(\alpha_1, \alpha_2) = 1$ . Then,  $\mathbb{Z}^{p,q} \cap \varphi_{\mathbf{u}}(\mathbb{Z}^{p,q})$  and  $\mathbb{Z}^{p,q} \cap R_{\mathbf{u}}(\mathbb{Z}^{p,q})$  are pseudo-square lattices.

The proof is completely similar to that given in Rodríguez *et al.* (2005).

A pseudo-square basis  $\{\mathbf{c}, \mathbf{d}\}$  of  $\mathbb{Z}^{p,q} \cap \varphi_{\mathbf{u}}(\mathbb{Z}^{p,q})$ , where  $\mathbf{c}, \mathbf{d} \in \mathbb{Z}^{p,q}$ , is given by

$$\mathbf{c} = \frac{1}{2}(\mathbf{u} - \mathbf{v}) = \varphi_{\mathbf{u}}(\mathbf{c}'), \tag{105}$$

$$\mathbf{d} = \frac{1}{2}(\mathbf{u} + \mathbf{v}) = \varphi_{\mathbf{u}}(\mathbf{d}'), \tag{106}$$

where  $\mathbf{v} = \alpha_2 \mathbf{e}_1 + \alpha_1 \mathbf{e}_2$  (v orthogonal to u),  $\mathbf{c}' = -\frac{1}{2}(\mathbf{u} + \mathbf{v})$ and  $\mathbf{d}' = \frac{1}{2}(\mathbf{v} - \mathbf{u})$ .

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

For instance, a basis and the coincidence index for a rotation  $R \in OC(\mathbb{Z}^{p,q})$  can be found, as illustrated in Table 1, where  $\mathbf{u} = \lambda(R(\mathbf{e}_1) - \mathbf{e}_1) \in \mathbb{Z}^{p,q}$  has relatively prime coefficients  $\alpha_1, \alpha_2, \lambda \in \mathbb{Z}$  and  $\mathbf{v} = \mathbf{u}\mathbf{e}_1\mathbf{e}_2$ .

### 6.2. Pseudo-rhombic lattices

Let  $\Gamma = \mathbb{Z}\mathbf{a}_1 + \mathbb{Z}\mathbf{a}_2$  be a pseudo-rhombic lattice in  $\mathbb{R}^{p,q}$ , *i.e.*,  $\mathbf{a}_1^2 = \mathbf{a}_2^2$ . We can assume, without generality loss, that  $\mathbf{a}_1^2 = \mathbf{a}_2^2 = 1$ . Notice that  $\{\mathbf{a}_1 + \mathbf{a}_2, \mathbf{a}_1 - \mathbf{a}_2\}$  is an orthogonal basis of  $\mathbb{R}^{p,q}$ .

By Propositions 3 and 4 the following corollary is immediate.

*Corollary 3.* Let  $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$  be a lattice in  $\mathbb{R}^{p,q}$  such that  $\mathbf{a}_1^2 = \mathbf{a}_2^2 = 1$ ,  $\mathbf{a}_1 \cdot \mathbf{a}_2 \neq \pm 1 \in \mathbb{Q}$ , then the following propositions hold:

(1) If  $T : \mathbb{R}^{p,q} \to \mathbb{R}^{p,q}$ ,  $T \in OC(\Gamma)$ , different from the identity, then there exists  $\mathbf{c} \in \Gamma$  such that

$$T(\mathbf{x}) = \begin{cases} \varphi_{\mathbf{c}}(\mathbf{x}) & \text{if } \det(T) = -1, \\ \varphi_{\mathbf{c}}\varphi_{\mathbf{d}_i}(\mathbf{x}) & \text{if } \det(T) = 1, \end{cases}$$
(107)

where *i* can be chosen as 1 or 2,  $\mathbf{d}_1 = \mathbf{a}_1 + \mathbf{a}_2$  and  $\mathbf{d}_2 = \mathbf{a}_1 - \mathbf{a}_2$ . (2) There exists  $\lambda \in \mathbb{N}$  such that  $\mathbf{v} = \lambda \mathbf{c} \cdot (\mathbf{a}_1 \wedge \mathbf{a}_2) \in \Gamma$ ,

where **v** is orthogonal to **c**.

(3)  $\Sigma(\varphi_{\mathbf{c}})$  divides  $\lambda(\mathbf{c}^2)$ .

