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Structures of coincidence symmetry groups

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The structure of the coincidence symmetry group of an arbitrary n-dimensional lattice in the n-dimensional Euclidean space is considered by describing a set of generators. Particular attention is given to the coincidence isometry subgroup (the subgroup formed by those coincidence symmetries that are elements of the orthogonal group). Conditions under which the coincidence isometry group can be generated by reflections defined by vectors of the lattice are discussed and an algorithm to decompose an arbitrary element of the coincidence isometry group in terms of reflections defined by vectors of the lattice is given.

1. Introduction

The mathematical theory of the coincidence site lattice (CSL) can be used to describe certain phenomena that arise in the physics of interfaces and grain boundaries [for a more detailed background in CSL theory, we refer readers to the references, especially Baake (1997), Bollmann (1970) and Grimmer (1973)]. Because of the success of the models for crystalline interfaces based on the properties of CSL and related lattices (Brandon *et al.*, 1964; Bollmann, 1970; Warrington & Bufalini, 1971; Grimmer, 1973, 1976), the focus of the CSL theory has been mostly on the coincidence of two lattices of the same dimensions (the coincidence of two lattices of different dimensions can be easily reduced to the same dimension case). Fortes (1983*a*,*b*) developed a matrix theory of CSL by using the normal form of an integer matrix. In his first paper, Fortes (1983*a*) gave a crystallographic interpretation of the invariant set of an integer matrix and applied it to solve the degree of coincidence problem of two lattices in arbitrary dimensions. In the subsequent paper (Fortes, 1983*b*), the theory was extended to include displacement shift complete (DSC) lattices and a method to calculate bases for these lattices *via* some special factorizations of the related matrices was provided. Duneau *et al.* (1992) further developed the matrix theory of CSL by using the normal form of an integer matrix and gave a method to decompose the corresponding matrix into associated shear transformations. Pleasants *et al.* (1996) used number theory to solve the planar coincidences for N-fold symmetry. Baake (1997) used the factorization properties of certain number fields to solve the coincidence problem for dimensions up to 4. Recently, Aragón *et al.* (2001) and Rodríguez *et al.* (2005) developed a different approach to coincidence isometry theory by using geometric algebra (Clifford algebra) as a tool. From the works in the literature, problems on the structures of the coincidence symmetry group of a given lattice can be formulated. In this paper, we consider the structure of the coincidence isometry group of a lattice in $\mathbb{R}^n$.

Let L be a lattice with basis $(a_1, \ldots, a_n)$, let V be the n-dimensional real vector space with the same basis, let $\mathcal{A}$ be a linear transformation of V and let A be the matrix of $\mathcal{A}$ under the basis $(a_1, \ldots, a_n)$. We call $\mathcal{A}$ a coincidence symmetry if $\mathcal{A}$ is an automorphism of V and $L \cap \mathcal{A}L$ is a sublattice of L with finite index. If $\mathcal{A}$ is a coincidence symmetry of L, we call A a coincidence matrix of L or, abusing the language, we also call A a coincidence symmetry. It is known (see §2) that A is a coincidence symmetry if and only if A is a rational matrix. The set of all coincidence symmetries (or the set of all $n \times n$ coincidence matrices) of L forms a group under the multiplication defined by composition (or the multiplication of matrices). If L is a lattice of the Euclidean space $\mathbb{R}^n$, then one can consider the isometries of $\mathbb{R}^n$ that are coincidence symmetries of L. In this case, one has the coincidence isometry subgroup formed by all the coincidence isometries (Baake, 1997). We analyze the structures of these groups by considering the decomposition of a matrix from both geometric and algebraic view points. Baake (1997) (see also Pleasants *et al.*, 1996) uses the factorization of numbers to reduce a symmetry to irreducible ones, while the approach developed by Aragón *et al.* (2001) and Rodríguez *et al.* (2005) relies on the decomposition of a matrix into a product of coincidence reflections. The results in Aragón *et al.* (2001) stated that, if the matrix is a product of coincidence reflections, then the corresponding symmetry is a coincidence isometry. In Rodríguez *et al.* (2005), it was conjectured that any coincidence isometry of the lattice spanned by the canonical basis of $\mathbb{R}^n$ is a product of coincidence reflections. We shall prove a theorem that includes this conjecture as a special case and use the theorem to describe the coincidence isometry group.

