

Crystallographic groups with cubic normal fundamental domain

By

LI YU*

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 $\{1, -1, \dots, n, -n\}$ 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

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

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*Department of Mathematics and IMS, Nanjing University, Nanjing, 210093, P.R.China, and

Department of Mathematics, Osaka City University, Osaka, 558-8585, Japan

e-mail: yuli@nju.edu.cn

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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 $\text{Isom}(\mathbb{R}^n) = O(n) \ltimes \mathbb{R}^n$, then any element of $\text{Isom}(\mathbb{R}^n)$ 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 $r : \text{Isom}(\mathbb{R}^n) \rightarrow O(n)$ 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 $\text{GL}(n, \mathbb{Z})$. 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 $\gamma \neq id_{\mathbb{R}^n} \in \Gamma$, $\gamma(\text{Int}D) \cap \text{Int}D = \emptyset$ where $\text{Int}D$ 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 $\mathbb{R}^n$.

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

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 $\tau_F : F \rightarrow F^*$ 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 $\{\gamma_F; F \text{ is a facet of } \mathcal{C}^n\}$.*

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 $[(\gamma, \mathcal{C}^n)]$, $\gamma \in \Gamma$.

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

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. $\Xi(f) = \{F \mid F \text{ is any facet of } \mathcal{C}^n \text{ with } f \subset F\}$. 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:

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

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

$$(2.2) \quad \Psi_F^f : \Xi(f) \rightarrow \Xi(f'), \text{ where } \Psi_F^f(F^\sharp) \cap F^* = \tau_F(F^\sharp \cap F) \text{ for } \forall F^\sharp \in \Xi(f).$$

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

$$(2.3) \quad (\Psi_F^f)^\perp : \Xi^\perp(f) \rightarrow \Xi^\perp(f'), (\Psi_F^f)^\perp(F^b) \cap f' = \tau_F(F^b \cap f) \text{ for } \forall F^b \in \Xi^\perp(f).$$

Since $\tau_F : F \rightarrow F^*$ 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:

$$\Psi_{F'}^{f'} \circ \Psi_F^f : \Xi(f) \rightarrow \Xi(f'') \text{ and } (\Psi_{F'}^{f'})^\perp \circ (\Psi_F^f)^\perp : \Xi^\perp(f) \rightarrow \Xi^\perp(f'').$$

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 $\tau_{F_4}\tau_{F_3}\tau_{F_2}\tau_{F_1}|_{f_1} : f_1 \rightarrow f_1$ coincides with id_{f_1} , and
- (b) the map $\Psi_{F_4}^{f_4} \circ \Psi_{F_3}^{f_3} \circ \Psi_{F_2}^{f_2} \circ \Psi_{F_1}^{f_1} : \Xi(f_1) \rightarrow \Xi(f_1)$ is the identity map.

Since the map $\tau_{F_4}\tau_{F_3}\tau_{F_2}\tau_{F_1}|_{f_1} : f_1 \rightarrow f_1$ 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 $(\Psi_{F_4}^{f_4})^\perp \circ (\Psi_{F_3}^{f_3})^\perp \circ (\Psi_{F_2}^{f_2})^\perp \circ (\Psi_{F_1}^{f_1})^\perp : \Xi^\perp(f_1) \rightarrow \Xi^\perp(f_1)$ is the identity map. In

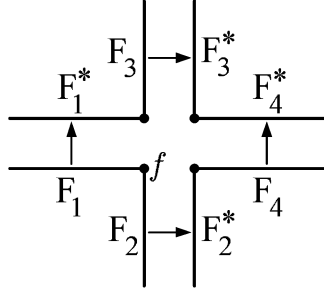


Figure 1.

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 $\tau_F : F \rightarrow F^*$ and $\tau_{F^*} : F^* \rightarrow F$ 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 $\tau_F : F \rightarrow F$ 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 $\{\tau_F : F \rightarrow F^*\}_{F \subset V^n}$ 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 $\tau_F : F \rightarrow F^*$ 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 $\text{Isom}(\mathbb{R}^n)$ 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 $\mathcal{P}$. $\square$

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 $\mathcal{P} = \{\hat{F}, \tau_F\}_{F \subset V^n}$ 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 $1 \leq j < k$. Moreover, when $k = 0$, we define $\tau_{F_k} \circ \cdots \circ \tau_{F_1}(f) := f$. Let $\hat{f}$ be the set of all faces of the valid form $\tau_{F_k} \circ \cdots \circ \tau_{F_1}(f)$ for some $k \geq 0$. We call $\hat{f}$ 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 $\hat{F}$.

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 $\hat{f}$ is called *perfect* if $\hat{f}$ 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.*

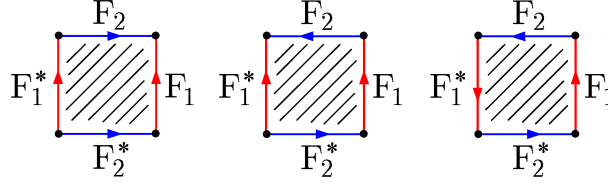


Figure 2.

