Counting Crystallographic Groups in Low Dimensions

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CONTENTS

We present the results of our computations concerning the space groups of dimension 5 and 6. We find 222 018 and 28 927 922 isomorphism types of these groups, respectively. Some overall statistics on the number of $\mathbb{Q}$-classes and $\mathbb{Z}$-classes in dimensions up to six are provided. The computations were done with the package CARAT, which can parametrize, construct and identify all crystallographic groups up to dimension 6.

1. INTRODUCTION AND DEFINITIONS

The classification of the isomorphism types of space groups in a given dimension is an old problem. Fedorov and Schönflies gave in 1895 a list of the 219 affine space-group types in three dimensions. This list was later extended to dimension 4 [Brown et al. 1978]. Continuing this work in this way (that is, giving a list of representatives) does not seem to be appropriate for higher dimensions, because the numbers grow rapidly. We suggest replacing this kind of classification by a set of algorithms which enables one to perform at least the following tasks:

- give a space group R a "name", that is, compute invariants/properties that determine the affine type of R uniquely;
- construct specific space groups on demand,
- count specific space groups, i.e., all space groups in a given $\mathbb{Z}$-class, as defined below.

As an example of this philosophy we calculated the number of space groups in dimensions 5 and 6, and the results are presented in this paper. A second application is given in [Cid and Schulz 2001], where the torsion-free space groups in dimension 5 and 6 are classified, which correspond to the compact Euclidean flat manifolds of that dimension.

The computer programs and data which can be used to obtain these results are part of CARAT, a

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software package available on the Internet at http://www-math.math.rwth-aachen.de/~LBFM/carat/. The package, the algorithms, a lot of the underlying theory and the terminology used in this paper is given in [Opgenorth et al. 1998].

Recall that the structure of a space group R is given by the exact sequence

$$0 \longrightarrow \mathbb{Z}^n \longrightarrow R \longrightarrow P \longrightarrow 1,$$

where $P \leq \mathrm{GL}_n(\mathbb{Z}) = \mathrm{Aut}(\mathbb{Z}^n)$ is finite and acts naturally on $\mathbb{Z}^n$. We call P the *point group* of R.

We say two space groups R and R' belong to the same

(i) affine class if they are isomorphic,
(ii) $\mathbb{Z}$-class if the corresponding point groups P and P' are conjugate in $\mathrm{GL}_n(\mathbb{Z})$,
(iii) $\mathbb{Q}$-class if the corresponding point groups P and P' are conjugate in $\mathrm{GL}_n(\mathbb{Q})$.

For a finite subgroup $G \leq \mathrm{GL}_n(\mathbb{Z})$ we define the space of invariant forms of G by

$$\mathcal{F}(G) = \{F \in \mathbb{Z}^{n\times n}_{\mathrm{sym}} \mid g^{\mathrm{tr}}Fg = F \text{ for all } g \in G\}.$$

Crystal families correspond to the transitive closure of $\sim$, defined as follows: For two finite subgroups $G, H \leq \mathrm{GL}_n(\mathbb{Z})$, we say $G \sim H$ if there exist subgroups $G' \leq G$ and $H' \leq H$ with $\mathcal{F}(G') = \mathcal{F}(G)$, $\mathcal{F}(H') = \mathcal{F}(H)$ and G' and H' belong to the same $\mathbb{Q}$-class. If one requires that the commuting algebras of G and G' as well of H and H' in $\mathbb{Q}^{n\times n}$ are the same, one gets strict families instead.

For strict families one can easily define a symbol by taking advantage of the following property of strict families: the natural representation of any group G in the strict family can be decomposed into rational irreducible representations Δ_i with multiplicities n_i, that is,

$$n_1\Delta_1 \dot{+} \cdots \dot{+} n_a\Delta_a.$$

The n_i and the strict families of the $\Delta_i(G)$ are characterising invariants of the strict family of G. As names for the strict families of irreducible groups of dimension d we choose the symbol $d - \alpha$, where α numbers the irreducible families of dimension d. Putting some order on these symbols, one assigns to G the symbol

$$(\underbrace{d_1\text{-}\alpha_1, \ldots, d_1\text{-}\alpha_1}_{n_1}; \underbrace{d_2\text{-}\alpha_2, \ldots, d_2\text{-}\alpha_2}_{n_2}; \ldots; \underbrace{d_a\text{-}\alpha_a, \ldots, d_a\text{-}\alpha_a}_{n_a}).$$

For crystal families one similarly defines a symbol, which differs from the above only in cases where a "," shows up: One first notes that a family is the union of strict families. For the symbol of an irreducible family one chooses a symbol d-α like above. In the symbol of a reducible family one uses these for the constituents of multiplicity one, and the symbols for the strict families for the other constituents. For instance for dimension 1 one has just one strict family (= family), which gets the symbol 1. For dimension 2, one has two irreducible families 2-1 (quadratic) and 2-2 (hexagonal): the first splits into two strict families 2-1 and 2-1′, and the second into strict families 2-2 and 2-2′. For dimension three one again has just one strict irreducible family, which therefore is also a family, and gets the symbol 3.