In §2, we briefly recall the relevant definitions and some known results. In §3, we prove a theorem about coincidence isometry groups of lattices L in $\mathbb{R}^n$, and apply it to describe the structure of the coincidence isometry group. Examples are given in §4.

2. Notation and definitions

The set of real numbers is denoted by $\mathbb{R}$, the set of real $n \times n$ matrices is denoted by $M_n(\mathbb{R})$ and the set of all non-singular $n \times n$ real matrices is denoted by $GL_n(\mathbb{R})$. Notation for matrices over the rational numbers $\mathbb{Q}$ and the integers $\mathbb{Z}$ are defined similarly. For example, $GL_n(\mathbb{Z})$ denotes the set of all invertible $n \times n$ integer matrices, so

$$GL_n(\mathbb{Z}) = \{n \times n \text{ integer matrices } A \text{ with } \det A = \pm 1\}.$$

We also consider the above sets of non-singular matrices as linear transformations. For example, we also regard $GL_n(\mathbb{R})$ as the set of all non-singular linear transformations of $\mathbb{R}^n$. If we do regard them as linear transformations, we shall specify the basis that relates the transformations to their matrices.

By an n-dimensional lattice L with basis $(a_1, \ldots, a_n)$, we mean the free abelian group $\oplus_{i=1}^n \mathbb{Z}a_i$. With the basis $(a_1, \ldots, a_n)$, we can always define a standard inner product on the n-dimensional real vector space $\oplus_{i=1}^n \mathbb{R}a_i$ by requiring $(a_1, \ldots, a_n)$ to be an orthonormal basis. This defines an isometry between the usual n-dimensional Euclidean space $\mathbb{R}^n$ and $\oplus_{i=1}^n \mathbb{R}a_i$. However, usually we need to consider a lattice in the n-dimensional Euclidean space $\mathbb{R}^n$ with canonical basis $(e_1, \ldots, e_n)$. In this case, we assume the lattice to be also n-dimensional since, if the lattice has dimension $m < n$, then we can always consider the m-dimensional subspace of $\mathbb{R}^n$ that contains the lattice of interest. Thus, a lattice $L \subset \mathbb{R}^n$ is given by an $n \times n$ non-singular matrix A and a basis of the lattice is

$$(a_1, \ldots, a_n) = (e_1, \ldots, e_n)A. \quad (1)$$

We call the matrix A the structure matrix of L and use the notation L_A if we want to specify the fact that the lattice L is given by the matrix A.

We adopt the definition that a sublattice $L' \subset L$ is a subgroup L' of finite index in the abelian group L. In the usual notation, this is $[L : L'] < \infty$. The CSL theory concerns the problems that arise when the intersection $L_1 \cap L_2$ of two lattices happens to be a sublattice of both lattices L_1 and L_2. If this is the case, we say that L_1 and L_2 are commensurate lattices.

Suppose that L_i is given by the structure matrix A_i, $i = 1, 2$, let the basis of L_i be $\mathbf{B}_i$. Then

$$\mathbf{B}_i = (e_1, \ldots, e_n)A_i, \quad i = 1, 2.$$

Theorem 2.1. *Grimmer*. The lattices L_1 and L_2 are commensurate if and only if $A_2^{-1}A_1$ is a rational matrix.

Proof. Let $L' = L_1 \cap L_2$ and let $\mathbf{B}'$ be a basis of L'. Then there are integer matrices N_i $(i = 1, 2)$ such that

$$\mathbf{B}_1 N_1 = \mathbf{B}' = \mathbf{B}_2 N_2.$$

Under the assumption that L_1 and L_2 are commensurate, *i.e.* $[L_i : L'] < \infty$ $(i = 1, 2)$, the matrices N_i are non-singular, thus, from $A_1N_1 = A_2N_2$, we obtain $A_2^{-1}A_1 = N_2N_1^{-1}$, implying that $A_2^{-1}A_1$ is a rational matrix. Conversely, if $A_2^{-1}A_1$ is a rational matrix, then there exists an integer $m > 0$ such that $mA_2^{-1}A_1$ is an integer matrix, say A. Then, from $mA_1 = A_2A$, we have $m\mathbf{B}_1 = \mathbf{B}_2A$. Hence, $mL_1 \subset L'$, which implies that $[L_1 : L'] \leq m^n$. Symmetrically, we also have $[L_2 : L'] < \infty$. Therefore, L_1 and L_2 are commensurate.

