RIMS Kôkyûroku Bessatsu
B39 (2013), 233–244

Crystallographic groups with cubic normal fundamental domain

By

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Abstract

We study the crystallographic groups in an n-dimensional Euclidean space whose normal fundamental domain can be chosen to be an n-dimensional cube (we call them cube-type crystallographic groups). We will show that defining a cube-type crystallographic group is equivalent to defining a combinatorial structure called facets-pairing structure on the n-cube. From this viewpoint, we can identify any cube-type crystallographic group in dimension n with a collection of permutations on the set $\{1, -1, \cdots, n, -n\}$ that satisfy some compatible relations.

§ 1. Introduction

An n-dimensional crystallographic group is a discrete, cocompact subgroup Γ of the isometry group of the n-dimensional Euclidean space $\mathbb{R}^n$. If Γ is also torsion free, then Γ is called a *Bieberbach group*. A Bieberbach group acts freely and properly discontinuously on $\mathbb{R}^n$, thus the orbit space $M_\Gamma := \mathbb{R}^n/\Gamma$ is a compact flat manifold with fundamental group Γ. In fact, any compact flat manifold arises in this way.

For an n-dimensional crystallographic group Γ, all the translations in Γ form a normal maximal abelian subgroup of finite index, denoted by L_Γ. Let $H_\Gamma = \Gamma/L_\Gamma$. Then we have a short exact sequence

$$0 \longrightarrow L_\Gamma \longrightarrow \Gamma \longrightarrow H_\Gamma \longrightarrow 1.$$

Received August 21, 2011. Revised December 13, 2011.
2000 Mathematics Subject Classification(s): 57S30, 57R15, 53A15
Key Words: *Crystallographic group, fundamental domain, cube, facets-pairing structure*
Supported by the Japanese Society for the Promotion of Sciences (grant no. P10018) and Natural Science Foundation of China (grant no.11001120). This work is also funded by the PAPD (priority academic program development) of Jiangsu higher education institutions.
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The groups L_Γ and H_Γ are called the *translation subgroup* of Γ and *holonomy group* (or *point-group*), respectively. More specifically, if we write the group of isometries of $\mathbb{R}^n$ as $\mathrm{Isom}(\mathbb{R}^n) = O(n) \ltimes \mathbb{R}^n$, then any element of $\mathrm{Isom}(\mathbb{R}^n)$ can be written uniquely as $L_b B$, where $B \in O(n)$ and L_b is a translation by $b \in \mathbb{R}^n$.

Let $r : \mathrm{Isom}(\mathbb{R}^n) \to O(n)$ be the canonical projection which sends any $L_b B$ to B. Then $L_\Gamma = \Gamma \cap \mathbb{R}^n$ and $H_\Gamma = r(\Gamma) < O(n)$. In addition, since L_Γ is a normal subgroup of Γ, and $(L_b B) L_a (L_b B)^{-1} = L_{Ba}$, we have an integral representation of H_Γ on $L_\Gamma \cong \mathbb{Z}^n$, called *holonomy representation* of Γ. This representation is faithful, so we can identify H_Γ with a subgroup of $\mathrm{GL}(n, \mathbb{Z})$. The reader is referred to [1] and [5] for more details on the above definitions.

Definition 1.1 (Fundamental Domain). For an n-dimensional crystallographic group Γ, a subset D of $\mathbb{R}^n$ is called a *fundamental domain* for Γ if it satisfies the following conditions.

(i) D is a closed set;

(ii) all the images $\{\gamma(D) \mid \forall\, \gamma \in \Gamma\}$ of the set D together cover the entire $\mathbb{R}^n$;

(iii) some (sufficiently small) neighborhood of each point of $\mathbb{R}^n$ intersects only finitely many of the sets $\gamma(D)$, $\gamma \in \Gamma$.

(iv) for any $\gamma \neq id_{\mathbb{R}^n} \in \Gamma$, $\gamma(\mathrm{Int}D) \cap \mathrm{Int}D = \varnothing$ where $\mathrm{Int}D$ is the interior of the set D.

It can be shown that any n-dimensional crystallographic group has a fundamental domain D which is a convex polyhedron in $\mathbb{R}^n$ (for example, the Dirichlet domain of Γ). In this case, we call D a *fundamental polyhedron* of Γ. A fundamental polyhedron is called *normal* if the intersection of any adjacent polyhedra in the decomposition $\mathbb{R}^n = \bigcup_{\gamma \in \Gamma} \gamma(D)$ is a face of each of them. If a fundamental domain D of Γ is not normal, we can always normalize D by introducing some extra faces (see chapter 2 in [4]).

In this paper, we will study crystallographic groups which have an n-dimensional cube as a normal fundamental polyhedron. Let $\mathcal{C}^n$ denote the following n-dimensional cube in the Euclidean space $\mathbb{R}^n$.

$$\mathcal{C}^n := \{(x_1, \cdots, x_n) \in \mathbb{R}^n \mid -\frac{1}{4} \leq x_i \leq \frac{1}{4},\ 1 \leq \forall\, i \leq n\}$$

It is easy to see that if a crystallographic group Γ has some n-dimensional cube as its normal fundamental polyhedron, there must exist a crystallographic group Γ' so that $\Gamma' \cong \Gamma$ and Γ' has $\mathcal{C}^n$ as a normal fundamental polyhedron. So without loss of generality, we introduce the following notion.

Definition 1.2. A crystallographic (Bieberbach) group Γ in dimension n is called *cube-type* if the cube $\mathcal{C}^n$ can serve as a normal fundamental polyhedron for Γ.

In the rest of this paper, we will study any n-dimensional cube-type crystallographic group Γ by some combinatorial structure on $\mathcal{C}^n$ that is canonically associated to Γ.