2. CONSTRUCTING THE $\mathbb{Q}$-CLASSES

In the given approach, constructing a set of representatives for the $\mathbb{Q}$-classes of finite subgroups of $\mathrm{GL}_n(\mathbb{Z})$ up to dimension 6 is the first difficulty. We solve it by taking a list of $\mathbb{Q}$-maximal subgroups of $\mathrm{GL}_n(\mathbb{Z})$ from [Plesken and Pohst 1977a; 1977b], and compute their subgroups via an algorithm described in [Cox et al. ≥ 2000] and implemented in the standard group theory package MAGMA [Bosma and Cannon 1993].

In principle, we could test each pair of these subgroups for $\mathrm{GL}_n(\mathbb{Q})$-conjugacy to obtain a set of representatives. For a short description of the $\mathrm{GL}_n(\mathbb{Q})$-conjugacy test used, see [Opgenorth et al. 1998]. To reduce the number of pairs which have to be considered for a $\mathrm{GL}_n(\mathbb{Q})$-conjugacy test, these invariants proved to be helpful:

(a) the family symbol [Plesken and Hanrath 1984];
(b) the order;
(c) the elementary divisors of the Gram matrix of the $\mathbb{Z}$-bilinear form $\Phi : \overline{\mathbb{Z}G} \times \overline{\mathbb{Z}G} \to \mathbb{Z}$ defined by

$$\Big(\sum_g a_g g, \sum_h b_h h\Big) \mapsto \sum_{g,h} a_g b_h \,\mathrm{Tr}(gh),$$

which is in line of the $\mathrm{GL}_n(\mathbb{Q})$-conjugacy test mentioned above.

This greatly reduces the number of pairs to be processed, and it was feasible to tackle them directly. We found 955 $\mathbb{Q}$-classes in dimension 5 and 7104 in dimension 6. The tables below show how they are distributed into crystal families. These computations took 4 weeks on an HP-9000/J282 and two HP-9000/730. An explicit list of representatives of the $\mathbb{Q}$-classes up to dimension 6 is now part of CARAT.

3. FROM $\mathbb{Q}$-CLASSES TO AFFINE CLASSES

The splitting of $\mathbb{Q}$-classes into affine classes (that is, isomorphism types of space groups) is done in two steps.

The first is to split the $\mathbb{Q}$-classes into $\mathbb{Z}$-classes, for which an algorithm has been described in [Opgenorth et al. 1998, Section 3.2.2].

The second step, splitting into affine classes each of the resulting 6079 $\mathbb{Z}$-classes in dimension 5 and 85311 in dimension 6, is classical [Zassenhaus 1948; Brown et al. 1978]. As a matter of fact, for given finite $G \leq \mathrm{GL}_n(\mathbb{Z})$, the isomorphism classes of space groups with point group $\mathrm{GL}_n(\mathbb{Z})$-conjugate to G are in bijection with the orbits of the normalizer $N := \mathrm{N}_{\mathrm{GL}_n(\mathbb{Z})}(G)$ on

$$H^2(G, \mathbb{Z}^n) \cong H^1(G, \mathbb{Q}^n/\mathbb{Z}^n).$$

The only slight problem here is that the number of orbits might be too large to compute them all, but in this case the lemma of Burnside is applied (bear in mind that although N might be infinite, $H^2(G, \mathbb{Z}^n)$ is not, and hence the acting group is finite).

4. RESULTS FOR DIMENSIONS 4, 5, AND 6

Table 2 gives the results of our computations concerning the crystallographic groups in dimension 5 and 6. For comparison, we give in Table 1 the known results for the dimensions 2, 3 and 4 [Brown et al. 1978]. Starting from the $\mathbb{Q}$-classes as input, the computations take respectively about 10 min, 6 hours, and 3 days in dimensions 4, 5, and 6 (timing again on a HP-9000/J282 workstation).

To interpret the family symbol, see [Plesken and Hanrath 1984] or call the appropriate CARAT routine. The first number following a comma or a semicolon or the number at the beginning denotes the dimension of an irreducible $\mathbb{Q}$-constituent. Equivalent constituents are separated by a comma, and inequivalent ones by a semicolon.

