Counting crystallographic groups in low dimensions

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Abstract

In this paper, we present results of our computations concerning the space groups of dimension 5 and 6. We find 222.018 resp. 28.927.922 isomorphism types of these groups. Some overall statistics on the number of $\mathbb{Q}$-classes and $\mathbb{Z}$-classes in the dimension up to six is added. 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 degree is an old problem. Fedorov and Schönflies gave a list of the 219 affine space-group types in three dimensions in 1895. This list has been extended to dimension 4 in 1978, see [BBNWZ 78]. Continuing this work in this way (i.e. 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", i.e. compute invariants/properties, which determine the affine type of R uniquely,
- construct specific space groups on demand,
- count specific space groups, i.e. all space group in a given $\mathbb{Z}$-class, as defined below.

As an example 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 [CS 99], where the torsion free space groups in dimension 5 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 the package CARAT, which is available via 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 [OPS 98]

Recall 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 $\mathbb{Z}^n$. P is called the point group of R.

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

(i) affine class iff they are isomorphic,

(ii) $\mathbb{Z}$-class iff the corresponding point groups P and P' are conjugate in $\mathrm{GL_n}(\mathbb{Z})$,

(iii) $\mathbb{Q}$-class iff 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 $\mathcal{F}(G) = \{F \in \mathbb{Z}^{n\times n}_{sym} | g^{tr} F g = F \text{ for all } g \in G\}$. 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, i. e. $n_1\dot{\Delta}_1 + \ldots + n_a\dot{\Delta}_a$. 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 degree d we choose the symbol $d-\alpha$, where α numbers the irreducible families of degree d. Putting some order on these symbols, one assigns the symbol

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

to G.

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 $d-\alpha$ 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 degree 1 one has just one strict family (= family), which gets the symbol 1. For degree 2, one has two irreducible families $2-1$ (quadratic) and $2-2$ (hexagonal), each one splitting into two restricted families $2-1$ and $2-1$‘, resp. $2-2$ and $2-2$‘. For degree 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 this problem by taking a list of $\mathbb{Q}$-maximal subgroups of $\mathrm{GL}_n(\mathbb{Z})$ from [PlP 77,80], and compute subgroups of them via an algorithm described in [CCH 99] and implemented in the standard group theory package MAGMA, cf. [BC 96].

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 used $\mathrm{GL}_n(\mathbb{Q})$-conjugacy test, see [OPS 98]. To reduce the number of pairs which have to be considered for a $\mathrm{GL}_n(\mathbb{Q})$-conjugacy test, the following invariants have proven to be helpful:

(a) family symbol (see [PlH 84]),

(b) order,

(c) elementary divisors of the Gram matrix of the $\mathbb{Z}$-bilinear form $\Phi : \overline{\mathbb{Z}G} \times \overline{\mathbb{Z}G} \to \mathbb{Z}$, $(\sum_g a_g g, \sum_h b_h h) \mapsto \sum_{g,h} a_g b_h \mathrm{Tr}(gh)$, 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 and 7104 $\mathbb{Q}$-classes in degree 5 and 6, resp. The tables below show how they distribute into crystal families. These computations took 4 weeks on an HP-9000/J282 and two HP-9000/730, and 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 (i.e. isomorphism types of space groups) is done in two steps.

The first step is to split the $\mathbb{Q}$-classes into $\mathbb{Z}$-classes, for which an algorithm has been described in [OPS 98, section 3.2.2].

The second step, splitting each of the resulting 6079 and 85311 $\mathbb{Z}$-classes in dimension 5 and 6, respectively, into affine classes, is classical, see [Zas 48], [BBNWZ 78]. 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 to the orbits of $N := \mathrm{N}_{\mathrm{GL}_n(\mathbb{Z})}(G)$ 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 ≤ 6

We now give the results of our computations concerning the crystallographic groups in dimension 5 and 6, and add the known results for the dimensions 2 to 4 (see [BBNWZ 78]) for comparison. Starting from the $\mathbb{Q}$-classes as input, the computations take about 10 min, 6 hours, and 3 days in dimensions 4, 5 resp. 6 (timing again on a HP-9000/J282 workstation).

As for the family symbol, see [PlH 84] or call the appropriate CARAT routine. Note, the first number following a comma or a semicolon or the number at the beginning denotes a degree of an irreducible $\mathbb{Q}$-constituent, equivalent constituents are seperated by a comma, and inequivalent by a semicolon.

family symbol	no. $\mathbb{Q}$-classes	no. $\mathbb{Z}$-classes	no. aff. classes	family symbol	no. $\mathbb{Q}$-classes	no. $\mathbb{Z}$-classes	no. aff. classes
1,1	2	2	2	1;1	2	4	7
2-1	2	2	3	2-2	4	5	5
				$\sum$	10	13	17

Table of the 2-dimensional crystallographic groups

family symbol	no. $\mathbb{Q}$-classes	no. $\mathbb{Z}$-classes	no. aff. classes	family symbol	no. $\mathbb{Q}$-classes	no. $\mathbb{Z}$-classes	no. aff. classes
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