§ 2. Facets-Pairing Structure on a Cube

Suppose Γ is an n-dimensional cube-type crystallographic group. Then by definition, $\mathbb{R}^n$ is tessellated by the family of cubes $\{\gamma(\mathcal{C}^n) \mid \forall\, \gamma \in \Gamma\}$. We call each $\gamma(\mathcal{C}^n)$ a *chamber*. Since $\mathcal{C}^n$ is a normal fundamental polyhedron, for each facet F of $\mathcal{C}^n$, there exists a unique chamber $\gamma_F(\mathcal{C}^n)$ ($\gamma_F \in \Gamma$) so that $\gamma_F(\mathcal{C}^n) \cap \mathcal{C}^n = F$. Then γ_F will map another facet F^* of $\mathcal{C}^n$ to F (it is possible that $F^* = F$). It is easy to see that $\gamma_{F^*} = \gamma_F^{-1}$ and $(F^*)^* = F$. Each γ_F is called an *adjacency transformation* in Γ.

So we have an involuntary permutation of the set of facets of $\mathcal{C}^n$ by associating F^* to F. Let $\tau_F : F \to F^*$ denote the restriction of γ_F^{-1} to F. It is clear that τ_F is a face-preserving isometry. The following two theorems contain some standard facts about fundamental polyhedra of crystallographic groups. Their proof may be found in Chapter 2 of [4].

Theorem 2.1 (see [4]). *The crystallographic group Γ is generated by adjacency transformations.*

There are two types of relations among the adjacency transformations of Γ.

Type-1: For any facet F of $\mathcal{C}^n$, $\gamma_{F^*}\gamma_F = id_{\mathbb{R}^n}$;

Type-2: For a codimension-two face f of $\mathcal{C}^n$, let $\gamma_{F_1}(\mathcal{C}^n)$, $\gamma_{F_2}\gamma_{F_1}(\mathcal{C}^n)$, $\gamma_{F_3}\gamma_{F_2}\gamma_{F_1}(\mathcal{C}^n)$ and $\gamma_{F_4}\gamma_{F_3}\gamma_{F_2}\gamma_{F_1}(\mathcal{C}^n)$ be the four chambers meeting at f. Then we have:

$$\gamma_{F_4}\gamma_{F_3}\gamma_{F_2}\gamma_{F_1} = id_{\mathbb{R}^n}.$$

The Type-2 relations are called *Poincaré relations.* We remark that the facets F_1, F_2, F_3, F_4 in a Type-2 relation may not be all distinct.

Theorem 2.2 (see [4]). *The Type-1 and Type-2 relations together form a set of abstract defining relations for the cube-type crystallographic group Γ on the generators $\{\gamma_F\,;\ F$ is a facet of $\mathcal{C}^n\}$.*

Since $\mathbb{R}^n$ is tiled by all the chambers of Γ, we can identify $\mathbb{R}^n$ with the quotient space $\Gamma\times\mathcal{C}^n/\mathcal{I}$ where $\mathcal{I}$ is the equivalent relation on $\Gamma\times\mathcal{C}^n$ generated by the equivalences of the form $(\gamma\gamma_F, x) \sim (\gamma, \gamma_F^{-1}(x)) = (\gamma, \tau_F(x))$ for any $\gamma \in \Gamma$ and any point x in a facet F of $\mathcal{C}^n$. Then the chambers of Γ can be represented by $[(\gamma, \mathcal{C}^n)]$, $\gamma \in \Gamma$.

$$\text{Let } \pi : \Gamma \times \mathcal{C}^n \to \mathbb{R}^n = \Gamma \times \mathcal{C}^n/\mathcal{I} \text{ denote the quotient map.} \tag{2.1}$$

For any proper face f of $\mathcal{C}^n$, let $\Xi(f)$ denote the set of facets of $\mathcal{C}^n$ that contain f, i.e. $\Xi(f) = \{F \,|\, F$ is any facet of $\mathcal{C}^n$ with $f \subset F\}$. And let $\Xi^{\perp}(f)$ be the set of facets of $\mathcal{C}^n$ that intersect f transversely. For any $F \in \Xi^{\perp}(f)$, $F \cap f$ must be a codimension-one face of f. So we have:

$$\Xi^{\perp}(f) = \{F \,|\, F \text{ is any facet of } \mathcal{C}^n \text{ so that } f \cap F \text{ is a codimension-one face of } f\}.$$

For an arbitrary facet $F \in \Xi(f)$, let $f' = \tau_F(f) \subset F^*$. Then we can define a map

$$\Psi^f_F : \Xi(f) \to \Xi(f'), \text{ where } \Psi^f_F(F^\sharp) \cap F^* = \tau_F(F^\sharp \cap F) \text{ for } \forall\, F^\sharp \in \Xi(f). \tag{2.2}$$

In particular, $\Psi^f_F(F) = F^*$. Similarly, we can define a map

$$(\Psi^f_F)^\perp : \Xi^\perp(f) \to \Xi^\perp(f'),\ (\Psi^f_F)^\perp(F^\flat) \cap f' = \tau_F(F^\flat \cap f) \text{ for } \forall\, F^\flat \in \Xi^\perp(f). \tag{2.3}$$

Since $\tau_F : F \to F^*$ is a face-preserving homeomorphism, Ψ^f_F and $(\Psi^f_F)^\perp$ are both bijections. Geometrically, Ψ^f_F and $(\Psi^f_F)^\perp$ just tell us how γ_F permutes the facets that contain f. Moreover, for any facet $F' \in \Xi(f')$, let $f'' = \tau_{F'}(f')$. So we have the composite maps:

$$\Psi^{f'}_{F'} \circ \Psi^f_F : \Xi(f) \to \Xi(f'') \text{ and } (\Psi^{f'}_{F'})^\perp \circ (\Psi^f_F)^\perp : \Xi^\perp(f) \to \Xi^\perp(f'').$$

Using these notions, we can interpret the above Type-1 and Type-2 relations among γ_F's into two types of relations among τ_F's as follows.