APPENDIX: CARAT

CARAT is an acronym for Crystallographic AlgoRithms And Tables. It handles enumeration and construction problems, as well as recognition and comparison problems for crystallographic groups up to dimension 6. Besides the above mentioned tables of $\mathbb{Q}$-classes, it contains a table of the Bravais groups (full automorphism groups of lattices) and their inclusions up to dimension 6. From this basic information the above tasks can be performed by a set of algorithms whose implementation are part of CARAT.

The most basic algorithms are:

(a) the Zassenhaus algorithm [1948] to split a $\mathbb{Z}$-class into affine classes;

(b) the sublattice algorithm, which for $G \leq \mathrm{GL}_n(\mathbb{Z})$ and $L \leq \mathbb{Z}^n$ a G-lattice computes the maximal G-sublattices of L [Plesken and Pohst 1977a; 1977b];

f.s.	$\mathbb{Q}$	$\mathbb{Z}$	aff.
1,1	2	2	2
1;1	2	4	7
2-1	2	2	3
2-2	4	5	5
$\sum$	10	13	17

f.s.	$\mathbb{Q}$	$\mathbb{Z}$	aff.
1,1,1	2	2	2
1,1;1	3	6	13
1;1;1	3	13	59
2-1;1	7	16	65
2-2;1	12	21	45
3	5	15	35
$\sum$	32	73	219

f.s.	$\mathbb{Q}$	$\mathbb{Z}$	aff.
1,1,1,1	2	2	2
1,1,1;1	3	6	13
1,1;1,1	2	6	12
1,1;1;1	4	25	207
1;1;1;1	5	54	1001
2-1′,2-1′	1	1	1
2-1,2-1	1	3	6
2-1;1,1	7	16	88
2-1;1;1	15	113	1670
2-1;2-1	11	41	302
2-2′,2-2′	2	2	2
2-2,2-2	2	5	5
2-2;1,1	12	21	49
2-2;1;1	22	84	471
2-2;2-1	22	40	108
2-2;2-2	26	63	87
3;1	16	85	471
4-1	37	73	205
4-1′	2	2	3
4-2	22	45	53
4-2′	2	2	2
4-3	7	16	20
4-3′	4	5	5
$\sum$	227	710	4783

TABLE 1. Families of two-dimensional (left), three-dimensional, and four-dimensional crystallographic groups. In each subtable, the first column gives the family symbols; the others give the number of $\mathbb{Q}$-classes, $\mathbb{Z}$-classes and affine classes.

f. symbol	ℚ	ℤ	aff.	f. symbol	ℚ	ℤ	aff.	f. symbol	ℚ	ℤ	aff.
1,1,1,1,1	2	2	2	2-1;1;1;1	33	912	84997	3;2-1	31	200	2147
1,1,1,1;1	3	6	13	2-1;2-1;1	59	728	29487	3;2-2	59	281	1333
1,1,1;1,1	3	9	21	2-2′,2-2′;1	5	7	12	4-1′;1	7	16	70
1,1,1;1;1	4	25	226	2-2,2-2;1	7	24	56	4-1;1	141	534	6976
1,1;1,1;1	4	38	396	2-2;1,1,1	12	21	49	4-2′;1	7	7	23
1,1;1;1;1	8	169	8083	2-2;1,1;1	35	146	1271	4-2;1	104	250	979
1;1;1;1;1	8	279	49659	2-2;1;1;1	45	432	10878	4-3′;1	12	21	45
2-1′,2-1′;1	3	6	14	2-2;2-1;1	119	592	7220	4-3;1	23	70	162
2-1,2-1;1	4	31	201	2-2;2-2;1	116	416	1940	5-1	13	39	112
2-1;1,1,1	7	16	90	3;1,1	16	85	565	5-2	10	40	89
2-1;1,1;1	24	232	6113	3;1;1	31	445	8789	∑	955	6079	222018