Grimmer's theorem immediately implies the following.

Corollary 2.2. Let L be a lattice with basis $(a_1, \ldots, a_n)$ and let A be an $n \times n$ non-singular real matrix. Then the lattice with basis $(a_1, \ldots, a_n)A$ and the lattice L are commensurate if and only if A is a rational matrix.

However, if we view the matrix A in the above corollary as the matrix of a linear transformation, then we need to specify under which basis this matrix is given. In Corollary 2.2, the matrix is given by using the basis $(a_1, \ldots, a_n)$. Let us consider a lattice L in $\mathbb{R}^n$ with the structure matrix A. Let $\mathcal{T}$ be a linear transformation of $\mathbb{R}^n$ and let T be the matrix of $\mathcal{T}$ under the canonical basis $(e_1, \ldots, e_n)$. Then the structure matrix of the lattice $\mathcal{T}(L)$ (the image of L under the transformation $\mathcal{T}$) is TA. Then by Theorem 2.1, the lattice $\mathcal{T}(L)$ and the lattice L are commensurate if and only if $A^{-1}TA$ is rational. This leads to the following definition.

Definition 2.3. Let $L_A \subset \mathbb{R}^n$ be a lattice with the structure matrix A. We call the group $AGL_n(\mathbb{Q})A^{-1}$ the coincidence symmetry group (CSG) of L_A.

The isometries of $\mathbb{R}^n$ [with the standard inner product (,)] that provide commensurate lattices to a lattice $L \subset \mathbb{R}^n$ are of special interest (*cf*. Baake, 1997; Aragón *et al.*, 2001; Rodríguez *et al.*, 2005). Let $O(n)$ be the set of orthogonal transformations of $\mathbb{R}^n$. The concept of coincidence isometry group was defined in Baake (1997) with the notation $OC(L)$, *i.e.*

$$OC(L) = \{\mathcal{R} \in O(n) : [L : L \cap \mathcal{R}L] < \infty\}.$$

For our purpose, we need a definition in terms of matrices under the canonical basis of $\mathbb{R}^n$. Let

$$O_n(\mathbb{R}) = \{A \in M_n(\mathbb{R}) : A^tA = I\}.$$

That is, $O_n(\mathbb{R})$ is the set of $n \times n$ orthogonal real matrices.

Suppose that $\mathcal{R} \in O(n)$ and $[L : L \cap \mathcal{R}(L)] < \infty$. Let R be the matrix of $\mathcal{R}$ under the canonical basis, then $R \in O_n(\mathbb{R})$. From the discussion preceding Definition 2.3, we conclude that the matrix $A^{-1}RA$ is rational. Thus we give the following definition.

Definition 2.4. Let $L_A \subset \mathbb{R}^n$ be a lattice with the structure matrix A. We call the group $O_n(\mathbb{R}^n) \cap (AGL_n(\mathbb{Q})A^{-1})$ the coincidence isometry group (CIG) of L_A.

Thus, the CIG of L is just the group $OC(L)$ and we will use both terms for our convenience.

Example. If $L = \mathbb{Z}^n$, then $A = I$ and $OC(L) = O_n(\mathbb{Q}) := O_n(\mathbb{R}^n) \cap GL_n(\mathbb{Q})$. We call the elements of $O_n(\mathbb{Q})$ rational orthogonal matrices.

In the next section, we analyze the structure of the coincidence isometry group of an arbitrary lattice L in $\mathbb{R}^n$.

3. Decomposition of elements of a CIG into reflections

The decomposition of an element of the CIG of a lattice $L \subset \mathbb{R}^n$ is central in the Clifford algebra approach to the coincidence site lattice problem developed in Aragón *et al.* (2001) and Rodríguez *et al.* (2005). It was conjectured (and proved for the planar lattices) in Rodríguez *et al.* (2005) that any coincidence isometry of the canonical lattice $\mathbb{Z}^n$ of $\mathbb{R}^n$ can be decomposed as a product of coincidence reflections (reflections that belong to the coincidence isometry group of L). Note that, for the lattice $\mathbb{Z}^n$, the corresponding CIG is $O_n(\mathbb{Q})$. Here, we prove a more general theorem that includes the lattice $\mathbb{Z}^n$ as a special case. It should be pointed out that, although the Cartan–Dieudonné theorem (Porteous, 1995, ch. 5) says that any orthogonal $n \times n$ real matrix can be decomposed into a product of at most n reflections, it is clear that a statement of coincidence isometries of certain lattices that can be decomposed into a product of coincidence reflections is not a direct consequence of the Cartan–Dieudonné theorem (*cf.* Example 4.2 below).

