Z. Kristallogr. **221** (2006) 77–82 / **DOI** 10.1524/zkri.2006.221.1.77

The four-dimensional magnetic point and space groups

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Received August 17, 2004; accepted February 1, 2005

Magnetic groups / Antisymmetry / Higher-dimensional crystallography / Quasicrystals

Abstract. This paper describes the classification of magnetic point and space groups which are also referred to as *antisymmetry groups* or *black-and-white groups*. These groups play an important role in the description of discrete point sets in which the points are not only characterized by their spatial coordinates but also by an additional property taking one of two possible values (*e.g.* spin *up* or *down*). Each operation of a magnetic group may or may not switch the value of this additional property. In this paper, the methods for classifying magnetic groups in arbitrary dimensions are described in an algorithmic fashion. Results of the full classification in four-dimensional space are given and the application of the magnetic groups in this dimension to quasicrystals is indicated.

Introduction

Since the classification of the 3-dimensional crystallographic space groups into 230 affine classes at the end of the 19th century, several developments have inspired the investigation of generalized concepts of crystallographic groups involving symmetry groups in dimensions exceeding 3.

One important motivation was the discovery of quasicrystals which have certain rotational symmetries and long-range order but no translational symmetry (see [13]). In particular, one observes rotations of order 5, 8, 10 or 12 which are in conflict with the crystallographic restriction in dimension 3. One possibility to describe structures with these types of symmetries is to regard their points as points of an integral lattice of higher degree, *i.e.* as integral linear combinations of a set of vectors which are linearly independent over the rational numbers but may become dependent over the real numbers. One thus looks at d-dimensional lattices embedded into the 2- or 3-dimensional Euclidean space. The groups acting on these lattices are described in a natural way by matrices giving the coordinates with respect to a lattice basis, which are therefore integral matrices of degree d. For example, rotations of order 5, 8, 10 or 12 may be represented by integral matrices of degree $d = 4$. Going one step further, one may immediately consider lattice points in an abstract d-dimensional space on which some higher-dimensional symmetry group acts. From this abstract space, a 2- or 3-dimensional point pattern can be obtained by a suitable projection method, *e.g.* by the cut-and-project method commonly used for quasicrystals (cf. [4]).

A second development arose from the study of crystals in which every crystal site is characterized not only by its spatial coordinates but also by some additional property. The most prominent of such properties are magnetic moments, electric dipole moments or simply types of atoms. In the case of a property that takes only two possible values, one often identifies these values with the colours *black* and *white* or with the spins *up* and *down*. The corresponding groups acting on the points are accordingly called *black-and-white groups* or *magnetic groups*. The 1651 3-dimensional magnetic space groups (also known as *Shubnikov groups*) were first classified by A. M. Zamorzaev [16] in 1953. It is worthwhile to note that it was already proposed by H. Heesch [3] in 1930 that 3-dimensional magnetic groups can be studied as reducible groups in dimension 4 and that this approach led him to the classification of the 122 3-dimensional magnetic point groups.

The combination of quasiperiodic symmetries and magnetic properties now suggests to look at magnetic groups in higher-dimensional spaces. In particular, magnetic substances with local 5-, 8-, 10- or 12-fold rotational symmetry can be described via 4-dimensional magnetic groups, which, following the philosophy of Heesch, can be studied as reducible groups in dimension 5. With the classification of the ordinary 5-dimensional space groups available (cf. [12] and [10]), one approach would be to select the groups in question from this list. This is in principle possible, but some subtle questions about equivalence arise, since the ordinary classes in dimension 5 may have to be split into several classes of magnetic groups because the coordinate representing the magnetic property has to be distinguished from the spatial coordinates. A more fundamental argument against this look-up approach is that it is desirable that information can be produced locally, *i.e.* that it is possible to compute only magnetic groups having certain symmetry properties, without relying on a full classification in a higher dimension.

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We therefore take the geometric and arithmetic classes of ordinary crystallographic point groups in dimension d as starting point and determine the d-dimensional magnetic point and space groups from there. Our approach is in line with the methods described in [8], however, some issues are described in a more algorithmic setting, following the philosophy of [10]. The methods described in the present paper have a natural generalization to colour groups, thus providing an algorithmic approach to the theory of colour symmetry as presented in [6].

