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Indices of coincidence isometries of the hypercubic lattice $\mathbb{Z}^n$

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The problem of computing the index of a coincidence isometry of the hypercubic lattice $\mathbb{Z}^n$ is considered. The normal form of a rational orthogonal matrix is analyzed in detail and explicit formulas for the indices of certain coincidence isometries of $\mathbb{Z}^n$ are obtained. These formulas generalize the known results for $n \le 4$.

1. Introduction

The theory of the coincidence site lattice (CSL) can be used to describe certain phenomena that arise in the physics of interfaces and grain boundaries (see Bollmann, 1970; Grimmer, 1973, 1976). Mathematically, CSL theory concerns the relationship between a lattice L and a transformed copy $\mathcal{A}L$ of L, where $\mathcal{A}$ is a linear transformation of the n-dimensional real vector space V spanned by L. 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. It is known (see §2) that $\mathcal{A}$ is a coincidence symmetry if and only if the matrix A of $\mathcal{A}$ under a basis of L 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 is interested in the isometries of $\mathbb{R}^n$ which are coincidence symmetries of L. In this case, we have the *coincidence isometry* subgroup formed by all the coincidence isometries (Baake, 1997).

One of the main problems in CSL theory is the computation of the index of coincidence of $L \cap \mathcal{A}L$ in L (also called degree). Fortes (1983*a*,*b*) provided a general approach to this problem by using the normal form of an integer matrix and Duneau *et al.* (1992) published a further study along a similar line. Although theoretically it is possible to compute the index of a coincidence transformation *via* the normal form of the corresponding integer matrix by Fortes's result, no general index formula in n dimensions is known even for the coincidence symmetries of the hypercubic lattice $\mathbb{Z}^n$. For the coincidence isometries, it is possible to give more explicit results. Pleasants *et al.* (1996) used number theory to treat the planar case. Baake (1997) provided a solution to this problem for the coincidence isometries for dimensions up to four by using the factorization properties of certain number systems. However, the method does not generalize to higher dimensions. Recently, the geometric algebra method was introduced into the study of CSL theory by Aragón *et al.* (2001) and Rodríguez *et al.* (2005). But only the planar case was treated. Zeiner (2006) provided a detailed analysis for the coincidence indices of hypercubic lattices in four dimensions.

In this paper, we derive several formulas for the index of a coincidence isometry of the lattice $\mathbb{Z}^n$ for arbitrary n. We analyze the normal form of the corresponding integer matrix of a coincidence isometry taking into account the orthogonal property. The main formulas are given in Theorems 3.1 and 3.2.

2. Preliminaries

The set of real numbers (respectively, integers and rational numbers) is denoted by $\mathbb{R}$ (respectively, $\mathbb{Z}$ and $\mathbb{Q}$), the set of all non-singular $n \times n$ real matrices is denoted by $GL_n(\mathbb{R})$ and the set of $n \times n$ real orthogonal matrices is denoted by $O_n(\mathbb{R})$. Notation for matrices over $\mathbb{Q}$ and $\mathbb{Z}$ are defined similarly. For a non-zero integer matrix Z, we denote by $\gcd(Z)$ the greatest common divisor of the non-zero entries of Z.

By an n-dimensional lattice L with basis $(a_1, \ldots, a_n)$, we mean the free Abelian group $\oplus_{i=1}^n \mathbb{Z}a_i$. In this paper, we only consider lattices in the n-dimensional Euclidean space $\mathbb{R}^n$, and we assume the lattices are also n-dimensional. Thus, a lattice $L \subset \mathbb{R}^n$ is given by an $n \times n$ non-singular matrix A (called the structure matrix of L), and a basis of the lattice is

$$(a_1, \ldots, a_n) = (e_1, \ldots, e_n)A, \tag{1}$$

where $(e_1, \ldots, e_n)$ is the canonical basis of $\mathbb{R}^n$.