Theorem 3.1. Let $L \subset \mathbb{R}^n$ be a lattice such that the reflection defined by an arbitrary nonzero vector of L is a coincidence isometry of L. Then any coincidence isometry of L can be decomposed as a product of at most n reflections defined by the vectors in L.

Proof. Let the structure matrix of L be A. Then

$$\mathbf{B} = (b_1, \ldots, b_n) := (e_1, \ldots, e_n)A$$

is a basis of L. Let $\mathcal{R} \in O(n)$ be a coincidence isometry of L. We use induction on n to prove the theorem. It is clear that the theorem holds for $n = 1$. Assume that it holds for all k such that $1 \le k < n$ and consider the case n. We consider two cases: $\mathcal{R}(b_1) = b_1$ or $\mathcal{R}(b_1) \neq b_1$.

In the first case, let

$$V = \{x \in \mathbb{R}^n : (x, b_1) = 0\}.$$

Then V is an $(n-1)$-dimensional subspace of $\mathbb{R}^n$ and V is invariant under $\mathcal{R}$, *i.e.* $\mathcal{R}(V) = V$. Thus, $\mathcal{R}$ restricts to an orthogonal transformation $\mathcal{R}'$ of the $(n-1)$-dimensional Euclidean subspace V. Compare the orthogonal projection $\mathcal{P} : \mathbb{R}^n \longrightarrow V$ defined by b_1:

$$\mathcal{P}(x) = x - \frac{(x, b_1)}{(b_1, b_1)} b_1, \quad \forall x \in \mathbb{R}^n, \tag{2}$$

with the reflection of $\mathbb{R}^n$ defined by b_1:

$$\mathcal{R}_{b_1}(x) = x - \frac{2(x, b_1)}{(b_1, b_1)} b_1, \quad \forall x \in \mathbb{R}^n. \tag{3}$$

We can see that, under the assumption of the theorem, for each b_i $(1 < i \le n)$, there exists an integer $m_i > 0$ such that $m_i \mathcal{P}(b_i) \in L$. Let $m = m_2 \ldots m_n$, then $m\mathcal{P}(L) \subset L$. Hence, $\mathcal{R}'$ is a coincidence isometry of the $(n-1)$-dimensional lattice $\mathcal{P}(L)$ [with basis $(\mathcal{P}(b_2), \ldots, \mathcal{P}(b_n))$] that satisfies the condition of the theorem. Therefore, by induction assumption, $\mathcal{R}'$ is a product of j reflections defined by some vectors $y_1, \ldots, y_j \in \mathcal{P}(L)$ such that $1 \le j \le n-1$. Let $x_i = my_i$, $1 \le i \le j$. Then all $x_i \in L$. Let the reflection of $\mathbb{R}^n$ defined by x_i be $\mathcal{R}_i$, then $\mathcal{R} = \mathcal{R}_1 \ldots \mathcal{R}_j$. Hence the theorem is proved in this case.

In the second case, $\mathcal{R}(b_1) \neq b_1$, thus $a := \mathcal{R}(b_1) - b_1 \neq 0$. Let $\mathcal{R}_a$ be the reflection defined by the vector a. Since $\mathcal{R}$ is a coincidence isometry of L, there exists an integer $t > 0$ such that $ta \in L$. However, $\mathcal{R}_a = \mathcal{R}_{ta}$, so $\mathcal{R}_a$ can be viewed as a reflection defined by a vector in L. Consider the coincidence isometry $\mathcal{R}_a\mathcal{R}$ of L. Note that $(b_1, b_1) = (\mathcal{R}(b_1), \mathcal{R}(b_1))$, we have (it can also be seen easily *via* a geometric diagram)

$$\begin{aligned}\mathcal{R}_a\mathcal{R}(b_1) &= \mathcal{R}(b_1) - \frac{2(\mathcal{R}(b_1), a)}{(a, a)} a \\ &= \mathcal{R}(b_1) - \frac{2(\mathcal{R}(b_1), \mathcal{R}(b_1) - b_1)}{(\mathcal{R}(b_1) - b_1, \mathcal{R}(b_1) - b_1)} (\mathcal{R}(b_1) - b_1) \\ &= b_1.\end{aligned}$$