Type-1': For any facet F of $\mathcal{C}^n$, $\tau_{F^*}\tau_F = id_F$;

Type-2': For a codimension-two face f_1 of $\mathcal{C}^n$, let $\gamma_{F_1}(\mathcal{C}^n)$, $\gamma_{F_2}\gamma_{F_1}(\mathcal{C}^n)$, $\gamma_{F_3}\gamma_{F_2}\gamma_{F_1}(\mathcal{C}^n)$ and $\gamma_{F_4}\gamma_{F_3}\gamma_{F_2}\gamma_{F_1}(\mathcal{C}^n) = \mathcal{C}^n$ be the four chambers meeting at f_1. Suppose $f_2 = \tau_{F_1}(f_1) \subset F_1^* \cap F_2$, $f_3 = \tau_{F_2}(f_2) \subset F_2^* \cap F_3$, $f_4 = \tau_{F_3}(f_3) \subset F_3^* \cap F_4$. Then $\tau_{F_4}(f_4) = f_1$ and we have:

(a) the map $\tau_{F_4}\tau_{F_3}\tau_{F_2}\tau_{F_1}|_{f_1} : f_1 \to f_1$ coincides with id_{f_1}, and

(b) the map $\Psi^{f_4}_{F_4} \circ \Psi^{f_3}_{F_3} \circ \Psi^{f_2}_{F_2} \circ \Psi^{f_1}_{F_1} : \Xi(f_1) \to \Xi(f_1)$ is the identity map.

Since the map $\tau_{F_4}\tau_{F_3}\tau_{F_2}\tau_{F_1}|_{f_1} : f_1 \to f_1$ is an isometry, it is uniquely determined by how it permutes the codimension-one faces of f_1. So Type-2'(a) is equivalent to saying that $(\Psi^{f_4}_{F_4})^\perp \circ (\Psi^{f_3}_{F_3})^\perp \circ (\Psi^{f_2}_{F_2})^\perp \circ (\Psi^{f_1}_{F_1})^\perp : \Xi^\perp(f_1) \to \Xi^\perp(f_1)$ is the identity map. In

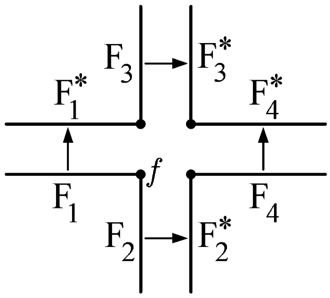

Figure 1.

addition, the Type-2'(b) here is actually a consequence of Type-2'(a), because there are always four chambers meeting at a codimension-two face of $\mathcal{C}^n$ in the tessellation of $\mathbb{R}^n$.

Notice that we can write Type-2'(a) equivalently as $\tau_{F_2}\tau_{F_1}|_{f_1} = \tau_{F_3}^{-1}\tau_{F_4}^{-1}|_{f_1}$. So the Type-1' and Type-2' conditions lead to a general notion on any nice manifold with corners as follows (also see [6]).

Definition 2.3 (Facets-Pairing Structure)**.** Suppose we have the following data on an n-dimensional nice manifold with corners V^n:

(I) each facet F of V^n is uniquely paired with a facet F^* (it is possible that $F^* = F$) and there are isometries $\tau_F : F \to F^*$ and $\tau_{F^*} : F^* \to F$ such that $\tau_{F^*} = \tau_F^{-1}$ (here F and F^* themselves are considered as manifolds with corners). If $F^* \neq F$, we call $\widehat{F} = \{F, F^*\}$ a *facet pair* and call F^* the *twin facet* of F. If $F^* = F$, the $\tau_F : F \to F$ is necessarily an involution on F (i.e. $\tau_F \circ \tau_F = id_F$). Then we define $\widehat{F} = \{F\}$ and call such an F a *self-involutive* facet.

(II) for any codimension-two face $f = F_1 \cap F_2$, if $\tau_{F_1}(f) = F_1^* \cap F_3$, $\tau_{F_2}(f) = F_2^* \cap F_4$, then $\tau_{F_3}\tau_{F_1}(f) = \tau_{F_4}\tau_{F_2}(f) = F_3^* \cap F_4^*$ (see Figure 1), and $\tau_{F_3}\tau_{F_1}(p) = \tau_{F_4}\tau_{F_2}(p)$ for $\forall\, p \in f$. Here it is possible that $F_3 = F_2^*$ or $F_4 = F_1^*$.

We call $\mathcal{P} = \{\widehat{F}, \tau_F\}_{F\subset V^n}$ a *facets-pairing structure* on V^n, and call $\{\tau_F : F \to F^*\}_{F\subset V^n}$ the *structure maps of* $\mathcal{P}$.

By our discussion above, any n-dimensional cube-type crystallographic group Γ determines a facets-pairing structure on the cube $\mathcal{C}^n$, denoted by $\mathcal{P}_\Gamma$. Conversely, we can prove the following.