By a sublattice $L' \subset L$, we mean a subgroup L' of finite index in the Abelian group L. 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 $(i = 1, 2)$ and let the basis of L_i be $\mathbf{B}_i$, *i.e.*

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

Then a theorem due to Grimmer states that L_1 and L_2 are commensurate if and only if $A_2^{-1}A_1$ is a rational matrix. This implies that, if L is a lattice with basis $(a_1, \ldots, a_n)$ and A is 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.

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 $\mathcal{T}(L)$ is TA. Thus the lattice $\mathcal{T}(L)$ and the lattice L are commensurate if and only if $A^{-1}TA$ is rational. The isometries of $\mathbb{R}^n$ that provide commensurate lattices to a lattice L are of special interest (*cf.* Baake, 1997; Aragón *et al.*, 2001; Rodríguez *et al.*, 2005); let us recall the relevant definitions. The following group was defined in Baake (1997):

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

The group $OC(L)$ is called the coincidence isometry group (CIG) of L. For $Y \in OC(L)$, let

$$\Sigma_L(Y) = [L : L \cap YL].$$

If the structure matrix of L is A, then the group $OC(L)$ is isomorphic to $O_n(\mathbb{R}^n) \cap (AGL_n(\mathbb{Q})A^{-1})$. If further A is a rational matrix (in particular, this is the case if $L = \mathbb{Z}^n$), then

$$OC(L) = O_n(\mathbb{Q}) := O_n(\mathbb{R}^n) \cap GL_n(\mathbb{Q}),$$

i.e. the corresponding group $OC(L)$ is formed by the rational orthogonal matrices. In this case, $OC(L)$ is generated by the reflections defined by the non-zero vectors of L (see Zou, 2006). For $Y \in O_n(\mathbb{Q})$, we write

$$Y = \frac{t}{q} Z, \tag{2}$$

where $t, q \in \mathbb{Z}_+$ such that $\gcd(t, q) = 1$ and Z is an integer matrix such that $\gcd(Z) = 1$. Then since $\det Z \in \mathbb{Z}$ and

$$\det Y = \left(\frac{t}{q}\right)^n \det Z = \pm 1,$$

we must have $t = 1$ and

$$Y = \frac{1}{q} Z. \tag{3}$$

Let q_i $(i = 1, \ldots, n)$ be the diagonal elements of the normal form of Z (Fortes, 1983*a*,*b*) and let

$$q_{(i)} = \frac{q}{\gcd(q, q_i)}. \tag{4}$$

Then Fortes's result says that

$$\Sigma_{\mathbb{Z}^n}(Y) = q_{(1)} q_{(2)} \ldots q_{(n)}. \tag{5}$$

Since $\gcd(Z) = 1$, $q_1 = 1$ and thus $q_{(1)} = q$. Furthermore, we have the following basic lemma.

Lemma 2.1. Let Y, Z and q be as in (3), and let q_i $(i = 1, \ldots, n)$ be the diagonal elements of the normal form of Z. Then $q_i q_{n-i+1} = q^2$.

Proof. From the discussion above, there are $P, Q \in GL_n(\mathbb{Z})$ (integer matrices with det $= \pm 1$) such that

$$PYQ = \frac{1}{q} \begin{pmatrix} 1 & & & \\ & q_2 & & \\ & & \ddots & \\ & & & q_n \end{pmatrix}. \tag{6}$$

Taking inverses, we have

$$\begin{aligned} Q^{-1} Y^{-1} P^{-1} &= q \begin{pmatrix} 1 & & & \\ & q_2^{-1} & & \\ & & \ddots & \\ & & & q_n^{-1} \end{pmatrix} \\ &= \frac{q}{q_n} \begin{pmatrix} q_n & & & \\ & q_n/q_2 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix}. \end{aligned} \tag{7}$$

Note that the last integer matrix has the normal form

$$\begin{pmatrix} 1 & & & \\ & q_n/q_{n-1} & & \\ & & \ddots & \\ & & & q_n \end{pmatrix}. \tag{8}$$

However, if we take transposes on both sides of (6), we have

$$Q^T Y^T P^T = \frac{1}{q} \begin{pmatrix} 1 & & & \\ & q_2 & & \\ & & \ddots & \\ & & & q_n \end{pmatrix}. \tag{9}$$

Since $Y^{-1} = Y^T$, by the uniqueness of the normal form, equations (7), (8) and (9) imply that $q_n = q^2$, which in turn implies the lemma. □

We will use this lemma to derive our index formulas in the next section.