Thus, by the first case, $\mathcal{R}_a\mathcal{R}$ is a product of at most $n-1$ reflections defined by some vectors of L, say $\mathcal{R}_a\mathcal{R} = \mathcal{R}_1 \ldots \mathcal{R}_j$ with $1 \le j \le n-1$. Then, since $\mathcal{R}_a^2 = I$, we conclude that $\mathcal{R} = \mathcal{R}_a\mathcal{R}_1 \ldots \mathcal{R}_j$ is a product of at most n reflections defined by vectors of L. This completes the proof of the theorem.

Note that the proof of Theorem 3.1 gives a practical way to actually decompose a coincidence isometry into a product of coincidence reflections. We give an example in §4.

It turns out that the condition in Theorem 3.1 is sufficient for any application purpose for which the computations involve only rational numbers. The following theorem gives a necessary and sufficient condition for a lattice to satisfy the condition in Theorem 3.1.

Theorem 3.2. Let $L \subset \mathbb{R}^n$ be a lattice with structure matrix $A = (a_{ij})$ and let $a_i, 1 \le i \le n$, be the column vectors of A. Then every nonzero vector of L defines a coincidence reflection of L if and only if the ratios

$$\frac{(a_j, a_i)}{(a_k, a_k)}, \quad 1 \le i, j, k \le n, \tag{4}$$

are all rational.

Proof. If every nonzero vector of L defines a coincidence reflection of L, then, in particular, every a_i $(1 \le i \le n)$ defines a coincidence reflection of L. Let $\mathcal{R}_i$ be the reflection defined by a_i. Then, since

$$\mathcal{R}_i(a_j) = a_j - \frac{2(a_j, a_i)}{(a_i, a_i)} a_i, \quad \forall j, \tag{5}$$

we must have

$$\frac{(a_j, a_i)}{(a_i, a_i)} \in \mathbb{Q}, \quad 1 \leq i, j \leq n. \tag{6}$$

If $(a_i, a_k) \neq 0$, then

$$\frac{(a_i, a_i)}{(a_k, a_k)} = \frac{(a_i, a_k)}{(a_k, a_k)} \frac{(a_i, a_i)}{(a_i, a_k)}$$

is a product of two rational numbers and hence is rational. If $(a_i, a_k) = 0$, consider the reflection $\mathcal{R}_c$ defined by $c = a_i - a_k$. By assumption, $\mathcal{R}_c$ is a coincidence reflection of L. Thus, from

$$\mathcal{R}_c(a_i) = a_i - \frac{2(a_i, c)}{(c, c)} c,$$

we have

$$\frac{(a_i, c)}{(c, c)} = \frac{(a_i, a_i)}{(a_i, a_i) + (a_k, a_k)} = \frac{1}{1 + \frac{(a_k, a_k)}{(a_i, a_i)}}$$

is rational. Hence we also have

$$\frac{(a_i, a_i)}{(a_k, a_k)} \in \mathbb{Q}.$$

Together with (6), this proves (4).

Conversely, if (4) holds, let $x = AX \in L$ be a nonzero vector, where $X = (x_1, \ldots, x_n)^t \in \mathbb{Z}^n$ is a column vector. Then, for any $1 \leq i \leq n$,

$$\frac{(a_i, x)}{(x, x)} = \frac{\sum_{j=1}^{n} x_j (a_i, a_j)}{\sum_{s,t=1}^{n} x_s x_t (a_s, a_t)} = \frac{\sum_{j=1}^{n} x_j \frac{(a_i, a_j)}{(a_i, a_i)}}{\sum_{s,t=1}^{n} x_s x_t \frac{(a_s, a_t)}{(a_i, a_i)}}$$

is rational. It follows that the reflection defined by x is a coincidence isometry of L. This completes the proof of the theorem.

A useful consequence of Theorem 3.2 is the following.

Corollary 3.3. Let $L \subset \mathbb{R}^n$ be a lattice with the structure matrix A. If $A^t A$ is a rational matrix, then every nonzero vector of L defines a coincidence reflection of L and hence every coincidence isometry of L can be decomposed into a product of at most n coincidence reflections defined by the vectors of L.