Magnetic point groups

As already suggested by Heesch [3], a d-dimensional magnetic point group can be realized as a $(d+1)$-dimensional rational matrix group which acts on the direct product of the d-dimensional space $\mathbb{R}^d$ with the 1-dimensional spin space (consisting of only 2 possible values). The matrices are of the form $\mathfrak{g} = \begin{pmatrix} g & 0 \\ 0 & \varepsilon \end{pmatrix}$ where g runs over all elements of a finite subgroup $G \leq GL(d, \mathbb{Q})$ and $\varepsilon = 1$ indicates that the element $\mathfrak{g}$ fixes the spin configuration while $\varepsilon = -1$ means that the spins are switched by $\mathfrak{g}$. There are now three possibilities (the first of which can be regarded as trivial):

(i) All ε are 1. In this case all spins are preserved and the group is isomorphic with G. These groups are called *junior* or *white* groups.

(ii) The identity element 1_G of G occurs both with $\varepsilon = 1$ and $\varepsilon = -1$, which means that all elements of G occur both with and without spin inversion. Such a group is isomorphic with the direct product $G \times C_2$ and is called a *senior* or *grey* group.

(iii) Precisely half of the elements of G occur only with $\varepsilon = 1$, the other half only with $\varepsilon = -1$. In this case, the map associating to each $g \in G$ its attached value ε is a group homomorphism $G \to C_2$. In particular, the set of elements with $\varepsilon = 1$ is a normal subgroup H of index 2 in G, namely the kernel of this homomorphism and the magnetic group is a (nontrivial) subdirect product of G and C_2 (recall that a subdirect product of two groups G_1 and G_2 is a subgroup S of the direct product $G_1 \times G_2$ such that the projections of S on the two components are surjective).

Note that many authors actually refer only to the subdirect products of case (iii) as magnetic, black-and-white or antisymmetry groups. To make a distinction we will term the groups of case (iii) *proper magnetic* groups in the sequel of this paper. A proper magnetic group is thus uniquely characterized by a pair (G, H) where H is the subgroup of index 2 in G preserving the spin configuration.

In order to classify the d-dimensional magnetic point groups one has to find the subgroups of index 2 for representatives of the point groups in dimension d. However, depending on the classification level, different notions of equivalence may be applied. The most natural classifications are those into geometric and arithmetic classes. For the classification into geometric classes, the group G represents its conjugates under $GL(d, \mathbb{Q})$. We call two magnetic point groups (G_1, H_1) and (G_2, H_2) *geometrically equivalent* if there exists a transformation $t \in GL(d, \mathbb{Q})$ such that $t^{-1}G_1t = G_2$ and $t^{-1}H_1t = H_2$. In particular, two magnetic point groups can only be geometrically equivalent if the groups G_1 and G_2 are geometrically equivalent as ordinary point groups. We can therefore restrict ourselves to the case $G_1 = G = G_2$ and check whether there exists $t \in GL(d, \mathbb{Q})$ such that $t^{-1}Gt = G$ and $t^{-1}H_1t = H_2$. Since the first condition means that t lies in the rational normalizer $N := N_{GL(d,\mathbb{Q})}(G)$ of G in $GL(d, \mathbb{Q})$, we conclude that two magnetic point groups (G, H_1) and (G, H_2) are geometrically equivalent if and only if H_1 and H_2 are conjugate under an element $t \in N$.

We therefore compute the orbits of the rational normalizer N of G on the subgroups H of index 2 in G and choose a representative H from each orbit. Each such orbit representative gives a representative of a geometric class of magnetic point groups.

In an analogous way the arithmetic classes of magnetic point groups are obtained. Here, a group G represents its conjugates under $GL(d, \mathbb{Z})$ and the stabilizer is its normalizer in $GL(d, \mathbb{Z})$. Hence, we take the orbit representatives of subgroups H of index 2 under the action of the integral normalizer $N_{GL(d,\mathbb{Z})}(G)$ of G.

A remark about the different normalizers seems appropriate. An algorithm to compute the integral normalizer $N_{GL(d,\mathbb{Z})}(G)$ of a group G is described in [11]. From this, the rational normalizer $N_{GL(d,\mathbb{Q})}(G)$ is obtained by adding elements in the centralizer of the group (which are not interesting in our case because they act trivially on the subgroups) and elements obtained from the G-invariant sublattices of $\mathbb{Z}^d$ which have G-actions lying in the same arithmetic class as G (see [15] for a more detailed discussion).