*Remark 3.* The condition  $\mathbf{a}_1 \cdot \mathbf{a}_2 \neq \pm 1$  is required to assure that  $\mathbf{d}_1$  and  $\mathbf{d}_2$  are both non-isotropic. Part (1) tells us that  $T \in OC(\Gamma)$  is at most the composition of two simple reflections of  $OC(\Gamma)$ . Furthermore, with these results, Proposition 11 of Rodríguez *et al.* (2005) becomes a corollary.

Since  $\varphi_{\mathbf{c}} = \varphi_{\lambda \mathbf{c}}$  for any  $\lambda \in \mathbb{R}$ , then we can assume that **c** has coordinates that are relatively prime with respect to the basis  $\{\mathbf{a}_1, \mathbf{a}_2\}$ .

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

$$\varphi_{\mathbf{c}}(\mathbf{x}) = -\mathbf{c}\mathbf{x}\mathbf{c}^{-1},\tag{108}$$

$$\varphi_{\mathbf{c}}\varphi_{\mathbf{d}_i}(\mathbf{x}) = R_{\mathbf{c}}(\mathbf{x}) = \mathbf{c}\mathbf{d}_i\mathbf{x}\mathbf{d}_i^{-1}\mathbf{c}^{-1}.$$
 (109)

In particular, if  $\varphi_{\mathbf{c}}(\mathbf{x}) \in OC(\Gamma)$  then, since  $\varphi_{\mathbf{d}}(\Gamma) = \Gamma$ ,

$$\Gamma \cap \varphi_{\mathbf{c}}(\Gamma) = \Gamma \cap R_{\mathbf{c}}(\Gamma), \tag{110}$$

$$\Sigma(\varphi_{\mathbf{c}}) = \Sigma(R_{\mathbf{c}}), \tag{111}$$

and a basis of  $\Gamma \cap R_{\mathfrak{c}}(\Gamma)$  can be obtained if a basis of  $\Gamma \cap \varphi_{\mathfrak{c}}(\Gamma)$  is known.

**6.2.1.** Coincidence index and basis of the CSL. The procedure for determining the coincidence index  $\Sigma(\varphi_e)$  and a basis of the CSL,  $\Gamma \cap \varphi_e(\Gamma)$ , of the pseudo-rhombic lattice follows the same lines as in the proof of Proposition 4. 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  $\mathbb{R}^{p,q}$ , such that  $\mathbf{a}_1^2 = \mathbf{a}_2^2$ . From Proposition 4, we know that there exists  $\mathbf{c} = \alpha_1 \mathbf{a}_1 + \alpha_2 \mathbf{a}_2 \in \Gamma$ , where  $gcd(\alpha_1, \alpha_2) = 1$ , such that  $\varphi_{\mathbf{c}} \in OC(\Gamma)$ . We know also that there exists a vector  $\mathbf{d} \in \Gamma$  such that  $\Gamma = \mathbb{Z}\mathbf{c} \oplus \mathbb{Z}\mathbf{d}$ ; in fact  $\mathbf{d} = -\beta_2 \mathbf{a}_1 + \beta_1 \mathbf{a}_2$ , where  $\alpha_1\beta_1 + \alpha_2\beta_2 = 1$ .

A basis of 
$$\Gamma \cap \varphi_{\mathbf{c}}(\Gamma)$$
 is

$$\{\mathbf{c}, m\varphi_{\mathbf{c}}(\mathbf{d})\},\tag{112}$$

where m is the least natural number such that

$$m\varphi_{\mathbf{c}}(\mathbf{d}) \in \Gamma \cap \varphi_{\mathbf{c}}(\Gamma).$$
 (113)

The natural number *m* is also the coincidence index  $\Sigma(\varphi_c)$ , and its value can be obtained from the rational components of

 $\varphi_{\mathbf{c}}(\mathbf{d})$  with respect to the basis  $\{\mathbf{a}_1, \mathbf{a}_2\}$  as indicated in Rodríguez *et al.* (2005), *i.e.* if

$$\varphi_{\mathbf{c}}(\mathbf{d}) = \frac{r_1}{n_1} \mathbf{a}_1 + \frac{r_2}{n_2} \mathbf{a}_2, \qquad (114)$$

where  $r_1, r_2, n_1, n_2 \in \mathbb{Z}$ , then

$$\Sigma(\varphi_{\mathbf{c}}) = m = \operatorname{lcm}(n_1, n_2), \tag{115}$$

where lcm stands for the least common multiple.

