Orbifold Triangulations and Crystallographic Groups

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Abstract

Given a triangulation of a 3-dimensional euclidean orbifold, e.g. in terms of the Delaney symbol of a periodic tiling, a method is discussed for identifying the isomorphism type of the corresponding space group. Of the 219 types of groups, 175 can be recognized solely by considering the orbifold graph associated with the given triangulation. Simple algebraic invariants distinguish between the remaining 44 cases. The graphs and invariants are listed.

1 Introduction

The motivation for the work reported in this paper is our interest in the classification of 3-dimensional periodic tilings and the following crucial question: Given an arbitrary 3-dimensional Delaney symbol [Dre84, Dre87] is it *realizable*, i.e. does it give rise to a periodic tiling, and if so, in which space can the tiling be realized? In particular, is the Delaney symbol *euclidean*, i.e. does it encode a tiling of euclidean space?

An *orbifold* is a Hausdorff, paracompact space $\mathcal{O}$ which is locally homeomorphic to the quotient space of $\mathbb{R}^n$ by a finite group action. To be precise, the given space is equipped with an atlas of charts $\phi_\alpha : U_\alpha/?_\alpha \to \mathcal{O}$, where U_α is an open set in $\mathbb{R}^n$ and $?_\alpha$ is a finite subgroup of the n-dimensional orthogonal group $O(n)$. These charts have to satisfy obvious compatibility conditions [Sco83][p. 422].

Let $\mathcal{Q}$ be a triangulation of a 3-dimensional orbifold $\mathcal{O}$, i.e. a triangulation of $\mathcal{O}$ that is compatible with the given atlas. We call $\mathcal{Q}$ *euclidean*, if it can be obtained as the orbit space of some 3-dimensional crystallographic space group acting on (a triangulation of) $\mathbb{E}^3$. In this paper we discuss the practical problem of determining the isomorphism type (or *affine crystallographic type* [Hah83]) of the space group ? associated with a given euclidean 3-dimensional orbifold $\mathcal{Q}$, where $\mathcal{Q}$ is given as an abstract orbifold triangulation, as defined

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below. In particular, we present a system of efficiently computable invariants that completely determine the isomorphism type.

In Section 2 we define orbifold triangulations and orbifold graphs, and then state in Theorem 2.2 that the 219 isomorphism types of 3-dimensional space groups give rise to precisely 189 different orbifold graphs (listed in Table 2), only 14 of which correspond to more than one group. In other words, 175 types of groups are characterized by their orbifold graph alone. In Section 3 we discuss how this work relates to the classification of space groups [Hah83]. Then, in Section 4 we introduce certain algebraic invariants, and state in Theorem 4.1 that they distinguish between the remaining 44 types of groups (listed in Table 3. Finally, in Section 5 we briefly describe our implementation of the concepts defined in this paper in terms of Delaney symbols.

The results presented here, and computer programs based on them, give rise to a strong necessary condition for a 3-dimensional orbifold triangulation or Delaney symbol to be euclidean, and thus will be a useful tool in the classification of 3-dimensional periodic tilings, as we shall demonstrate in a forthcoming paper [DH96a].

For an enumeration of all 3-dimensional euclidean orbifolds whose underlying space is $\mathbb{S}^3$, see [Dun88]. Note that our definition of an orbifold graph and Lemma 2.1 is similar to works presented in [Bal90]. The role of orbifolds in crystallography is discussed in [JBD96].

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2 Orbifold Graphs

Let $\mathcal{S}$ be a finite 3-dimensional simplical complex and let $\mathcal{S}_0$, $\mathcal{S}_1$, $\mathcal{S}_2$ and $\mathcal{S}_3$ denote the set of 0-, 1-, 2- and 3-dimensional simplices in $\mathcal{S}$, called *vertices*, *edges*, *facets* and *chambers*, respectively.