Theorem 2.4. *Any facets-pairing structure $\mathcal{P}$ on $\mathcal{C}^n$ canonically determines an n-dimensional cube-type crystallographic group Γ so that $\mathcal{P}_\Gamma = \mathcal{P}$.*

Proof. For any facet F of $\mathcal{C}^n$, the isometry $\tau_F : F \to F^*$ determines a unique isometry γ_F of $\mathbb{R}^n$ so that $\gamma_F(\mathcal{C}^n) \cap \mathcal{C}^n = F$ and γ_F^{-1} agrees with τ_F on F. Let Γ be the subgroup of Isom($\mathbb{R}^n$) generated by all these γ_F's. Then by the definition of facets-pairing structure, these γ_F's satisfy the Type-1 and Type-2 relations. In addition, for any codimension-two face f, there exist facets F_1, F_2, F_3, F_4 (may not be all distinct) so that $\gamma_{F_1}(\mathcal{C}^n)$, $\gamma_{F_2}\gamma_{F_1}(\mathcal{C}^n)$, $\gamma_{F_3}\gamma_{F_2}\gamma_{F_1}(\mathcal{C}^n)$ and $\gamma_{F_4}\gamma_{F_3}\gamma_{F_2}\gamma_{F_1}(\mathcal{C}^n) = \mathcal{C}^n$ form a "circuit" around f in $\mathbb{R}^n$. Since the sum of the dihedral angles of $\tau_{F_1}(f), \tau_{F_2}\tau_{F_1}(f), \tau_{F_3}\tau_{F_2}\tau_{F_1}(f)$ and $\tau_{F_4}\tau_{F_3}\tau_{F_2}\tau_{F_1}(f) = f$ equals 2π, Γ is an n-dimensional crystallographic group (see p.165 of [4]). It is clear that $\mathcal{C}^n$ is a normal fundamental polyhedron of Γ and, the facets-pairing structure on $\mathcal{C}^n$ induced by Γ is exactly $\mathcal{P}$. □

By Theorem 2.2 and Theorem 2.4, defining a cube-type crystallographic group of dimension n is equivalent to defining a facets-pairing structure on $\mathcal{C}^n$.

Example 2.5. If we define $F^* = F$ and $\tau_F = id_F$ for each facet F of $\mathcal{C}^n$, what we get is obviously a facets-pairing structure on $\mathcal{C}^n$, denoted by $\mathcal{P}_0$. We call $\mathcal{P}_0$ the *trivial facets-pairing structure*. The crystallographic group corresponding to $\mathcal{P}_0$ is a *Coxeter group* generated by the reflections about all the facets of $\mathcal{C}^n$.

§ 3. Cube-type Bieberbach Groups

Cube-type *Bieberbach* groups are torsion-free cube-type crystallographic groups. In this section, we will interpret the "torsion-freeness" of a cube-type crystallographic group into some condition on the corresponding facets-pairing structure on $\mathcal{C}^n$. First, let us introduce some new notions in a facets-pairing structure.

Definition 3.1 (Face Family). Suppose $\mathcal{P} = \{\widehat{F}, \tau_F\}_{F \subset V^n}$ is a facets-pairing structure on a nice manifold with corners V^n. For any face f of V^n, $\tau_{F_k} \circ \cdots \circ \tau_{F_1}(f)$ is called *valid* if $f \subset F_1$ and $\tau_{F_j} \circ \cdots \circ \tau_{F_1}(f) \subset F_{j+1}$ for each $1 \le j < k$. Moreover, when $k = 0$, we define $\tau_{F_k} \circ \cdots \circ \tau_{F_1}(f) := f$. Let $\widehat{f}$ be the set of all faces of the valid form $\tau_{F_k} \circ \cdots \circ \tau_{F_1}(f)$ for some $k \ge 0$. We call $\widehat{f}$ the *face family* containing f in $\mathcal{P}$. Obviously, each proper face of V^n is contained in a unique face family of $\mathcal{P}$. In particular, the face family containing a facet F is just $\widehat{F}$.

Definition 3.2 (Perfect Facets-Pairing Structure). In a facets-pairing structure $\mathcal{P}$ on a nice manifold with corners V^n, a codimension-l face family $\widehat{f}$ is called *perfect* if $\widehat{f}$ consists of exactly 2^l different faces of V^n. Moreover, $\mathcal{P}$ is called *perfect* if all its face families are perfect. Note that a perfect facets-pairing structure should have no self-involutive facets.

Theorem 3.3. *An n-dimensional cube-type crystallographic group Γ is torsion free if and only if the corresponding facets-pairing structure $\mathcal{P}_\Gamma$ on $\mathcal{C}^n$ is perfect.*

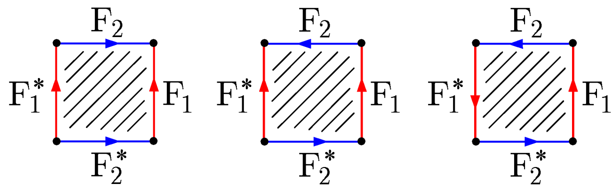

Figure 2.

Proof. For any codimension-l face f of $\mathcal{C}^n$, there are exactly 2^l chambers of Γ meeting f in the tiling of $\mathbb{R}^n$. Let $\pi : \Gamma \times \mathcal{C}^n \to \mathbb{R}^n = \Gamma \times \mathcal{C}^n/\mathcal{I}$ be the quotient map which defines the tiling of $\mathbb{R}^n$ by chambers of Γ (see (2.1)). Then

$$\pi^{-1}(\pi(id_{\mathbb{R}^n}, f)) = \{(\gamma_{F_1} \circ \cdots \circ \gamma_{F_k}, \tau_{F_k} \circ \cdots \circ \tau_{F_1}(f)) \ ; \ \tau_{F_k} \circ \cdots \circ \tau_{F_1}(f) \text{ is any valid form}\}.$$

In addition, let $\theta : \Gamma \times \mathcal{C}^n \to \Gamma$ be the map defined by $\theta(\gamma, x) = \gamma$. Then the set $\Gamma_f := \theta(\pi^{-1}(\pi(id_{\mathbb{R}^n}, f))) \subset \Gamma$ consists of exactly 2^l elements. Note that this implies that the face family $\widehat{f}$ has at most 2^l components.