Now, consider a vector  $\mathbf{u} \in \Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$ . From Theorem 4 we know that  $\varphi_{\mathbf{u}}$  is a coincidence reflection provided that

$$\frac{(\mathbf{u} \cdot \mathbf{a}_i)}{\mathbf{u}^2} \in \mathbb{Q}.$$
(116)

With this condition the reasoning follows the same lines as in the last part of the Section 6.2 of Rodríguez *et al.* (2005); given  $\mathbf{c} = \alpha_1 \mathbf{a}_1 + \alpha_2 \mathbf{a}_2 \in \Gamma$ , where  $gcd(\alpha_1, \alpha_2) = 1$ , then by substituting in (116) we get that  $\varphi_{\mathbf{c}} \in OC(\Gamma)$  provided that  $\mathbf{a}_1 \cdot \mathbf{a}_2 \in \mathbb{Q}$ ; if  $\mathbf{a}_1 \cdot \mathbf{a}_2 \notin \mathbb{Q}$  then we need  $\mathbf{d}_1 = \mathbf{a}_1 + \mathbf{a}_2$  and  $\mathbf{d}_2 = \mathbf{a}_1 - \mathbf{a}_2$ , and in this last case we have that

$$OC(\Gamma) = \{I, \varphi_{\mathbf{d}_1}, \varphi_{\mathbf{d}_2}, \varphi_{\mathbf{d}_1}\varphi_{\mathbf{d}_2}\}.$$
(117)

### 6.3. Pseudo-rectangular lattices

Let  $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$  be a pseudo-rectangular lattice, *i.e.*,  $\mathbf{a}_1 \cdot \mathbf{a}_2 = 0$ . Without loss of generality, we can suppose that  $\mathbf{a}_1^2 = 1$ . From Propositions 3 and 4 the following corollary is immediate.

*Corollary 4.* Let  $\Gamma = \mathbb{Z}\mathbf{a}_1 \oplus \mathbb{Z}\mathbf{a}_2$  be a pseudo-rectangular lattice in  $\mathbb{R}^{p,q}$ ,  $\mathbf{a}_1 \cdot \mathbf{a}_2 = 0$ ,  $\mathbf{a}_1^2 = 1$  and  $\mathbf{a}_2^2 \in \mathbb{Q}$ . Then the following propositions hold:

(1) If  $T : \mathbb{R}^{p,q} \to \mathbb{R}^{p,q}$ ,  $T \in OC(\Gamma)$ , different from the identity, then there exists  $\mathbf{c} \in \Gamma$  such that

$$T(\mathbf{x}) = \begin{cases} \varphi_{\mathbf{c}}(\mathbf{x}) & \text{if } \det(T) = -1, \\ \varphi_{\mathbf{c}}\varphi_{\mathbf{a}_{i}}(\mathbf{x}) & \text{if } \det(T) = 1, \end{cases}$$
(118)

where *i* can be chosen as 1 or 2.

(2) There exists  $\lambda \in \mathbb{N}$  such that  $\mathbf{v} = \lambda \mathbf{c} \cdot (\mathbf{a}_1 \wedge \mathbf{a}_2) \in \Gamma$ , where  $\mathbf{v}$  is orthogonal to  $\mathbf{c}$ .

(3)  $\Sigma(\varphi_{\mathbf{c}})$  divides  $\lambda(\mathbf{c}^2)$ .

Part (1) generalizes Proposition 9 of Rodríguez et al. (2005).

**6.3.1.** Coincidence index and basis of the CSL. The procedure for determining the coincidence index  $\Sigma(\varphi_e)$  and a basis of the CSL,  $\Gamma \cap \varphi_e(\Gamma)$ , follows the same lines as in the case of the pseudo-rhombic lattice. For that reason, here we only summarize the results without further details.

Let

$$\varphi_{\mathbf{c}}(\mathbf{x}) = -\mathbf{c}\mathbf{x}\mathbf{c}^{-1},\tag{119}$$

$$R_{\mathbf{c}}(\mathbf{x}) = \mathbf{c}\mathbf{a}_i \mathbf{x} \mathbf{a}_i^{-1} \mathbf{c}^{-1}, \qquad (120)$$

$$R_{\mathbf{c}}(\Gamma) \cap \Gamma = \varphi_{\mathbf{c}}(\Gamma) \cap \Gamma, \qquad (121)$$

where  $\mathbf{c} \in \Gamma$ . Again, as in equation (115), we have that

$$\Sigma(\varphi_{\mathbf{c}}) = m = \operatorname{lcm}(n_1, n_2), \qquad (122)$$

where  $n_1$  and  $n_2$  correspond to equation (114).