We call $\mathcal{S}$ a *3-dimensional compact pseudo-manifold*, if the following conditions hold:

- Every simplex $s \in \mathcal{S}$ is contained in some chamber $c \in \mathcal{S}_3$.
- Every facet $f \in \mathcal{S}_2$ is contained in at most two chambers.
- The link of any vertex $v \in \mathcal{S}_0$ or edge $e \in \mathcal{S}_1$ is connected.

Moreover, $\mathcal{S}$ is called *connected*, if we have:

- Any two chambers $c, c' \in \mathcal{S}_3$ are connected by a chain of chambers, in which any two consecutive chambers share a common facet.

Let $\mathcal{S}$ be 3-dimensional compact connected pseudo-manifold. A simplex $s \in \mathcal{S}$ is called *unprotected*, if its interior lies on the boundary of the topological realization $|\mathcal{S}|$, and *protected*, otherwise.

Let n be an *edge-labeling of* $\mathcal{S}$, i.e. a map $n : \mathcal{S}_1 \to \mathbb{N} \backslash \{0\}$. In this situation the *link* of a vertex is a 2-dimensional complex that inherits a labeling of its vertices from the edge-labeling of $\mathcal{S}$. Hence it is a 2-dimensional orbifold. We call the system $\mathcal{Q} := (\mathcal{S}, n)$ an *orbifold triangulation*, if for each vertex $v \in \mathcal{S}_0$, the link of v is a *spherical* orbifold, i.e. an orbit space $\mathbb{S}^2/?$ with ? a finite subgroup of $O(3)$. Note that then, the open stars of vertices can be used to define an orbifold atlas for $|\mathcal{S}|$, and, vice versa, an orbifold atlas of $|\mathcal{S}|$ that is compatible with the triangulation defines an edge-labeling of $\mathcal{S}$.

Let $\mathcal{Q} = (\mathcal{S}, n)$ be a (3-dimensional) orbifold triangulation. The associated *orbifold graph* G is a node-labeled graph $G = (V, E)$, with node set V and edge set E. We define $V := \mathcal{S}$, and label each node by the name of the orbifold which is given by the corresponding link. We use Conway's orbifold notation [Con92, BH96], as summarized in Table 1. For the different types of simplices this means:

- Each vertex $v \in \mathcal{S}_0$ is labeled by the name of the associated 2-dimensional orbifold.
- Each edge $e \in \mathcal{S}_1$ is labeled vv or $*vv$, with $v = n(e)$, depending on whether e is protected, or not.
- each facet $f \in \mathcal{S}_2$ is labeled 1 or $1*$, depending on whether f is protected, or not.
- Each chamber $c \in \mathcal{S}_3$ is labeled 1.

Two distinct nodes $A, B \in V$ are joined by an edge $\{A, B\} \in E$, if and only if $A \subset B$ or $B \subset A$.

Obviously, one can define the concept of an *orbifold graph* independently of a given orbifold triangulation, as a node-labeled graph, whose labeling fulfills certain compatibility conditions, but we omit the details. An orbifold graph G is called *reduced*, if no two adjacent nodes have the same label. Any orbifold graph G can be transformed into a reduced graph $G^* = (V^*, E^*)$ as follows:

Two nodes A, B are called *equivalent*, if and only if there they are connected by a chain of adjacent nodes, that all have the same label (including A and B). Let V^* be the set of all such equivalence classes. We join two classes C and C' by an edge in E^*, if and only if there exist $A \in C$ and $B \in C$ such that A and B are adjacent in G.

Note that G^* contains precisely one *trivial node* labeled 1, adjacent to all other nodes. Obviously, this node can be omitted. We call $\mathcal{S}$ *orientable*, if $|\mathcal{S}|$ is orientable as a pseudo-manifold. Additionally, we attach one further piece of information to the graph of an orbifold triangulation $\mathcal{Q}$, namely whether the complex $\mathcal{S}$ is *non-orientable*, *weakly-orientable* (i.e. orientable and not all facets are protected), or *strongly-orientable* (i.e. orientable and all facets are protected).