3. Index formulas

In this section, we assume $L = \mathbb{Z}^n$ and write $\Sigma(Y)$ for $\Sigma_{\mathbb{Z}^n}(Y)$. We begin with an immediate consequence of Lemma 2.1.

Theorem 3.1. Let Y, Z, q be as in (3), and let δ_i be the greatest common divisor of the determinants of the $i \times i$ minors of Z $(i = 1, \ldots, n)$. Then,

$$\Sigma(Y) = \frac{q^m}{\delta_m}, \tag{10}$$

where $m = [n/2]$ is the integer part of $n/2$.

Proof. Since the diagonal elements of the normal form of Z satisfy $q_i \mid q_{i+1}$, by Lemma 2.1, $q_i \mid q$ if $i \leq m$, and $q \mid q_i$ if $i > m$. Thus the $q_{(i)}$ defined in (4) are given by

$$q_{(i)} = \begin{cases} q/q_i & \text{if } i \leq m, \\ 1 & \text{if } i > m. \end{cases}$$

Therefore, since the greatest common divisors of the determinants of the minors of Z and its normal form are the same (see for example pp. 458 and 485 in Artin, 1991), using (5), we have

$$\Sigma(Y) = \frac{q^m}{q_1 \ldots q_m} = \frac{q^m}{\delta_m}.$$

□

Remark. Note that since $\delta_1 = 1$, for $n \leq 3$, formula (10) simplifies to the known result $\Sigma(Y) = q$ (see Baake, 1997). Note also that, for $n = 4$ and 5, the formula is the same: $\Sigma(Y) = q^2/\delta_2$.

Since the group $OC(\mathbb{Z}^n)$ is generated by reflections defined by the non-zero vectors of $\mathbb{Z}^n$, we now turn to the reflections. Let

$$0 \neq v = \sum_i^n a_i e_i, \quad a_i \in \mathbb{Z}, \quad 1 \leq i \leq n. \tag{11}$$

Since we are interested in the reflection defined by v, we can always assume that $\gcd(a_1, \ldots, a_n) = 1$. Under the canonical basis, the reflection of $\mathbb{R}^n$ defined by v has the matrix

$$R_v = I - 2\frac{vv^T}{v^T v} = \frac{1}{v^T v}(v^T vI - 2vv^T), \tag{12}$$

where v^T is the transpose of v.

Lemma 3.1. Let v be as above. Then

$$\gcd(v^T vI - 2vv^T) = \begin{cases} 1 & \text{if } v^T v \text{ is odd,} \\ 2 & \text{if } v^T v \text{ is even.} \end{cases} \tag{13}$$

Proof. The ith row of the matrix $v^T vI - 2vv^T$ is

$$r_i = (-2a_i a_1, \ldots, v^T v - 2a_i^2, \ldots, -2a_i a_n).$$

Let $d_i = \gcd(r_i)$ or $\gcd(r_i/2)$ according to whether $v^T v$ is odd or even. We claim that, if a prime p divides d_i, then it divides a_i. In fact, if

$$t_i = \gcd(a_1, \ldots, a_{i-1}, a_{i+1}, \ldots, a_n),$$

then

$$d_i = \begin{cases} \gcd(2a_i t_i, v^T v - 2a_i^2) & \text{if } v^T v \text{ is odd,} \\ \gcd(a_i t_i, (v^T v - 2a_i^2)/2) & \text{if } v^T v \text{ is even.} \end{cases}$$