Table of the 3-dimensional crystallographic groups

family symbol	no. $\mathbb{Q}$-classes	no. $\mathbb{Z}$-classes	no. aff. classes	family symbol	no. $\mathbb{Q}$-classes	no. $\mathbb{Z}$-classes	no. aff. classes
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 of the 4-dimensional crystallographic groups

family symbol	no. $\mathbb{Q}$-classes	no. $\mathbb{Z}$-classes	no. aff. classes	family symbol	no. $\mathbb{Q}$-classes	no. $\mathbb{Z}$-classes	no. aff. classes
1,1,1,1,1	2	2	2	1,1,1,1;1	3	6	13
1,1,1;1,1	3	9	21	1,1,1;1;1	4	25	226
1,1;1,1;1	4	38	396	1,1;1;1;1	8	169	8083
1;1;1;1;1	8	279	49659	2-1',2-1';1	3	6	14
2-1,2-1;1	4	31	201	2-1;1,1,1	7	16	90
2-1;1,1;1	24	232	6113	2-1;1;1;1	33	912	84997
2-1;2-1;1	59	728	29487	2-2',2-2';1	5	7	12
2-2,2-2;1	7	24	56	2-2;1,1,1	12	21	49
2-2;1,1;1	35	146	1271	2-2;1;1;1	45	432	10878
2-2;2-1;1	119	592	7220	2-2;2-2;1	116	416	1940
3;1,1	16	85	565	3;1;1	31	445	8789
3;2-1	31	200	2147	3;2-2	59	281	1333
4-1';1	7	16	70	4-1;1	141	534	6976
4-2';1	7	7	23	4-2;1	104	250	979
4-3';1	12	21	45	4-3;1	23	70	162
5-1	13	39	112	5-2	10	40	89
				$\sum$	955	6079	222018

Table of the 5-dimensional crystallographic groups

family symbol	no. $\mathbb{Q}$-classes	no. $\mathbb{Z}$-classes	no. aff. classes	family symbol	no. $\mathbb{Q}$-classes	no. $\mathbb{Z}$-classes	no. aff. classes
1,1,1,1,1,1	2	2	2	1,1,1,1,1;1	3	6	13
1,1,1,1;1,1	3	9	21	1,1,1,1;1;1	4	25	228
1,1,1;1,1,1	2	8	17	1,1,1;1,1;1	5	60	866
1,1,1;1;1;1	8	177	10537	1,1;1,1;1,1	3	41	396
1,1;1,1;1;1	8	374	34875	1,1;1;1;1;1	15	1439	934891
1;1;1;1;1;1	15	2273	8599496	2-1',2-1',2-1'	1	1	1
2-1',2-1';1,1	3	9	23	2-1',2-1';1;1	5	35	276
2-1',2-1';2-1	5	14	90	2-1,2-1,2-1	1	3	8
2-1,2-1;1,1	4	40	354	2-1,2-1;1;1	10	311	8989
2-1,2-1;2-1	10	131	2306	2-1;1,1,1,1	7	16	90
2-1;1,1,1;1	24	232	7012	2-1;1,1;1,1	15	207	7647
2-1;1,1;1;1	64	3244	738504	2-1;1;1;1;1	78	9938	11255381
2-1;2-1;1,1	59	869	71105	2-1;2-1;1;1	218	12717	4258991
2-1;2-1;2-1	113	2355	234229	2-2',2-2',2-2'	2	2	2
2-2',2-2';1,1	5	9	15	2-2',2-2';1;1	7	20	71
2-2',2-2';2-1	7	8	16	2-2',2-2';2-2	15	27	43
2-2,2-2,2-2	2	6	6	2-2,2-2;1,1	7	27	67
2-2,2-2;1;1	15	114	673	2-2,2-2;2-1	15	51	146
2-2,2-2;2-2	25	122	180	2-2;1,1,1,1	12	21	49
2-2;1,1,1;1	35	146	1330	2-2;1,1;1,1	22	126	1214
2-2;1,1;1;1	84	1177	66716	2-2;1;1;1;1	101	3121	665233
2-2;2-1',2-1'	8	11	21	2-2;2-1,2-1	14	69	319
2-2;2-1;1,1	119	592	13308	2-2;2-1;1;1	433	7580	592666
2-2;2-1;2-1	277	2131	47956	2-2;2-2;1,1	116	428	2658
2-2;2-2;1;1	358	3004	55848	2-2;2-2;2-1	358	1524	8212
2-2;2-2;2-2	264	1379	2534	3,3	5	36	109
3;1,1,1	16	85	571	3;1,1;1	51	904	29343
3;1;1;1	65	3004	382566	3;2-1;1	179	3744	218443
3;2-2;1	293	2973	54405	3;3	60	806	10538
4-1';1,1	7	16	95	4-1';1;1	15	113	1809
4-1';2-1	17	67	540	4-1';2-2	22	40	108
4-1;1,1	141	562	12500	4-1;1;1	365	4760	446887
4-1;2-1	399	2868	92178	4-1;2-2	576	1950	12345
4-2';1,1	7	7	25	4-2';1;1	15	30	249
4-2';2-1	17	23	68	4-2';2-2	28	45	52
4-2;1,1	104	250	1223	4-2;1;1	315	1604	21599
4-2;2-1	343	1123	5359	4-2;2-2	481	1747	2388
4-3';1,1	12	21	49	4-3';1;1	22	84	471
4-3';2-1	22	40	108	4-3';2-2	34	67	67
4-3;1,1	23	62	157	4-3;1;1	46	296	1696
4-3;2-1	49	155	490	4-3;2-2	69	236	268
5-1;1	43	228	1561	5-2;1	32	222	956
6-1	93	519	2538	6-2	125	334	441
6-2'	4	5	5	6-3	15	34	45
6-3'	4	5	5	6-4	2	9	23
6-4'	2	6	11				
				$\sum$	7104	85311	28927922

Table of the 6-dimensional crystallographic groups

5 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 the following three:

(a) the Zassenhaus algorithm to split a $\mathbb{Z}$-class into affine classes, see [Zas 48],

(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, see [PlP 77,80],

(c) the lattice automorphism and isometry algorithm to compute isometries/automorphism groups of quadratic forms, see [PlS 97].

Building up from these, CARAT contains an implementation of the normalizer (and $\mathbb{Z}$-equivalence) algorithm, see [Op 99], which is 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 iff 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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