f. symbol	ℚ	ℤ	aff.	f. symbol	ℚ	ℤ	aff.	f. symbol	ℚ	ℤ	aff.
1,1,1,1,1,1	2	2	2	2-2′,2-2′;2-2	15	27	43	4-1;1,1	141	562	12500
1,1,1,1,1;1	3	6	13	2-2,2-2,2-2	2	6	6	4-1;1;1	365	4760	446887
1,1,1,1;1,1	3	9	21	2-2,2-2;1,1	7	27	67	4-1;2-1	399	2868	92178
1,1,1,1;1;1	4	25	228	2-2,2-2;1;1	15	114	673	4-1;2-2	576	1950	12345
1,1,1;1,1,1	2	8	17	2-2,2-2;2-1	15	51	146	4-2′;1,1	7	7	25
1,1,1;1,1;1	5	60	866	2-2,2-2;2-2	25	122	180	4-2′;1;1	15	30	249
1,1,1;1;1;1	8	177	10537	2-2;1,1,1,1	12	21	49	4-2′;2-1	17	23	68
1,1;1,1;1,1	3	41	396	2-2;1,1,1;1	35	146	1330	4-2′;2-2	28	45	52
1,1;1,1;1;1	8	374	34875	2-2;1,1;1,1	22	126	1214	4-2;1,1	104	250	1223
1,1;1;1;1;1	15	1439	934891	2-2;1,1;1;1	84	1177	66716	4-2;1;1	315	1604	21599
1;1;1;1;1;1	15	2273	8599496	2-2;1;1;1;1	101	3121	665233	4-2;2-1	343	1123	5359
2-1′,2-1′,2-1′	1	1	1	2-2;2-1′,2-1′	8	11	21	4-2;2-2	481	1747	2388
2-1′,2-1′;1,1	3	9	23	2-2;2-1,2-1	14	69	319	4-3′;1,1	12	21	49
2-1′,2-1′;1;1	5	35	276	2-2;2-1;1,1	119	592	13308	4-3′;1;1	22	84	471
2-1′,2-1′;2-1	5	14	90	2-2;2-1;1;1	433	7580	592666	4-3′;2-1	22	40	108
2-1,2-1,2-1	1	3	8	2-2;2-1;2-1	277	2131	47956	4-3′;2-2	34	67	67
2-1,2-1;1,1	4	40	354	2-2;2-2;1,1	116	428	2658	4-3;1,1	23	62	157
2-1,2-1;1;1	10	311	8989	2-2;2-2;1;1	358	3004	55848	4-3;1;1	46	296	1696
2-1,2-1;2-1	10	131	2306	2-2;2-2;2-1	358	1524	8212	4-3;2-1	49	155	490
2-1;1,1,1,1	7	16	90	2-2;2-2;2-2	264	1379	2534	4-3;2-2	69	236	268
2-1;1,1,1;1	24	232	7012	3,3	5	36	109	5-1;1	43	228	1561
2-1;1,1;1,1	15	207	7647	3;1,1,1	16	85	571	5-2;1	32	222	956
2-1;1,1;1;1	64	3244	738504	3;1,1;1	51	904	29343	6-1	93	519	2538
2-1;1;1;1;1	78	9938	11255381	3;1;1;1	65	3004	382566	6-2	125	334	441
2-1;2-1;1,1	59	869	71105	3;2-1;1	179	3744	218443	6-2′	4	5	5
2-1;2-1;1;1	218	12717	4258991	3;2-2;1	293	2973	54405	6-3	15	34	45
2-1;2-1;2-1	113	2355	234229	3;3	60	806	10538	6-3′	4	5	5
2-2′,2-2′,2-2′	2	2	2	4-1′;1,1	7	16	95	6-4	2	9	23
2-2′,2-2′;1,1	5	9	15	4-1′;1;1	15	113	1809	6-4′	2	6	11
2-2′,2-2′;1;1	7	20	71	4-1′;2-1	17	67	540				
2-2′,2-2′;2-1	7	8	16	4-1′;2-2	22	40	108	∑	7104	85311	28927922

TABLE 2. Families of five-dimensional (top) and six-dimensional (bottom) crystallographic groups. The first column gives the family symbols; the others give the number of ℚ-classes, ℤ-classes and affine classes.

(c) the lattice automorphism and isometry algorithm to compute isometries/automorphism groups of quadratic forms [Plesken and Souvignier 1997].

Building up from these algorithms, CARAT offers an implementation of the normalizer (and $\mathbb{Z}$-equivalence) algorithm [Opgenorth 2001], based mainly on (c), to construct isometries between so called G-perfect forms. Combining this with the sublattice algorithm (b) one gets an algorithm to split a $\mathbb{Q}$-class into $\mathbb{Z}$-classes. Note that the normalizer algorithm also provides input necessary for the extension algorithm (a).

In the data bank of $\mathbb{Q}$-classes, each class has a name, from which certain invariants can be read off. CARAT automatically extends this name to a name of the isomorphism class of a space group, via a name of the $\mathbb{Z}$-class by using the above algorithms as numbering devices. Two space groups are isomorphic if and only if CARAT produces the same name for both of them.

To use CARAT one need not learn a new language; instead uses the Unix command line to call the various programs, each of which comes with an online help. It should be portable to any Unix machine.

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