So if $p \mid d_i$ but $p \nmid a_i$, then $p \mid t_i$, implies that $p \mid \sum_{k \neq i}^n a_k^2$. However, this would imply that p also divides

$$a_i^2 = 2a_i^2 - v^T v + \sum_{k \neq i}^n a_k^2,$$

which is a contradiction. Now the lemma follows since by our assumption $\gcd(a_1, \ldots, a_n) = 1$. □

It follows from this lemma that if we write

$$R_v = \frac{1}{q} T_v \tag{14}$$

as in (3), then $q = v^T v$ or $v^T v/2$ depending on whether $v^T v$ is odd or even. Moreover, we have the following lemma:

Lemma 3.2. Assume that $n > 2$. If $q_1, q_2, \ldots, q_n$ are the diagonal elements of the normal form of T_v, then $q_2 = q$.

Remark. Note that for $n = 2$ we have $q_2 = q^2$ by Lemma 2.1. Note also that it follows from this lemma that $q_2 = \ldots = q_{n-1} = q$.

Proof. To prove the lemma, recall that $q_i = \delta_i/\delta_{i-1}$, where δ_i is the greatest common divisor of the determinants of all $i \times i$ minors of T_v (see for example pp. 458 and 485 in Artin, 1991). Since $\delta_1 = 1$, we need to prove $\delta_2 = q$. We give the detail for the case that $v^T v$ is odd, since it will be clear from the discussion that the same argument works for the even case. Consider the 2×2 minors of T_v. If a 2×2 minor M does not involve any diagonal element, then $\det(M) = 0$. If it involves diagonal element(s), then there are basically two possibilities:

$$\begin{pmatrix} v^T v - 2a_i^2 & -2a_i a_j \\ -2a_t a_i & -2a_t a_j \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} v^T v - 2a_i^2 & -2a_i a_j \\ -2a_j a_i & v^T v - 2a_j^2 \end{pmatrix}.$$

It is clear that the determinants of both matrices have the factor $v^T v$, hence our claim follows. □

We now give a formula for the index of a reflection.

Theorem 3.2. Let

$$0 \neq v = \sum_{i=1}^n a_i e_i \in \mathbb{Z}^n \quad \text{with} \quad \gcd(a_1, \ldots, a_n) = 1.$$

Then

$$\Sigma(R_v) = \begin{cases} v^T v & \text{if } v^T v \text{ is odd,} \\ v^T v/2 & \text{if } v^T v \text{ is even.} \end{cases} \tag{15}$$

Proof. This is an immediate consequence of Lemmas 2.1, 3.1 and 3.2. □

This theorem provides the base for using induction to obtain some interesting results. As an example, we will prove a proposition.

For $i = 1, \ldots, k$, let

$$0 \neq v_i = \sum_{j=1}^n a_{ji} e_j \in \mathbb{Z}^n \quad \text{with} \quad \gcd(a_{1i}, \ldots, a_{ni}) = 1.$$

Define the integers r_i to be $v_i^T v_i$ or $v_i^T v_i/2$ depending on whether $v_i^T v_i$ is odd or even.

Proposition 3.1. Assume that $\gcd(r_i, r_j) = 1$ for $i \neq j$. Then

$$\Sigma(R_{v_1} \ldots R_{v_k}) = r_1 \ldots r_k.$$

This proposition follows from Theorem 3.2 and the following lemma:

Lemma 3.3. Let $R_i \in O_n(\mathbb{Q})$ $(i = 1, 2)$ be reflections and write $R_i = (1/r_i)S_i$ as in (3). Assume that $\gcd(r_1, r_2) = 1$ and the normal forms of S_i are

$$\begin{pmatrix} 1 & & & \\ & r_i & & \\ & & \ddots & \\ & & & r_i^2 \end{pmatrix}, \quad i = 1, 2.$$

If we write $R_1R_2 = (1/r)R$ as in (3), then $r = r_1r_2$ and the matrix R has the normal form

$$\begin{pmatrix} 1 & & & \\ & r & & \\ & & \ddots & \\ & & & r^2 \end{pmatrix}.$$