If we assume $\mathcal{P}_\Gamma$ is perfect, the face family of f consists of exactly 2^l different faces of $\mathcal{C}^n$. This implies that for any $\gamma_{F_1} \circ \cdots \circ \gamma_{F_k} \neq id_{\mathbb{R}^n} \in \Gamma_f$, the $\tau_{F_k} \circ \cdots \circ \tau_{F_1}(f)$ is a face on $\mathcal{C}^n$ different from f. Under this condition, we claim that the action of Γ on $\mathbb{R}^n$ has to be free. Otherwise, since Γ can be generated by γ_F's, there exists a sequence of facets $F_1, \cdots, F_r$ of $\mathcal{C}^n$ so that $\gamma_{F_1} \circ \cdots \circ \gamma_{F_r} \neq id_{\mathbb{R}^n}$ and $\gamma_{F_1} \circ \cdots \circ \gamma_{F_r}(x) = x$ for some $x \in \mathcal{C}^n$. Suppose x is contained in the relative interior of a face f. Then since each γ_{F_i} is face-preserving, we must have $\gamma_{F_1} \circ \cdots \circ \gamma_{F_r}(f) = f$. Then $\gamma_{F_r}^{-1} \circ \cdots \circ \gamma_{F_1}^{-1}(f) = f$. By definition, $\tau_F = \gamma_F^{-1}|_F : F \to F^*$ for any facet F, so we have $\tau_{F_r} \circ \cdots \circ \tau_{F_1}(f) = f$, which leads to a contradiction.

Conversely, we assume the action of Γ on $\mathbb{R}^n$ is free. To prove $\mathcal{P}_\Gamma$ is perfect on $\mathcal{C}^n$, it suffices to show that for any proper face f of $\mathcal{C}^n$ and any $\gamma_{F_1} \circ \cdots \circ \gamma_{F_k} \neq id_{\mathbb{R}^n} \in \Gamma_f$, the $\tau_{F_k} \circ \cdots \circ \tau_{F_1}(f)$ is a face on $\mathcal{C}^n$ different from f. Indeed, $\tau_{F_k} \circ \cdots \circ \tau_{F_1}(f) = f$ implies that $\gamma_{F_k}^{-1} \circ \cdots \circ \gamma_{F_1}^{-1}(f) = f$. So we have $\gamma_{F_1} \cdots \gamma_{F_k}(f) = f$. By Brouwer's fixed point theorem, $\gamma_{F_1} \circ \cdots \circ \gamma_{F_k}$ must have a fixed point which contradicts our assumption that Γ acts freely on $\mathbb{R}^n$. So the theorem is proved. □

Example 3.4. Figure 2 shows three different facets-pairing structures on $\mathcal{C}^2$. Only the left and the middle one are perfect. The cube-type crystallographic groups corresponding to these facets-pairing structures are shown in Example 4.7.

§ 4. Combinatorics of Facets-Pairing Structures on a Cube

In this section, we will study the combinatorics of a facets-pairing structure on a cube, which will help us to understand the geometry of the corresponding cube-type crystallographic group. First, let us introduce some auxiliary notations.

Let $[\pm n] := \{\pm 1, \cdots, \pm n\} = \{1, -1, 2, -2, \cdots, n, -n\}$. A map $\sigma : [\pm n] \to [\pm n]$ is called a *signed permutation* on $[\pm n]$ if σ is a bijection and $\sigma(-k) = -\sigma(k)$ for any $k \in [\pm n]$. The set of all signed permutations on $[\pm n]$ with respect to the composition of maps forms a group, denoted by $\mathfrak{S}_n^{\pm}$ (also called *Hyperoctahedral group*). In addition, we can consider $\mathfrak{S}_n^{\pm}$ as a subgroup of $\mathrm{GL}(n, \mathbb{Z})$ by sending $\sigma \in \mathfrak{S}_n^{\pm}$ to a matrix P_σ where

$$(i,j)\text{-entry of } P_\sigma = \begin{cases} \mathrm{sign}(\sigma(i)), j = \sigma(i); \\ 0, \qquad\qquad \text{otherwise.} \end{cases}$$

Such a matrix $P_\sigma \in \mathrm{GL}(n, \mathbb{Z})$ is called a *signed permutation matrix*. Since any P_σ is an orthogonal matrix, we have $P_{\sigma^{-1}} = P_\sigma^{-1} = P_\sigma^t$. In fact, the set of all n-dimensional signed permutation matrices is exactly $\mathrm{GL}(n, \mathbb{Z}) \cap O(n)$.

Let $\mathbf{F}(i)$ and $\mathbf{F}(-i)$ be the facets of $\mathcal{C}^n$ which lie in the hyperplanes $\{x_i = \frac{1}{4}\}$ and $\{x_i = -\frac{1}{4}\}$ of $\mathbb{R}^n$, respectively. Moreover, for any $j_1, \cdots, j_s \in [\pm n]$ whose absolute values $|j_1|, \cdots, |j_s|$ are pairwise distinct, we define

$$\mathbf{F}(j_1, \cdots, j_s) := \mathbf{F}(j_1) \cap \cdots \cap \mathbf{F}(j_s) \subset \mathcal{C}^n.$$

Then $\mathbf{F}(j_1, \cdots, j_s)$ is a face of $\mathcal{C}^n$ with codimension s. Conversely, for any proper codimension-s face f of $\mathcal{C}^n$, there exists $j_1, \cdots, j_s \in [\pm n]$ so that $\mathbf{F}(j_1, \cdots, j_s)$ equals f. Obviously, $\mathbf{F}(j_1, \cdots, j_s) = \mathbf{F}(j'_1, \cdots, j'_s)$ if and only if $\{j_1, \cdots, j_s\} = \{j'_1, \cdots, j'_s\}$.

Fact: The symmetry group of $\mathcal{C}^n$ is isomorphic to the signed permutation group $\mathfrak{S}_n^{\pm}$. This is because each symmetry of $\mathcal{C}^n$ is uniquely determined by how it permutes the $2n$ facets $\{\mathbf{F}(j)\}_{j \in [\pm n]}$ of $\mathcal{C}^n$.