Proof. Keep the notation of Theorem 3.2. Under the assumption that $A^t A$ is rational, all (a_i, a_j), $1 \leq i, j \leq n$, are rational, hence condition (4) holds.

A special case of Corollary 3.3 is when the matrix A is rational.

Corollary 3.4. If A is rational, then every nonzero vector of L defines a coincidence reflection of L and hence every coincidence isometry of L can be decomposed into a product of at most n coincidence reflections defined by the vectors of L.

The decomposition of a coincidence isometry of the lattice $L = \mathbb{Z}^n$ into a product of coincidence reflections is just a special case of Corollary 3.3.

By Theorem 3.1 and Theorem 3.2, we immediately obtain the following.

Theorem 3.5. If the structure matrix A of a lattice $L \subset \mathbb{R}^n$ satisfies condition (4), then $OC(L)$ is generated by the reflections defined by the nonzero vectors of L.

As an application, we have the following.

Theorem 3.6. For $n > 1$, $OC(\mathbb{Z}^n)$ is infinitely generated.

To prove Theorem 3.6, we need the following fact about the rational numbers:

Lemma 3.7. Let S be a finite subset of the rational numbers $\mathbb{Q}$ and let P be the set of all the prime integers that show up in the denominators of the reduced forms of the elements of S. If only addition, subtraction and multiplication are allowed, then S cannot produce rational numbers whose denominators of the reduced forms contain prime factors not in P.

Now we are ready to prove Theorem 3.6.

Proof of Theorem 3.6. Assume that $n > 1$ and let $G = OC(\mathbb{Z}^n)$. Under the assumption of the theorem, every nonzero vector $v \in \mathbb{Z}^n$ generates an element $\mathcal{R}_v \in G$. By Corollary 2.2, the matrix of $\mathcal{R}_v$ under the canonical basis $(e_1, \ldots, e_n)$ is a rational matrix. Since the inverse of an orthogonal matrix is its transpose, G is generated as a group by the rational matrices defined by the reflections of the nonzero vectors of $\mathbb{Z}^n$ involving only addition, subtraction and multiplication of rational numbers. If G is finitely generated, then there is a finite subset S of G whose elements are rational matrices that generates G. Let P be the set of all the prime integers that show up in the denominators of the reduced forms of the rational numbers involved in the elements of S. To prove the theorem, by Lemma 3.7, we only need to show that there is a nonzero vector $v \in \mathbb{Z}^n$ such that the matrix of $\mathcal{R}_v$ under the canonical basis involves rational numbers whose reduced forms contain prime factors in the denominators that are not in P.

We consider vectors of the form

$$v = e_1 + y e_2, \quad y \in \mathbb{Z},$$

and consider the fraction that shows up in

$$\mathcal{R}_v(e_1) = e_1 - \frac{2}{1 + y^2}(e_1 + y e_2). \tag{7}$$

Suppose p is the largest element in P. If we let $y = p_1 \ldots p_r$ be the product of the first r primes $\leq p$, then all the prime factors of the denominator of the fraction in (7) are not in P. This completes the proof of Theorem 3.6.

It should be pointed out that a detailed analysis of the group of $OC(\mathbb{Z}^2)$ is contained in Baake (1997).

4. Examples

We consider two examples in this section. In the first example, we show how to use the procedure in the proof of Theorem 3.1 to decompose a coincidence isometry into a product of coincidence reflections. In the second example, we consider special types of lattices in $\mathbb{R}^2$ and determine their coincidence isometry groups.

Example 4.1. Let $L \subset \mathbb{R}^2$ be the rhombic lattice defined by the matrix

$$A = \begin{pmatrix} 1 & \frac{2}{3} \\ 0 & \frac{\sqrt{5}}{3} \end{pmatrix}.$$

Let

$$R = \begin{pmatrix} -\frac{19}{21} & -\frac{4\sqrt{5}}{21} \\ \frac{4\sqrt{5}}{21} & -\frac{19}{21} \end{pmatrix}.$$

Then, R is an orthogonal matrix and

$$A^{-1}RA = \begin{pmatrix} -\frac{9}{7} & -\frac{4}{7} \\ \frac{4}{7} & -\frac{11}{21} \end{pmatrix}.$$