Proof. Let the normal form of R be

$$\begin{pmatrix} d_1 & & & \\ & d_2 & & \\ & & \ddots & \\ & & & d_n \end{pmatrix}.$$

Then we know that $d_1 = 1$ and $d_n = r^2$, so it remains to prove that $d_2 = r$. Consider

$$R_1R_2 = \frac{1}{r_1r_2}S_1S_2.$$

If the normal form of S_1S_2 is

$$\begin{pmatrix} c_1 & & & \\ & c_2 & & \\ & & \ddots & \\ & & & c_n \end{pmatrix},$$

then $r = r_1r_2/c_1$ and $d_i = c_i/c_1$. For an integer matrix A, denote by $\delta_i(A)$ the greatest common divisor of the determinants of the $i \times i$ minors of A. Then $\delta_i(S_1S_2)$ are identical to those of (compare with the proof of Lemma 2.1)

$$R' = \begin{pmatrix} 1 & & & \\ & r_1 & & \\ & & \ddots & \\ & & & r_1^2 \end{pmatrix} S_2', \tag{16}$$

where S_2' is obtained from S_2 by left multiplying by an element from $GL_n(\mathbb{Z})$. Therefore, $\gcd(S_2') = 1$ and $\delta_i(S_2') = \delta_i(S_2)$. Thus, if a prime p divides $c_1 = \gcd(R')$, it must divide r_1. Similarly, p also divides r_2. But $\gcd(r_1, r_2) = 1$, so $\gcd(R') = c_1 = 1$. Thus, $r = r_1r_2$ and $d_2 = c_2$.

Now $c_2 = \delta_2(R')/c_1 = \delta_2(R')$. Since every 2×2 minor of R' contains at least one row of S_2' multiplied by r_1 or r_1^2, we see that $r_1r_2 = r_1\delta_2(S_2') \mid \delta_2(R')$ implies that $r \mid d_2$. But $d_2 \le r$ by Lemma 2.1, so $d_2 = r$. □

It should be pointed out that without the assumption that $\gcd(r_i, r_j) = 1$, the result of Proposition 3.1 does not hold. This can be seen by noting that the square of a reflection is the identity.

4. Concluding remarks

It is known that certain positive integers cannot be the coincidence isometry indices for the lattice $\mathbb{Z}^n$ when $n \le 4$. In particular, it is well known that, in dimension 3, the indices assume precisely the odd positive integers (Grimmer, 1973). One may ask what happens when $n \ge 4$. This question can be answered by using the results of the present work together with some known facts about the square sums of integers. Recall that a theorem due to Legendre and Gauss says that a positive integer can be expressed as a sum of three squares if and only if it is not the form $4^m(8k + 7)$ (Adler & Coury, 1995, p. 236). It follows from this theorem that every *odd* positive integer can be written as a sum of four integers with gcd = 1. To see this, note that, for $n \ge 0$, if

$$4n + 1 = a^2 + b^2 + c^2,$$

then since every square is congruent to 0 or 1 modulo 4, exactly one of a, b and c is odd. Assume that c is odd and write

$$a = 2u, \quad b = 2v, \quad c = 2t + 1,$$

then

$$(u + v)^2 + (u - v)^2 + t^2 + (t + 1)^2 = 2n + 1.$$

Thus, by Theorem 3.2, the indices provided by $OC(\mathbb{Z}^n)$ $(n \le 4)$ cover all the positive odd integers, although these indices do not include the powers of 2^k for $k > 1$ (see Baake, 1997). However, for $n = 5$, all the positive integers are covered. To see this, note that, since $2^k - 1$ is odd, from the above discussion, 2^k can be expressed as a sum of five squares with gcd = 1, so Theorem 3.2 and Proposition 3.1 imply the result.

The index formulas for the coincidence isometries of the lattice $\mathbb{Z}^n$ provided in this work are quite explicit. However, the computations are more involved in the general cases and one should not expect to have formulas as explicit. The connection between the coincidence index formulas and the related formulas in number theory deserves further attention (see Baake, 1997).

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