Theorem 4.1. *For any n-dimensional cube-type crystallographic group Γ, its holonomy group $H_\Gamma < O(n)$ is generated by some signed permutation matrices and its translation subgroup $L_\Gamma \subset \frac{1}{2}\mathbb{Z}^n$.*

Proof. For any facet $\mathbf{F}(j)$ of $\mathcal{C}^n$, suppose $\mathbf{F}(j)^* = \mathbf{F}(j')$, i.e. $\gamma_{\mathbf{F}(j)}$ maps $\mathbf{F}(j')$ to $\mathbf{F}(j)$ and $\gamma_{\mathbf{F}(j)}(\mathcal{C}^n) \cap \mathcal{C}^n = \mathbf{F}(j)$. We can write $\gamma_{\mathbf{F}(j)} = L_{b_j} B_j$ where $B_j \in O(n)$ and L_{b_j} is the translation along a vector b_j in $\mathbb{R}^n$. Notice that B_j must preserve the cube $\mathcal{C}^n$, i.e. B_j induces a symmetry of $\mathcal{C}^n$. So B_j is a signed permutation matrix. And since Γ is generated by the set $\{\gamma_{\mathbf{F}(j)}, j \in [\pm n]\}$, the holonomy group H_Γ is generated by $\{B_j, j \in [\pm n]\}$. In addition, observe that we must have $B_j(\mathbf{F}(j')) = \mathbf{F}(-j)$ and L_{b_j} is the translation which moves $\mathbf{F}(-j)$ to $\mathbf{F}(j)$. So

$$b_j = \begin{cases} \frac{1}{2}\delta_j, \quad\ j > 0; \\ -\frac{1}{2}\delta_{|j|}, j < 0. \end{cases}$$

where $\delta_i = (0, \cdots, 0, \overset{i}{1}, 0, \cdots, 0)^t \in \mathbb{Z}^n$ for any $1 \leq i \leq n$. For any translation $L_b \in L_\Gamma = \Gamma \cap \mathbb{R}^n$, if we write L_b as a product of elements in $\{\gamma_{\mathbf{F}(j)}, j \in [\pm n]\}$, it is easy to see that $b = \frac{1}{2}(k_1\delta_1 + \cdots + k_n\delta_n)$ for some $k_1, \cdots, k_n \in \mathbb{Z}$. So $L_\Gamma \subset \frac{1}{2}\mathbb{Z}^n$. □

Remark. In the above theorem, suppose $\eta : H_\Gamma \to \mathrm{GL}(n, \mathbb{Z})$ is the holonomy representation of Γ. In general, $\eta(H_\Gamma) < \mathrm{GL}(n, \mathbb{Z})$ may not consist of signed permutation matrices although $H_\Gamma < O(n)$ does.

Suppose $\mathcal{P}$ is a facets-pairing structure on $\mathcal{C}^n$. For any facet $\mathbf{F}(j)$ of $\mathcal{C}^n$, let the twin facet of $\mathbf{F}(j)$ in $\mathcal{P}$ be $\mathbf{F}(\omega(j))$ where $\omega(j) \in [\pm n]$. Then $\omega \circ \omega = id_{[\pm n]}$. In other words, ω is an involuntary permutation on $[\pm n]$.

The structure maps of $\mathcal{P}$ are a collection of isometries between facets of $\mathcal{C}^n$

$$\{\tau_j \triangleq \tau_{\mathbf{F}(j)} : \mathbf{F}(j) \to \mathbf{F}(\omega(j))\}_{j \in [\pm n]}$$

which satisfy the conditions in Definition 2.3. To each τ_j, we can associate a map

$$\sigma_j : [\pm n] \backslash \{\pm j\} \to [\pm n] \backslash \{\pm \omega(j)\}, \ j \in [\pm n]$$

$$\text{with } \ \tau_j(\mathbf{F}(j,k)) = \mathbf{F}(\omega(j), \sigma_j(k)), \ \forall\, k \in [\pm n]\backslash\{\pm j\}. \tag{4.1}$$

Obviously, σ_j is a bijection and $\sigma_j(-k) = -\sigma_j(k)$, and $\mathcal{P}$ is completely determined by $\{\omega, \sigma_j\}_{j \in [\pm n]}$. So in the rest of this paper, we write $\mathcal{P} = \{\omega, \sigma_j\}_{j \in [\pm n]}$.

Next, we interpret the condition (I) and (II) in the Definition 2.3 into conditions on $\{\omega, \sigma_j\}_{j \in [\pm n]}$. We can show that the condition (I) is equivalent to:

$$\sigma_{\omega(j)} \circ \sigma_j(k) = k, \ \forall\, k \in [\pm n]\backslash\{\pm j\}, \forall\, j \in [\pm n] \tag{4.2}$$

The condition(II) is equivalent to the following two conditions (see section 3 of [6]).

$$\sigma_{\sigma_j(k)}(\omega(j)) = \omega(\sigma_k(j)), \ \forall\, |j| \neq |k| \text{ where } j, k \in [\pm n]; \tag{4.3}$$

$$\sigma_{\sigma_j(k)}(\sigma_j(l)) = \sigma_{\sigma_k(j)}(\sigma_k(l)), \ \forall\, |j| \neq |k| \neq |l| \text{ where } j, k, l \in [\pm n]. \tag{4.4}$$

The following theorem follows easily from our discussion above.