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 $\pi : \Gamma \times \mathcal{C}^n \rightarrow \mathbb{R}^n = \Gamma \times \mathcal{C}^n / \mathcal{I}$ 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 $\theta : \Gamma \times \mathcal{C}^n \rightarrow \Gamma$ 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 $\hat{f}$ 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 $F_1, \dots, F_r$ 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, $\tau_F = \gamma_F^{-1}|_F : F \rightarrow F^*$ 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. $\square$

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 $[\pm n] := \{\pm 1, \dots, \pm n\} = \{1, -1, 2, -2, \dots, n, -n\}$. A map $\sigma : [\pm n] \rightarrow [\pm n]$ 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 $\text{GL}(n, \mathbb{Z})$ by sending $\sigma \in \mathfrak{S}_n^\pm$ to a matrix P_σ where

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

Such a matrix $P_\sigma \in \text{GL}(n, \mathbb{Z})$ 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 $\text{GL}(n, \mathbb{Z}) \cap O(n)$.

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 $j_1, \dots, j_s \in [\pm n]$ whose absolute values $|j_1|, \dots, |j_s|$ are pairwise distinct, we define

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

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

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

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

where $\delta_i = (0, \dots, 0, \overset{i}{1}, 0, \dots, 0)^t \in \mathbb{Z}^n$ 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 $b = \frac{1}{2}(k_1\delta_1 + \dots + k_n\delta_n)$ for some $k_1, \dots, k_n \in \mathbb{Z}$. So $L_\Gamma \subset \frac{1}{2}\mathbb{Z}^n$. $\square$

Remark. In the above theorem, suppose $\eta : H_\Gamma \rightarrow \text{GL}(n, \mathbb{Z})$ is the holonomy representation of Γ . In general, $\eta(H_\Gamma) < \text{GL}(n, \mathbb{Z})$ 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 $\omega \circ \omega = \text{id}_{[\pm n]}$. 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 $\mathcal{C}^n$

$$\{\tau_j \stackrel{\Delta}{=} \tau_{\mathbf{F}(j)} : \mathbf{F}(j) \rightarrow \mathbf{F}(\omega(j))\}_{j \in [\pm n]}$$

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

$$\sigma_j : [\pm n] \setminus \{\pm j\} \rightarrow [\pm n] \setminus \{\pm \omega(j)\}, \quad j \in [\pm n]$$

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

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:

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

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

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

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

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 $\sigma_j : [\pm n] \setminus \{\pm j\} \rightarrow [\pm n] \setminus \{\pm \omega(j)\}$ 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 $\tilde{\sigma}_j : [\pm n] \rightarrow [\pm n]$ by:

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

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

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

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

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

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 $\tilde{\sigma}_j$ is a signed permutation on $[\pm n]$. So $\tilde{\sigma}_j$ determines a unique symmetry of the cube $\mathcal{C}^n$, denoted by $\tilde{\tau}_j : \mathcal{C}^n \rightarrow \mathcal{C}^n$ where $\tilde{\tau}_j(\mathbf{F}(k)) = \mathbf{F}(\tilde{\sigma}_j(k))$ for any $k \in [\pm n]$. Then (4.1) becomes:

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

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

Corollary 4.4. Any regular facets-pairing structure on $\mathcal{C}^n$ corresponds to a tuple of elements $(\omega; T_1, T_{-1}, \dots, T_n, T_{-n})$ 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 $h : \mathcal{C}^n \rightarrow \mathcal{C}^n$ 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 $(\omega; \tilde{\sigma}_1, \tilde{\sigma}_{-1}, \dots, \tilde{\sigma}_n, \tilde{\sigma}_{-n})$ and $(\omega'; \tilde{\sigma}'_1, \tilde{\sigma}'_{-1}, \dots, \tilde{\sigma}'_n, \tilde{\sigma}'_{-n})$ 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:

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

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 $s_1, \dots, s_n$ on $\mathbb{R}^n$ is defined by:

$$s_i^A(x_1, \dots, x_n) := ((-1)^{A_{i1}}x_1, \dots, (-1)^{A_{i,i-1}}x_{i-1}, x_i + \frac{1}{2}, (-1)^{A_{i,i+1}}x_{i+1}, \dots, (-1)^{A_{in}}x_n)$$

where $A_{ij}^i \in \mathbb{Z}_2$ denote the (i, j) entry of A . Let $\Gamma(A)$ be the subgroup of $\text{Isom}(\mathbb{R}^n)$ generated by $s_1^A, \dots, s_n^A$, 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 $\mathbf{F}(i)$, $1 \leq i \leq n$, $\gamma_{\mathbf{F}(i)} = s_i^A$. 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 $r = \text{rank}_{\mathbb{Z}_2}(A)$.

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 $\{\omega_0, \tilde{\sigma}_j^A\}_{j \in [\pm n]}$ where

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

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

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.

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