Since the determination of the space groups requires the normalizers of the point groups, we have to compute the normalizers of the magnetic point groups as well. For a magnetic point group (G, H), its normalizer is the stabilizer $S := \mathrm{Stab}_N(H)$ of H in the normalizer N of G. In the process of computing the orbit representatives for the subgroups of index 2 in G we get this stabilizer almost for free by the following method: Let N be generated by the elements $n_1, n_2, \ldots, n_s$. We get the orbit of H under N be repeatedly applying the generators n_j of N to the conjugate subgroups H_i of H found so far until no new conjugates occur. Each time we find a new conjugate H_i we record an element $t_i \in N$ which conjugates H to H_i. Ultimately, we obtain a set $\{t_1, t_2, \ldots, t_r\}$ of coset representatives for the cosets of S in N which correspond to the conjugates $H_1, \ldots, H_r$ of H under N. If we denote by $\overline{n}$ the element t_i such that $n^{-1}Hn = t_i^{-1}Ht_i$, then the set $\{t_i n_j (\overline{t_i n_j})^{-1} \mid 1 \leq i \leq r,\ 1 \leq j \leq s\}$ is a set of generators for S, called *Schreier generators*.

Magnetic space groups

Having analyzed the situation for magnetic point groups, we can analogously apply the case distinction of *white*, *grey* and *proper magnetic* groups to space groups. We thus obtain the following three cases for a magnetic space group $\mathfrak{G}$:

(i) $\mathfrak{G}$ is a white group, *i.e.* no element of the group changes the spin arrangement. In this case $\mathfrak{G}$ is an ordinary space group and the white groups are clearly in 1-1 correspondence with the space groups.

(ii) $\mathfrak{G}$ is a grey group, *i.e.* the identity element of an ordinary space group $\mathcal{G}$ occurs with and without spin inversion in $\mathfrak{G}$. This means that $\mathfrak{G} \cong \mathcal{G} \times C_2$ and also the grey groups are in 1-1 correspondence with the ordinary space groups.

(iii) The elements in $\mathfrak{G}$ preserving the spin arrangement form a subgroup of index 2, but the pure spin inversion is not contained in $\mathfrak{G}$. Ignoring the action of $\mathfrak{G}$ on the spins turns $\mathfrak{G}$ into an ordinary space group $\mathcal{G}$ and the elements of $\mathfrak{G}$ which fix the spin arrangement form a subgroup $\mathcal{H}$ of index 2 in $\mathcal{G}$.

The interesting case (iii) of proper magnetic space groups can be split into two subcases:

(a) The translation subgroup of $\mathcal{H}$ is a subgroup of index 2 in the translation subgroup of $\mathcal{G}$ and consequently every element of the point group of $\mathcal{G}$ occurs in the point group of $\mathcal{H}$. In this case, $\mathcal{H}$ is called a *class-equal (klassengleich)* subgroup of $\mathcal{G}$.

(b) The translation subgroup of $\mathcal{H}$ is equal to the translation subgroup of $\mathcal{G}$ and thus the point group of $\mathcal{H}$ is a subgroup of index 2 of the point group of $\mathcal{G}$. In this case, $\mathcal{H}$ is called a *lattice-equal (zellengleich)* or *translation-equal* subgroup of $\mathcal{G}$.

Starting from arithmetic classes of point groups, the magnetic space groups with class-equal and lattice-equal subgroups fixing the spin arrangement are determined by slightly differing approaches.

Class-equal subgroups

We start with a grey point group $G \times C_2$ by adding the matrix $\iota := \begin{pmatrix} 1_G & 0 \\ 0 & -1 \end{pmatrix}$ for the spin inversion as a generator to the group $\left\{ \begin{pmatrix} g & 0 \\ 0 & 1 \end{pmatrix} \mid g \in G \right\}$, where $G \leq GL(d, \mathbb{Z})$ is a representative of an arithmetic class in dimension d. To obtain the magnetic space groups with this group as point group, we compute the vector systems for this group via a slight modification of the Zassenhaus algorithm (cf. [18]) setting the translation component for the additional spin coordinate to 0. As usual, the representatives for the equivalence classes of space groups are found as orbit representatives for the action of the normalizer of G on the vector systems. Note that in this case only the ordinary normalizer $N_{GL(d,\mathbb{Z})}(G)$ is required, since we are dealing with a grey group.