Theorem 4.2. *For any facets-pairing structure $\mathcal{P}$ on $\mathcal{C}^n$, the corresponding data $\{\omega, \sigma_j\}_{j \in [\pm n]}$ must satisfy* (4.2) (4.3) *and* (4.4)*. Conversely, given any involuntary permutation ω on $[\pm n]$ and bijections $\sigma_j : [\pm n]\backslash\{\pm j\} \to [\pm n]\backslash\{\pm\omega(j)\}$ for $\forall j \in [\pm n]$ with $\sigma_j(-k) = -\sigma_j(k)$, which satisfy* (4.2) (4.3) *and* (4.4)*, the $\{\omega, \sigma_j\}_{j \in [\pm n]}$ canonically determines a facets-pairing structure on $\mathcal{C}^n$.*

From the definition of $\mathcal{P}$, it is not clear whether $\omega(-j)$ should equal $-\omega(j)$ for $j \in [\pm n]$. But if we assume $\omega(-j) = -\omega(j)$ for all $j \in [\pm n]$, then each σ_j canonically determines a signed permutation $\widetilde{\sigma}_j : [\pm n] \to [\pm n]$ by:

$$\widetilde{\sigma}_j(k) := \begin{cases} \sigma_j(k), & k \neq \pm j; \\ \omega(k), & k = \pm j. \end{cases} \tag{4.5}$$

In this case, (4.2) (4.3) and (4.4) are equivalent to the following conditions on $\{\omega, \widetilde{\sigma}_j\}_{j\in[\pm n]}$.

$$\widetilde{\sigma}_{\omega(j)} \circ \widetilde{\sigma}_j = id_{[\pm n]}, \quad \forall\, j \in [\pm n]. \tag{4.6}$$

$$\widetilde{\sigma}_{\widetilde{\sigma}_j(k)}(\omega(j)) = \omega(\widetilde{\sigma}_k(j)), \ \forall\, j,k \in [\pm n]. \tag{4.7}$$

$$\widetilde{\sigma}_{\widetilde{\sigma}_j(k)}(\widetilde{\sigma}_j(l)) = \widetilde{\sigma}_{\widetilde{\sigma}_k(j)}(\widetilde{\sigma}_k(l)), \ \forall\, j,k,l \in [\pm n]. \tag{4.8}$$

Note if we set $l = j$ in (4.8), we obtain (4.7). So (4.7) is actually contained in (4.8).

Definition 4.3. A facets-pairing structure $\mathcal{P} = \{\omega, \tau_j\}_{j\in[\pm n]}$ on $\mathcal{C}^n$ is called *regular* if $\omega(-j) = -\omega(j)$ for all $j \in [\pm n]$. In other words, ω is an involuntary signed permutation on $[\pm n]$. Geometrically, this means that if $\mathbf{F}(j)$ is paired with $\mathbf{F}(\omega(j))$, then $\mathbf{F}(-j)$ is paired with $\mathbf{F}(-\omega(j))$.

If $\mathcal{P} = \{\omega, \sigma_j\}_{j\in[\pm n]}$ is a regular facets-pairing structure on $\mathcal{C}^n$, each $\widetilde{\sigma}_j$ is a signed permutation on $[\pm n]$. So $\widetilde{\sigma}_j$ determines a unique symmetry of the cube $\mathcal{C}^n$, denoted by $\widetilde{\tau}_j : \mathcal{C}^n \to \mathcal{C}^n$ where $\widetilde{\tau}_j(\mathbf{F}(k)) = \mathbf{F}(\widetilde{\sigma}_j(k))$ for any $k \in [\pm n]$. Then (4.1) becomes:

$$\widetilde{\tau}_j(\mathbf{F}(j,k)) = \mathbf{F}(\widetilde{\sigma}_j(j), \widetilde{\sigma}_j(k))). \tag{4.9}$$

Obviously, $\tau_j = \widetilde{\tau}_j|_{\mathbf{F}(j)}$. So for a regular facets-pairing structure $\mathcal{P}$, we also write $\mathcal{P} = \{\omega, \widetilde{\sigma}_j\}_{j\in[\pm n]}$ where $\omega, \widetilde{\sigma}_j \in \mathfrak{S}_n^{\pm}$.

Corollary 4.4. *Any regular facets-pairing structure on $\mathcal{C}^n$ corresponds to a tuple of elements $(\omega; T_1, T_{-1}, \cdots, T_n, T_{-n})$ in $\mathfrak{S}_n^{\pm}$ which satisfy the following conditions.*

(a) $\omega \circ \omega = id_{[\pm n]}$ for $\forall\, j \in [\pm n]$.

(b) $T_j(j) = \omega(j)$ and $T_{\omega(j)} \circ T_j = id_{[\pm n]}$, $\forall\, j \in [\pm n]$,

(c) $T_{T_j(k)} \circ T_j = T_{T_k(j)} \circ T_k$, $\ \forall\, j,k \in [\pm n]$.

The following question on cube-type crystallographic groups seems a little bold to ask. But no counterexample of this question is known to the author so far.

Question: for any n-dimensional cube-type crystallographic group Γ, is the corresponding facets-pairing structure P_Γ on $\mathcal{C}^n$ always regular?

Besides, there is a natural equivalence relation among all facets-pairing structures on $\mathcal{C}^n$ induced by the symmetries of $\mathcal{C}^n$ as defined below.

Definition 4.5. Two facets-pairing structures $\mathcal{P}$ and $\mathcal{P}'$ on $\mathcal{C}^n$ are called *strongly equivalent* if there exists a symmetry $h : \mathcal{C}^n \to \mathcal{C}^n$ such that $\mathcal{P}' = h(\mathcal{P})$. Suppose $\mathcal{P} = \{\omega, \tau_j\}_{j\in[\pm n]}$ and $\mathcal{P}' = \{\omega', \tau'_j\}_{j\in[\pm n]}$. Then we have: $\tau_j = h^{-1} \circ \tau'_{j'} \circ h$ where $\mathbf{F}(j') = h(\mathbf{F}(j))$ for each $j \in [\pm n]$.

