COMPUTING WITH CRYSTALLOGRAPHIC GROUPS

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Algorithms are presented for the computation with crystallographic groups of arbitrary dimension, in particular for the determination of the Wyckoff positions and maximal subgroups of a space group, and for the determination of all space group types for a given point group. These algorithms have been implemented in the computer algebra system GAP, and are made publically available. The capabilities of this software package are illustrated by a number of examples.

1 Introduction

Information about crystallographic groups, in particular space groups, is usually made available in the form of printed lists, such as in the International Tables,[1] or in the book on four-dimensional crystallographic groups.[2] For higher dimensions, this approach becomes quickly impractical, as the number of such groups grows very rapidly with the dimension. Since some of the higher-dimensional space groups are of practical importance as symmetry groups of quasicrystals and modulated cystals, we suggest here a more promising approach. Instead of providing pre-computed tables one should rather provide *software* that can selectively compute the entries of these tables whenever the need arises. Such an approach has several advantages. There is no need to decide beforehand which are the "interesting" groups. Moreover, the user can work in any basis that seems suitable for the problem at hand, and is not bound to the choice of basis made by the authors of the table. And finally, having the information available in electronic form makes it easy to further process the data by other programs.

Such a software system, called CrystGap,[3] has been implemented on top of GAP,[4] a freely available computer algebra system which is particularly strong in group theoretical computations. CrystGap is distributed together with the current 3.4.4 release of GAP.[4] Building CrystGap on top of GAP has several advantages over a standalone package. The most important one is that many group theoretical algorithms are already implemented in GAP and are ready to be used, so that one does not have to reinvent the wheel all the time. Since these algorithms have been selected and implemented by experts in the field, it is likely that they are more efficient than anything one would write for a standalone package. A further advantage is that GAP also contains a number of group databases. Of particular interest for a crystallographic groups package

are a table with representavtives of all space group types of dimensions 2, 3 and 4, and tables with Z-class or Q-class representatives of maximal irreducible finite integral matrix groups for many dimensions. From the tables of finite integral matrix groups one can determine representatives of all point groups of a given dimension, and from these the corresponding space groups types can be computed by means of the Zassenhaus algorithm, which is also provided.

In the following, we first sketch the algorithms used in CrystGap. These algorithms have been described in more detail in a previous paper.[5] Some of the capabilites of CrystGap are then illustrated with a few examples. A further example of an application of CrystGap can be found in a separate paper.[6]

2 Sketch of the algorithms

Since space groups are not finite, computing with them is not entirely trivial. These problems are solved by using the fact that the subgroup T of pure translations of a space group S is normal, and that the sequence of homomorphisms $0 \to T \to S \to P \to 1$ is exact, where $P \cong S/T$ is the point group of S.

An important piece of information about a space group is its set of Wyckoff positions.[7] To determine these, one takes the full lift of a representative of each of the subgroup conjugacy classes of the point group (which are efficiently computed by GAP), and determines the set of points left invariant modulo lattice translations. These points form an array of affine subspaces. In some cases the resulting points have an even bigger stabilizer, but otherwise the S-orbit of any one of these affine subspaces forms a Wyckoff position.

For the computation of maximal subgroups, two different procedures are used, depending on whether the space group is solvable or not. In the solvable case one first divides S by p times the translation subgroup, where p is some prime, and computes the maximal subgroups of the resulting finite group, using a special power-commutator presentation for which very efficient methods exist. The other translations are added again later. In this way, the maximal subgroups of p-power index are obtained. In the non-solvable case, one has to distinguish between translation-equal and class-equal subgroups. For translation-equal subgroups it is enough to lift the maximal subgroups of the point group to S, whereas in the class-equal case one first has to compute the P-invariant subgroups of given index of T, and then determine the conjugacy class representatives of their complements in S.

There is one class of algorithms in GAP which is essential for most of the computations described above. GAP provides facilities to conveniently compute the orbit and the stabilizer of arbitrary, user-defined group actions, provided the orbit of the group action remains finite.

3 Examples

CrystGap can deal with space groups expressed in any basis. It is not necessary to use a primitive lattice basis. This makes it easy to explore the subgroup structure of a space group by iteratively computing maximal subgroups without any change of basis. As an example we show part of the subgroup lattice of the 6D icosahedral space group $I\bar{5}\bar{3}\frac{2}{m}$ (Fig. 1). Shown are all class-equal subgroups (having an isomorphic point group) whose index is a power of 2 (and not bigger than 64). There are three symmorphic subgroups $P\bar{5}\bar{3}\frac{2}{m}$, and three non-symmorphic subgroups $P\bar{5}\bar{3}\frac{2}{q}$, all of index 2. They correspond to the three different embeddings of the P lattice in the I lattice. The three subgroups $F\bar{5}\bar{3}\frac{2}{q}$ (index 4) and the four subgroups $I\bar{5}\bar{3}\frac{2}{m}$ (index 64), on the other hand, are conjugates of each other by translations. They are conjugated in the affine normalizer of the top level group $I\bar{5}\bar{3}\frac{2}{m}$.