A basis of  $\Gamma \cap \varphi_{\mathbf{c}}(\Gamma)$  is

$$[\mathbf{c}, m\varphi_{\mathbf{c}}(\mathbf{d})], \tag{123}$$

where *m* is the least natural number such that equation (113) is fulfilled,  $\mathbf{c}$  and  $\mathbf{d}$  are defined in §6.2.1.

Finally, to characterize  $OC(\Gamma)$  we notice that since  $\mathbf{a}_1^2 = 1$ , the reasoning follows the same lines as in Section 5.2 of Rodríguez *et al.* (2005) to obtain that if  $\mathbf{a}_2^2 \notin \mathbb{Q}$ , then

$$OC(\Gamma) = \{I, \varphi_{\mathbf{a}_1}, \varphi_{\mathbf{a}_2}, \varphi_{\mathbf{a}_2}, \varphi_{\mathbf{a}_1}\}.$$
 (124)

### 7. Conclusions

We have generalized our previous work on coincidence lattices to cover the case of the space  $\mathbb{R}^{p,q}$  for p + q = 2. This required a consideration of the Cartan–Dieudonné theorem and the development of a constructive view leading to explicit expressions for the simple reflections factoring a given orthogonal transformation.

We have formulated the CSL problem for lattices in  $\mathbb{R}^{p,q}$ (p+q=2) using Clifford algebras in a metric-independent way and have constructed explicitly the bases and coincidence indices for several interesting cases. We also show that in this case any coincidence isometry can be decomposed as a product of at most two reflections by vectors of the lattice.

In this way we argue that Clifford algebra is the right tool for this and other important problems in crystallography.

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### References

- Ablamowicz, R., Lounesto, P. & Maks, J. (1991). Found. Phys. 21, 735–748.
- Aragón, G., Aragón, J. L., Dávila, F., Gómez, A. & Rodíguez, M. A. (2001). Geometric Algebra with Applications in Science and Engineering, edited by E. Bayro-Corrochano & G. Sobczyk, pp. 371–386. Boston: Birkhäuser.
- Aragón-González, G., Aragón, J. L. & Rodríguez-Andrade, M. A. (2006). J. Math. Phys. 47, 013509.
- Artin, E. (1957). *Geometric Algebra*. New York: Interscience Publishers.
- Baake, M. (1997). The Mathematics of Aperiodic Order, edited by R. V. Moody, pp. 9–44. Dordrecht: Kluwer Academic Publishers.
- Bayro-Corrochano, E. & Sobczyk, G. (2001). Editors. *Geometric Algebra with Applications in Science and Engineering*. Boston: Birkhäuser.
- Chevalley, C. C. (1954). *The Algebraic Theory of Spinors*. Cambridge: Columbia University Press.

Hestenes, D. (2007). J. Math. Phys. 48, 023514.

- Hestenes, D. & Sobczyk, G. (1985). Clifford Algebra to Geometric Calculus. A Unified Language for Mathematics and Physics. Holland: D. Reidel Publishing Co.
- Hitzer, E. & Perwass, C. (2005). Proceedings of the International Conference on Numerical Analysis and Applied Mathematics 2005, edited by T. E. Simos, G. Sihoyios & C. Tsitouras, pp. 937–941. Weinheim: Wiley-VCH.
- Lounesto, P. (2001). *Clifford Algebras and Spinors*, 2nd ed. Cambridge University Press.
- Mackay, A. L. (2002). Struct. Chem. 13, 215-220.
- Porteous, I. (1995). *Clifford Algebras and the Classical Groups*. Cambridge University Press.
- Reed, B. W., Minich, R. W., Rudd, R. E. & Kumar, M. (2004). Acta Cryst. A60, 263–277.
- Riesz, M. (1993). Clifford Numbers and Spinors: with Riesz's Private Lectures to E. Folke Bolinder and a Historical Review by Pertti Lounesto. New York: Springer.
- Rodríguez, M. A., Aragón, J. L. & Verde-Star, L. (2005). Acta Cryst. A61, 173–184.
- Rotman, J. J. (1995). An Introduction to the Theory of Groups, 4th ed. New York: Springer.
- Sadoc, J.-F. & Charvolin, J. (1989). Acta Cryst. A45, 10-20.
- Snapper, E. & Troyer, R. J. (1971). *Metric Affine Geometry*. New York: Dover.
- Zou, Y. M. (2006a). Acta Cryst. A62, 109-114.
- Zou, Y. M. (2006b). Acta Cryst. A62, 454-458.