Suppose $(\omega; \widetilde{\sigma}_1, \widetilde{\sigma}_{-1}, \cdots, \widetilde{\sigma}_n, \widetilde{\sigma}_{-n})$ and $(\omega'; \widetilde{\sigma}'_1, \widetilde{\sigma}'_{-1}, \cdots, \widetilde{\sigma}'_n, \widetilde{\sigma}'_{-n})$ are two tuples of elements of $\mathfrak{S}_n^{\pm}$ corresponding to regular facets-pairing structures $\mathcal{P}$ and $\mathcal{P}'$ on $\mathcal{C}^n$, respectively. Then $\mathcal{P}$ is strongly equivalent to $\mathcal{P}'$ if and only if there is an element $S \in \mathfrak{S}_n^{\pm}$ so that:

$$\omega = S^{-1}\omega' S; \quad \widetilde{\sigma}_j = S^{-1}\widetilde{\sigma}'_{S(j)}S, \quad \forall\, j \in [\pm n].$$

Remark. Let Γ_i be the crystallographic groups determined by a facets-pairing structures $\mathcal{P}_i$ on $\mathcal{C}^n$, $i = 1, 2$. If $\mathcal{P}_1$ is strongly equivalent to $\mathcal{P}_2$, then Γ_1 is obviously isomorphic to Γ_2. But conversely, Γ_1 and Γ_2 are isomorphic can not guarantee that $\mathcal{P}_1$ and $\mathcal{P}_2$ are strongly equivalent.

Finally, let us discuss an interesting class of cube-type crystallographic groups introduced in [3]. For any $n \times n$ binary matrix A with zero diagonal, a set of Euclidean motions $s_1, \cdots, s_n$ on $\mathbb{R}^n$ is defined by:

$$s_i^A(x_1, \cdots, x_n) := ((-1)^{A_1^i}x_1, \cdots, (-1)^{A_{i-1}^i}x_{i-1}, x_i + \frac{1}{2}, (-1)^{A_{i+1}^i}x_{i+1}, \cdots, (-1)^{A_n^i}x_n)$$

where $A_j^i \in \mathbb{Z}_2$ denote the (i, j) entry of A. Let $\Gamma(A)$ be the subgroup of $\mathrm{Isom}(\mathbb{R}^n)$ generated by $s_1^A, \cdots, s_n^A$, and let $M(A) = \mathbb{R}^n/\Gamma(A)$ be the orbit space of the action of $\Gamma(A)$ on $\mathbb{R}^n$. It is easy to see that $\Gamma(A)$ is a cube-type crystallographic group. By our notation in Section 2, for any facet $\mathbf{F}(i)$, $1 \le i \le n$, $\gamma_{\mathbf{F}(i)} = s_i^A$. In addition, it is easy to see that the holonomy group $H_{\Gamma(A)}$ of $\Gamma(A)$ is isomorphic to $(\mathbb{Z}_2)^r$ where $r = \mathrm{rank}_{\mathbb{Z}_2}(A)$.

We denote the facets-pairing structure on $\mathcal{C}^n$ corresponding to $\Gamma(A)$ by $\mathcal{P}_A$. Indeed, $\mathcal{P}_A$ is a regular facets-pairing structure defined by $\{\omega_0, \widetilde{\sigma}_j^A\}_{j\in[\pm n]}$ where

$$\omega_0(j) = -j, \quad \forall\, j \in [\pm n]; \tag{4.10}$$

$$\widetilde{\sigma}_j^A(k) = \begin{cases} (-1)^{A_{|k|}^{|j|}} \cdot k, k \in [\pm n], & k \neq \pm j; \\ -k, & k = \pm j. \end{cases} \tag{4.11}$$

Proposition 4.6 (Theorem 6.1 of [6]). *For two $n \times n$ binary matrix A_1 and A_2 with zero diagonal, the facets-pairing structures $\mathcal{P}_{A_1}$ and $\mathcal{P}_{A_2}$ are strongly equivalent if and only if A_1 and A_2 are conjugate by a permutation matrix.*

It is shown in [2] that $\Gamma(A_1)$ is isomorphic to $\Gamma(A_2)$ as abstract group if and only if A_1 can be turned into A_2 via three types of matrix operations, one of which is the conjugation by permutation matrices. So there are many examples of $\Gamma(A_1)$ being isomorphic to $\Gamma(A_2)$ but $\mathcal{P}_{A_1}$ is not strongly equivalent to $\mathcal{P}_{A_2}$.

In addition, it is shown in [3] that $\Gamma(A)$ is torsion-free if and only if A is a *Bott matrix*, which means that there exists an $n \times n$ permutation matrix P so that PAP^{-1} is a strictly upper triangular binary matrix. So $\mathcal{P}_A$ is perfect if and only if A is a Bott matrix (another proof of this statement is given in Theorem 6.6 of [6]).

Example 4.7. For the following matrix A, the representation of $\Gamma(A)$ via the Poincaré relations is:

(i) For $A = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$, $\Gamma(A) = \{\gamma_1, \gamma_2 \mid \gamma_2^{-1}\gamma_1\gamma_2 = \gamma_1\}$, $M(A) \cong T^2$ (torus).

(ii) For $A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, $\Gamma(A) = \{\gamma_1, \gamma_2 \mid \gamma_2\gamma_1\gamma_2 = \gamma_1\}$, $M(A) \cong K^2$ (Klein bottle).

(iii) For $A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\Gamma(A) = \{\gamma_1, \gamma_2 \mid \gamma_2\gamma_1\gamma_2 = \gamma_1^{-1}, \gamma_2\gamma_1^{-1}\gamma_2 = \gamma_1\}$, $M(A) \cong \mathbb{R}P^2$ (real projective plane).

The facets-pairing structures $\mathcal{P}_A$ corresponding to these three binary matrices are shown from the left to the right in Figure 2.

Acknowledgement: the author wants to thank professor Mikiya Masuda for his hospitality while this work was done in Osaka City University in 2011.

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