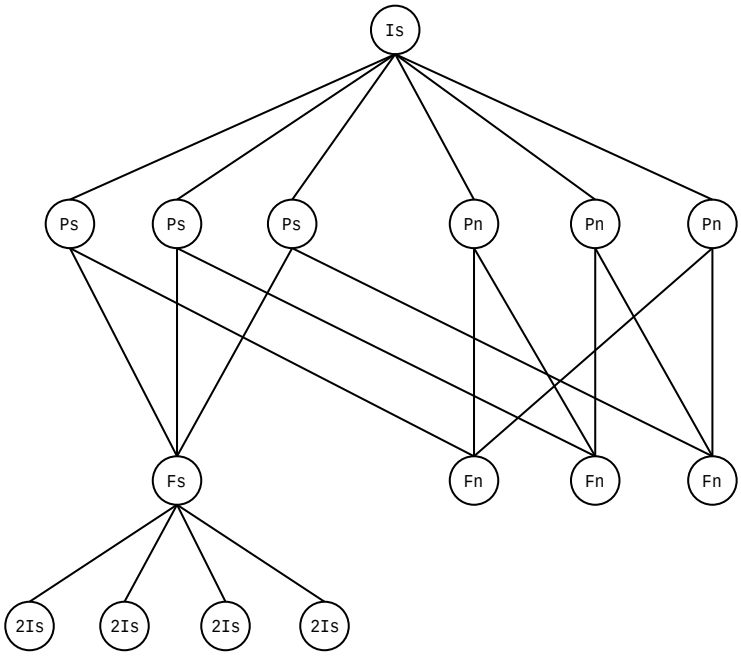

Figure 1: Part of the subgroup lattice of $I\bar{5}\bar{3}\frac{2}{m}$ (class-equal subgroups only). A vertex label Ls means a symmorphic space group of type $L\bar{5}\bar{3}\frac{2}{m}$, a label Ln a non-symmorphic space group of type $L\bar{5}\bar{3}\frac{2}{q}$, where the lattice L is either I, P or F. $2I$ denotes the I lattice scaled by a factor 2. For the I lattice there exists only a symmorphic space group.

CrystGap offers the possibility to display the set of Wyckoff positions of a space group, together with their incidence relations, in the form of a graph (Fig. 2). For instance, a special line contains a special point if and only if the two corresponding vertices of the graph are connected. Such a graph allows to quickly seize the situation. By clicking with the mouse on one of the vertices a menu pops up, with the help of which one can inquire various properties of the corresponding Wyckoff position and its stabilizer.

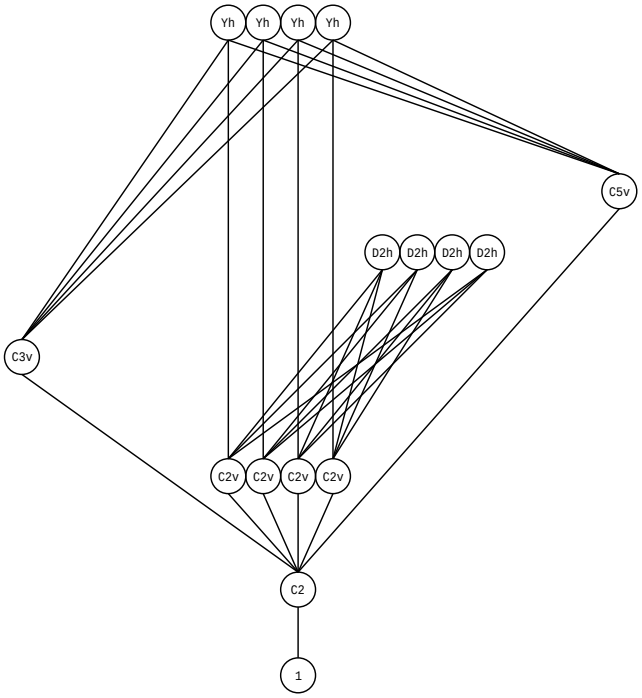

Figure 2: Structure of the Wyckoff psitions of the 6D icosahedral space group $F\bar{5}\bar{3}\frac{2}{m}$. There are special points with stabilizers $Y_h = \bar{5}\bar{3}m$ and $D_{2h} = mmm$ (4 each), special lines with stabilizers $C_{5v} = \bar{5}m$, $C_{3v} = \bar{3}m$ (1 kind each) and $C_{2v} = mm$ (4 kinds), one kind of mirror plane, and the general position. Connections in the graph indicate incidence relations.

Without giving an example, we mention that CrystGap supports also colour space groups. Space groups can be coloured by specifying the subgroup which leaves one of the colours (colour 1) invariant. The permutation group induced by the colour group on the set of colours can also be computed. With the maximal subgroups routine, it is also possible to determine all inequivalent colourings with a given number of colours.

4 Conclusion

We have presented a freely available software package for the computation with crystallographic groups. There are other packages which offer some of these functions as well. While the performance of our package compares well[5] with the package of Fuksa & Engel[8] (which computes Wyckoff positions only), a performance comparison with the package of Thiers et al.[9] could not yet be made, as the latter is currently available only over the Web.[10] What is presently missing, but planned for the future, is a routine to compute the normalizer of an arbitrary point group in $GL(n, \mathbb{Z})$, needed in the Zassenhaus algorithm and for the computation of the affine normalizer of a space group.

Acknowledgments

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