The reduced orbifold graph is independent of the given triangulation:

Lemma 2.1 *Let $\mathcal{Q} = (\mathcal{S}, n)$ be a 3-dimensional euclidean orbifold triangulation obtained from the action of a crystallographic space group ? on a triangulation $\mathcal{S}'$ of $\mathbb{E}^3$. The associated reduced orbifold graph $G^* = (V^*, E^*)$ depends only on ? .*

Proof. (Sketch) The described reduction process determines a stratification of the triangulated orbifold into strata of points whose stabilizer groups have the same type. This follows from the fact that the point stabilizer group is

(i)	(ii)	(i)	(ii)	(i)	(ii)	(i)	(ii)
1	1	2×	$\bar{4}$	432	432	∗322	$\bar{6}2m$
1∗	m	322	32	44	4	∗33	$3m$
1×	$\bar{1}$	33	3	4∗	$4/m$	∗332	$\bar{4}3m$
22	2	332	23	622	622	∗422	$4/mmm$
222	222	3∗	$3/m$	66	6	∗432	$m\bar{3}m$
2∗	$2/m$	3∗2	$m\bar{3}$	6∗	$6/m$	∗44	$4mm$
2∗2	$\bar{4}2m$	3×	$\bar{3}$	∗22	$mm2$	∗622	$6/mmm$
2∗3	$\bar{3}m$	422	422	∗222	mmm	∗66	$6mm$

Table 1: Conway's orbifold notation (i) and standard crystallographic notation (ii) for the crystallographic point-groups.

invariant on the interior of the simplices, as $\mathcal{S}$ comes from a ?-invariant triangulation. Hence, the reduced graph depends only on the type of the orbifold and not on the given triangulation. □

From now on, we will always assume the considered orbifold graphs are reduced. The orbifold graph (together with the information on orientability) is a useful space-group invariant. We have the following result:

Theorem 2.2 *The 219 isomorphism types of 3-dimensional crystallographic space groups give rise to 189 isomorphism types of orbifold graphs. Exactly 175 graphs each correspond to precisely one type of group, whereas the remaining 14 each are compatible with two or more types of groups.*

Proof. In Table 2 we list all 189 different orbifold graphs and for each such graph we indicate the corresponding type(s) of group(s). □

3 International Tables

How do orbifold graphs relate to the descriptions of symmetry groups given in the *International Tables of Crystallography* [Hah83]? In Table 2 we list the *Wyckoff letters* associated with each of the nodes of the given orbifold graph G. In most cases, there is a one-to-one correspondence between Wyckoff letters and nodes. A slight discrepancy can arise when a 3-fold axis is present in ?, as then different nodes in the orbifold graph may correspond to different segments of the *same* Wyckoff site. For example, a 2-fold rotational axis in ? that passes through a point group of type 322 in general gives rise to two different nodes in G, which both correspond to the same Wyckoff site or letter, see [JBD96] for details.

We can resolve this discrepancy as follows. Let G be the (reduced) orbifold graph G of some crystallographic group ?. Two nodes v and w both labeled Y are called *Wyckoff equivalent*, if there exists a node x labeled X that is adjacent to both v and w such that one of the following conditions hold:

- $X = 322$ and $Y = 22$,
- $X = 332$ and $Y = 33$,
- $X = *322$ and $Y = *22$,
- $X = *332$ and $Y = *33$, or
- $X = *33$ and $Y = 1*$.

This generates an equivalence relationship on the node set of G, and the equivalence classes correspond to the Wyckoff positions of the associated symmetry group. Let us call the graphs obtained by identifying nodes with respect to this equivalence relationship *Wyckoff graphs*. By inspection of all graphs listed in Table 2, we obtain the following result:

Lemma 3.1 *The crystallographic space groups give rise to precisely 189 types of Wyckoff graphs.*

4 Abelian Invariants

Given a 3-dimensional orbifold triangulation. Using standard techniques from algebraic topology, a finite presentation in terms of generators and relations of the corresponding space group, or, in general, the group of deck-transformations of the corresponding universal orbifold cover, can easily be computed. The isomorphism type of the largest abelian quotient group, which is derived as the quotient by its commutator subgroup, is a simple group invariant. This *commutator factor group* is a finitely generated abelian group, i.e. it can be represented uniquely as a (finite) direct sum of infinite cyclic groups and cyclic groups of prime-power orders. We will call the isomorphism type of the commutator factor group of a given group ? the *abelian type* of ?.