We now have two possibilities: Either the vector system element for the spin inversion ι is trivial, which means that the space group contains spin inversion and is therefore a grey group. Or the vector system element for the spin inversion is non-trivial, which means that the translation subgroup of the group preserving the spin configuration is of index 2 in the full translation subgroup. In the latter case we have therefore constructed a proper magnetic space group with class-equal subgroup fixing the spin configuration.

Note that the special case of G being a Bravais group gives as a byproduct the black-and-white Bravais lattices, whose enumeration was already described in [9].

Lattice-equal subgroups

To obtain proper magnetic space groups with lattice-equal subgroups fixing the spin configuration we start with a proper magnetic point group (G, H). As in the case of class-equal subgroups, the vector systems for this group are computed using the modified Zassenhaus algorithm, setting again the spin component to 0. To get representatives for the equivalence classes of magnetic space groups, we have to compute the orbits of the normalizer of the point group on the vector systems. This time, the normalizer is the normalizer of the magnetic point group (G, H) which we obtain as the stabilizer of H in the integral normalizer of G (as described earlier). In general, this normalizer is smaller than the ordinary normalizer of G, hence the orbits on the vector systems may split into smaller orbits under the normalizer of the magnetic point group. This splitting of orbits reflects the fact that the subgroup H may be oriented in different ways relative to the translation subgroup of the space group.

Enantiomorphism

Two point or space groups are called an enantiomorphic pair if they are equivalent under a general linear or affine transformation but not under an orientation-preserving transformation. Note that by this definition enantiomorphism is an abstract concept applicable in arbitrary dimensions. However, its interpretation as *handedness* does not always carry through the projection process into 2- or 3-dimensional physical space. In fact, enantiomorphism in the higher-dimensional space is a stronger property, since operations are regarded as orientation-preserving which may not preserve orientations in the projection (for example the product of two reflections one of which has a normal vector orthogonal to the physical space).

For ordinary point groups, determining enantiomorphism comes down to deciding whether the normalizer of a group contains elements of negative determinant (see [15]). The same is true for magnetic point groups, provided the correct normalizer is considered. For a proper magnetic point group given by a pair (G, H), we have already seen that the normalizer is the stabilizer of H in the normalizer of G.

For magnetic space groups, the situation is analogous to that of ordinary space groups. If the point group is enantiomorphic because its normalizer contains only orientation-preserving transformations, all space groups with this point group are enantiomorphic. Note that for a proper magnetic point group (G, H) we again have to use the correct normalizer, *i.e.* the stabilizer of H in the normalizer of G. If the magnetic point group is itself not enantiomorphic, enantiomorphism may still occur for some of the space groups, namely in the case that the linear part of the stabilizer of a space group contains only elements of positive determinant.

Results

The techniques described above have been used to reconstruct the known classification results for magnetic groups in dimensions 1, 2 and 3 and to obtain the corresponding results in dimension 4.

Table 1 gives the numbers of proper magnetic point and space groups as well as the total numbers of magnetic groups, including the white and grey groups. Note that the full number of magnetic groups on a classification level is obtained as the number of proper magnetic groups plus two times the number of ordinary groups on this level (corresponding to the white and grey groups). For the proper magnetic space groups, the numbers of groups with class-equal and lattice-equal subgroup fixing the spin arrangement, respectively, are also distinguished. The numbers given refer to equivalence classes under general linear and affine transformations, the numbers of enantiomorphic pairs are given in brackets.

In order to relate the results given to other results in the literature it is worthwhile to note that in the notation of Bohm symbols $G_{nst\dots}$ (cf. [14], [17], [5]) the geometric classes of white point groups correspond to the groups $G_{d,0}$, the geometric classes of all magnetic point groups to $G_{d+1,d,0}$, the classes of white space groups to G_d and the classes of all magnetic space groups to the groups $G_{d+1,d}$.

Note that for dimension 3 there is a slight discrepancy in the literature concerning the number of magnetic space group types when disregarding enantiomorphism. While [17] states that there are 1160 proper magnetic and 1598 magnetic space groups, [5] gives the correct number of 1594 magnetic groups.

Application to quasicrystals

The 4-dimensional point and space groups are of particular interest in connection with quasicrystals displaying octagonal, pentagonal, decagonal or dodecagonal symmetries.