Thus, R is a coincidence isometry of the lattice L (the coincidence index is 21). Denote the column vectors of A by a_1, a_2. Let

$$b_1 = R(a_1) - a_1 = \begin{pmatrix} \frac{-40}{21} \\ \frac{4\sqrt{5}}{21} \end{pmatrix}.$$

Then the matrix of the reflection $\mathcal{R}_{b_1}$ under the canonical basis is

$$R_1 = \begin{pmatrix} -\frac{19}{21} & \frac{4\sqrt{5}}{21} \\ \frac{4\sqrt{5}}{21} & \frac{19}{21} \end{pmatrix}$$

and

$$R_1 R = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \qquad (8)$$

Let

$$b_2 = 2a_1 - 3a_2 = \begin{pmatrix} 0 \\ -\sqrt{5} \end{pmatrix}.$$

Then b_2 is a scalar multiple of the projection of a_2 with respect to the orthogonal projection defined by a_1. The matrix R_2 of the reflection defined by b_2 under the canonical basis is the matrix on the right-hand side of (8) and $R = R_1 R_2$.

Example 4.2. Let $L \subset \mathbb{R}^2$ be a lattice with the structure matrix

$$A = \begin{pmatrix} a & 1 \\ 0 & b \end{pmatrix}, \qquad (9)$$

where a and b are arbitrary positive real numbers. Let the column vectors of A be a_1, a_2. For this matrix, condition (4) is equivalent to

$$a, \frac{a}{1+b^2} \in \mathbb{Q} \Longleftrightarrow a, b^2 \in \mathbb{Q}.$$

If this is the case, $OC(L)$ is generated by the reflections defined by the nonzero vector of L.

If $a \notin \mathbb{Q}$, but $a/(1+b^2) \in \mathbb{Q}$, then $b^2 \notin \mathbb{Q}$. To find the condition for a reflection to be a coincidence reflection, we only need to consider vectors of the form $v = xe_1 + e_2, x \in \mathbb{R}$ (these vectors need not be in L). Consider

$$\begin{aligned} \frac{(v, a_1)}{(v, v)} v &= \frac{ax}{1+x^2} v = \frac{x(bx-1)}{b(1+x^2)} a_1 + \frac{ax}{b(1+x^2)} a_2, \\ \frac{(v, a_2)}{(v, v)} v &= \frac{x+b}{1+x^2} v = \frac{(x+b)(bx-1)}{ab(1+x^2)} a_1 + \frac{x+b}{b(1+x^2)} a_2. \end{aligned} \qquad (10)$$

If at least one of $x + b$ and $bx - 1$ is 0, then the fractions involved in (10) are all rational numbers and the reflection defined by v is a coincidence reflection of L. In the first case, the vector v is orthogonal to a_2; in the second case, the vector v is parallel to a_2. Assume that both $x + b$ and $bx - 1$ are nonzero, and suppose that v defines a coincidence reflection of L. Then the second equation in (10) implies that $x \neq 0$. Furthermore, (10) implies that

$$\frac{ax}{x+b}, \quad \frac{bx-1}{a} \in \mathbb{Q}. \qquad (11)$$

Since $a/(1+b^2) \in \mathbb{Q}$, (11) implies that

$$\frac{x(1+b^2)}{x+b}, \quad \frac{bx-1}{1+b^2} \in \mathbb{Q}. \qquad (12)$$

The second condition in (12) implies that there exists a $q \in \mathbb{Q}$ such that

$$x = \frac{q(1+b^2)+1}{b}. \qquad (13)$$

Substituting (13) into the first condition of (12), we have $b^2 \in \mathbb{Q}$, which contradicts our assumption. Thus, the only coincidence reflections are defined by a vector that is parallel to a_2 or a vector that is perpendicular to a_2.

Similarly, we can discuss the case that $a \in \mathbb{Q}$ but $b^2 \notin \mathbb{Q}$ and the case that both $a, a/(1+b^2) \notin \mathbb{Q}$. In the first case, the only coincidence reflections are defined by a_1 or a nonzero vector that is orthogonal to a_1. In the second case, there is no coincidence reflection for L. To determine the group $OC(L)$, it remains to consider rotations. If

$$R = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

is a coincidence isometry of L, then

$$\begin{aligned} R(a_1) &= \begin{pmatrix} a\cos\theta \\ a\sin\theta \end{pmatrix} = xa_1 + ya_2 = \begin{pmatrix} ax + y \\ by \end{pmatrix}, \\ R(a_2) &= \begin{pmatrix} \cos\theta - b\sin\theta \\ \sin\theta + b\cos\theta \end{pmatrix} = x'a_1 + y'a_2 = \begin{pmatrix} ax' + y' \\ by' \end{pmatrix}, \end{aligned}$$

for some $x, x', y, y' \in \mathbb{Q}$. In particular, we have

$$by = a\sin\theta, \quad ax' = -\left(b + \frac{1}{b}\right)\sin\theta. \tag{14}$$