The set of all (conjugacy classes of) index two subgroups of a given finitely presented group can be determined by standard methods from computational group theory, namely by enumerating all essentially different actions of the given group on a set of order two and then interpreting this set as the set of cosets with respect to a certain subgroup of index two [S+93].

We have the following result:

Theorem 4.1 *Of the* 44 *types of 3-dimensional space groups that cannot be distinguished by their orbifold graphs alone,* 33 *can be recognized by their orbifold graph together with their abelian type. For the* 11 *remaining cases, a successful strategy is to consider as an additional invariant the set of all different abelian types of index two subgroups of the group in question.*

PROOF. In Table 3, for each of the 44 space groups that cannot be distinguished by their orbifold graphs alone, we list the corresponding abelian types and, where necessary, the additional invariants. □

5 Computation

We have implemented the concepts introduced in this paper in terms of Delaney symbols. Our C++ program OGRAPH takes as input a list of 3-dimensional Delaney symbols and produces as output the corresponding reduced orbifold graphs. Based on [NM95], it uses [McK90] to determine whether computed graphs are isomorphic. A second program, based on [S^+93], computes the abelian invariants associated with a given Delaney symbol [Del94].

Using a program for computing periodic Delone tilings [DH96b], we can obtain Delaney symbols for each of the 219 types of space groups. Applying the above mentioned programs to this data produces the results listed in Theorem 2.2 and Theorem 4.1.

Putting this all together gives rise to a program that takes as input a 3-dimensional Delaney symbol and produces as output either "none", or the name of one of the 219 types of 3-dimensional space groups. In the former case, the Delaney symbol cannot be euclidean, whereas in the latter case, either the associated symmetry group is of the named type, or the Delaney symbol is not euclidean. This program will have useful applications in classification problems concerning 3-dimensional tilings of the type described in [DHM93].

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Captions

Fig. 1
The orbifold graph $Q121$.

Table 2

Here we list the 189 isomorphism types of orbifold graphs arising from the 219 isomorphism types of 3-dimensional space groups. The graphs are ordered by the following features: First number of nodes, then occurring labels, number of edges, orientability, and finally, adjacencies of nodes. The Wyckoff letters were not used in sorting. To understand how to read the graphs, consider for example, graph 51: The first line `Q51 (n=4,e=2,or=0)` indicates that the graph has `n=4` nodes, `e=2` edges and the underlying manifold is non-orientable `or=0` (whereas `or=1` or `or=2` would indicate the weakly- or strongly-orientable case, respectively). The nodes of the graph are numbered `0,1,...,n-1` and there is one line per node. Each line starts with the node number, followed by the Wyckoff letter associated with the node, the next entry is the node label, i.e. a 2-dimensional symmetry group in orbifold notation, which is followed by the list of adjacent nodes. E.g., `1 c: 22 2 3` indicates that node number 1 has Wyckoff letter c, label 22 and is adjacent to nodes 2 and 3. Below each graph we list the numbers of the possible crystallographic groups [Hah83]. E.g., `Groups: 114 122` indicates that groups 114 and 122 correspond to the given graph. Finally, if two groups differ only by their left- or righthandeness, then we list them together; for example, `Groups: 180 (181)` indicates that the listed graph corresponds to the isomorphic pair 180 and 181.

Table 3

Here we list the 44 sets of abelian invariants needed to identify the crystallographic group for those 14 orbifold graphs that correspond to more than one group. For each such group listed in the first column, we list its abelian type in the second column. Where necessary, the third column contains the different abelian types of all its index 2 subgroups. In the last column we indicate the number of the group (or the isomorphic pair) [Hah83].