There are different methods how a discrete point set representing a 2-dimensional quasicrystal can be obtained, amongst which the cut-and-project method described in [4]. The idea of this method is as follows: A 2-dimensional subspace V of $\mathbb{R}^4$ is chosen as physical space. In the orthogonal space $V^\perp$ a bounded region B is selected, which is called the *acceptance region*. Now only those points of $\mathbb{R}^4$ whose orthogonal projection into $V^\perp$ lie in B are projected into V. For the illustrations displayed below we chose B to be the projection of the Voronoi-cell around the origin with respect to the underlying 4-dimensional lattice. In these examples the Voronoi-cell is a regular 24-cell and its projection a regular octagon.

It is clear that in order to obtain 2-dimensional quasicrystals with symmetries of order 8, 5, 10 or 12 by the cut-and-project method we have to look at the crystal families of rationally irreducible point groups in dimension 4.

On the one hand there are the octagonal, decagonal and dodecagonal crystal families containing dihedral groups with rotations of order 8, 10 and 12, respectively. These groups are rationally irreducible but have invariant subspaces of dimension 2 over the real numbers which are the obvious choices for the physical space in the cut-and-project method. The groups can be analyzed in a straightforward manner as suggested in [6], and for example the octagonal crystal family has already been discussed in the more general setting of spin groups in [7] and [2].

On the other hand the diisohexagonal (XXI), icosahedral (XXII) and hypercubic (XXIII) crystal families (in the terminology of [1]) of absolutely irreducible point groups also contain symmetries of orders 8, 10 or 12 (note that the hypercubic family admits symmetries of order 8 as well as of order 12). Table 2 displays the numbers of magnetic groups for these crystal families, showing that they provide us with a wealth of examples of interesting patterns.

Although the groups in these families do not have proper invariant subspaces themselves, they contain subgroups acting on 2-dimensional subspaces. If such a subspace is chosen as physical space, the pattern obtained by the cut-and-project method will display the symmetries of

Table 1. Classification results for magnetic point and space groups.

	Number of classes in dimension			
	1	2	3	4
Geometric classes	5	31	122	1025 (+177)
white/grey	2	10	32	227 (+44)
proper magnetic	1	11	58	571 (+89)
Arithmetic classes	5	43	294	3653 (+311)
white/grey	2	13	73	710 (+70)
proper magnetic	1	17	148	2233 (+171)
Space-group types	7	80	1594 (+57)	61553 (+674)
white/grey	2	17	219 (+11)	4783 (+111)
proper magnetic	3	46	1156 (+35)	51987 (+452)
class-equal	2	20	500 (+17)	21872 (+70)
lattice-equal	1	26	656 (+18)	30115 (+382)

Table 2. Classification results for absolutely irreducible crystal families in dimension 4.

	XXI	XXII	XXIII
Geometric classes	104 (+49)	23	141 (+77)
white/grey	22 (+10)	7	37 (+20)
proper magnetic	60 (+29)	9	67 (+37)
Arithmetic classes	220 (+78)	54	300 (+122)
white/grey	45 (+15)	16	73 (+30)
proper magnetic	130 (+48)	22	154 (+62)
Space-group types	250 (+86)	64	1266 (+386)
white/grey	53 (+17)	20	205 (+63)
proper magnetic	144 (+52)	24	856 (+260)
class-equal	0	0	195 (+47)
lattice-equal	144 (+52)	24	661 (+213)

the subgroup while the other symmetries of the full group remain hidden. Of course, the subgroups we are interested in are cyclic groups of orders 8, 5, 10 or 12 and the corresponding dihedral groups of orders 16, 10, 20 or 24. For these groups, the physical space can be determined as follows:

Let $g \in GL(4, \mathbb{Z})$ be an element of order m for $m \in \{8, 5, 10, 12\}$ and let $\zeta_m = \mathrm{e}^{\frac{2\pi i}{m}}$, then the matrix $g + g^{-1}$ has a 2-dimensional eigenspace for the eigenvalue $\zeta_m + \zeta_m^{-1}$ and g acts as a rotation of order m on this eigenspace. For the above values of m, these eigenvalues are easily computed, namely: $\zeta_8 + \zeta_8^{-1} = 2\cos\left(\frac{\pi}{4}\right) = \sqrt{2}$, $\zeta_5 + \zeta_5^{-1} = 2\cos\left(\frac{2\pi}{5}\right) = \frac{1}{2}(-1+\sqrt{5})$, $\zeta_{10} + \zeta_{10}^{-1} = 2\cos\left(\frac{\pi}{5}\right) = \frac{1}{2}(1+\sqrt{5})$ and $\zeta_{12} + \zeta_{12}^{-1} = 2\cos\left(\frac{\pi}{6}\right) = \sqrt{3}$. We thus choose the physical space V as the eigenspace for the eigenvalue $\zeta_m + \zeta_m^{-1}$ of $g + g^{-1}$ and get the orthogonal complement $V^{\perp}$ as the eigenspace for the other eigenvalue of $g + g^{-1}$. Note that the irrationality of the eigenvalues guarantees that the cut-and-project method yields a non-periodic pattern.