If $\sin\theta \neq 0$, (14) implies that

$$\frac{b^2+1}{a^2} = -\frac{x'}{y} \in \mathbb{Q}. \tag{15}$$

However, if one of a and $a/(1+b^2)$ is rational and the other one is irrational, then (15) does not hold. If both are irrational, then

$$(ax+y)^2 + (by)^2 = a^2$$

together with (15) will also lead to a contradiction. Therefore, $\sin\theta = 0$ and $R = \pm I$.

To summarize, we have the following.

Proposition 4.3. Suppose the structure matrix of $L \subset \mathbb{R}^2$ is given by (9).

1. If $a, b^2 \in \mathbb{Q}$, then $OC(L)$ is generated by the reflections defined by the nonzero vectors of L.
2. If $a \in \mathbb{Q}$ but $b^2 \notin \mathbb{Q}$, then $OC(L) = \{\pm I, \pm R_{a_1}\} \cong \mathbb{Z}_2^2$.
3. If $a \notin \mathbb{Q}$ but $a/(1+b^2) \in \mathbb{Q}$, then $OC(L) = \{\pm I, \pm R_{a_2}\} \cong \mathbb{Z}_2^2$.
4. If $a, a/(1+b^2) \notin \mathbb{Q}$, then $OC(L) = \{\pm I\} \cong \mathbb{Z}_2$.

It should be pointed out that there are many ways to decompose an orthogonal matrix into products of reflections. To see this, we just need to note that the identity matrix is the product of any reflection with itself. It can be seen (say, by considering planar lattices and rotations) that, for any integer $m > 0$, there are orthogonal transformations $\mathcal{R}$ of $\mathbb{R}^n$ such that $\mathcal{R}^k$ are not coincidence isometries of the canonical lattice $\mathbb{Z}^n$ for all $1 \le k < m$, but $\mathcal{R}^m$ is a coincidence isometry of $\mathbb{Z}^n$. The same is true for reflections, *i.e.* there are reflections $\mathcal{R}_i$ ($1 \le i \le m$) such that any partial product of the $\mathcal{R}_i$'s is not a coincidence isometry but the product $\mathcal{R}_1 \ldots \mathcal{R}_m$ is a coincidence isometry.

References

Aragón, G., Aragón, J. L., Dávila, F., Gömez, A. & Rodríguez, M. A. (2001). *Geometric Algebra with Applications in Science and Engineering*, edited by E. Byro-Corrochano & G. Sobczyk, pp. 371–386. Boston: Birkhäuser.

Baake, M. (1997). *The Mathematics of Aperiodic Order*, edited by R. V. Moody, pp. 9–44. Dordrecht: Kluwer Academic Publishers.

Bollmann, W. (1970). *Crystal Defects and Crystalline Interfaces.* Berlin: Springer.

Brandon, D. G., Ralph, B., Ranganathan, S. & Wald, M. S. (1964). *Acta Metall.* **12**, 813–821.

Duneau, M., Oguey, C. & Tahal, A. (1992). *Acta Cryst.* A**48**, 772–781.

Fortes, M. A. (1983*a*). *Acta Cryst.* A**39**, 348–350.

Fortes, M. A. (1983*b*). *Acta Cryst.* A**39**, 351–357.

Grimmer, H. (1973). *Scr. Metall.* **7**, 1295–1300.

Grimmer, H. (1976). *Acta Cryst.* A**32**, 783–785.

Pleasants, P. A. B., Baake, M. & Roth, J. (1996). *J. Math. Phys.* **37**, 1029–1058.

Porteous, I. R. (1995). *Clifford Algebras and Classical Groups.* Cambridge University Press.

Rodríguez, M. A., Aragón, J. L. & Verde-Star, L. (2005). *Acta Cryst.* A**61**, 173–184.

Warrington, D. H. & Bufalini, P. (1971). *Scr. Metall.* **5**, 771–776.