We now give two examples of 2-dimensional black-and-white point sets obtained from proper magnetic space groups by the cut-and-project method. Both examples are obtained from the same point group G, a group of order 16 in the hypercubic crystal system which contains a cyclic group of order 8 as a subgroup. As explained above we choose a 2-dimensional subspace invariant under an element of order 8 as physical space in order to obtain point patterns displaying 8-fold rotational symmetry.

The first example shows the effect of choosing different subgroups fixing the spin configuration in the lattice-equal case. The group G has three subgroups of index 2 from which we obtain three proper magnetic point groups. Applying the space groups with trivial vector system for these three magnetic point groups to a point in general position (*i.e.* with trivial stabilizer) gives the patterns displayed in Fig. 1. The points of the underlying translation lattice are indicated by little crosses.

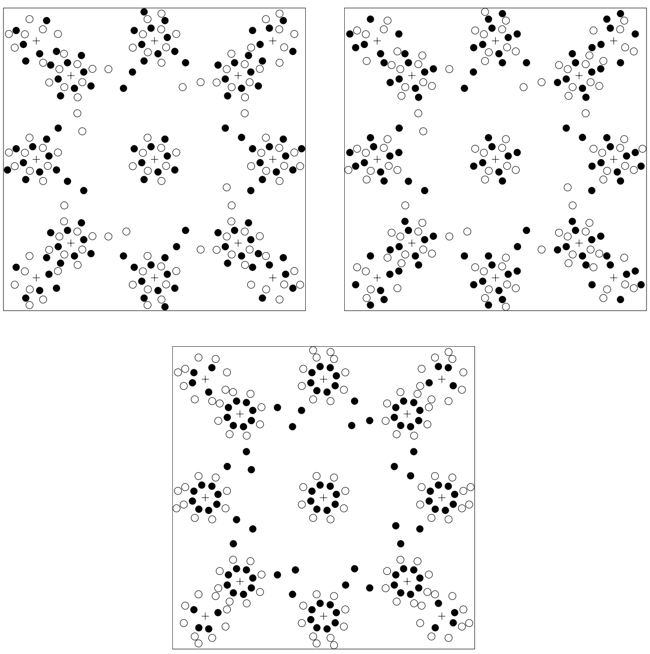

Fig. 1. Lattice-equal magnetic groups for different subgroups.

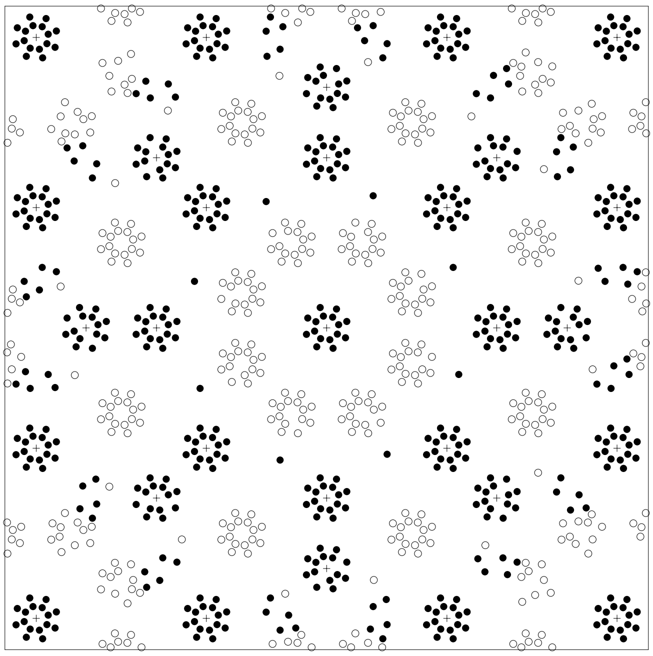

Fig. 2. Class-equal magnetic group.

In the second example we look at the class-equal case for the same point group G. Here we have to choose a non-trivial vector system, since the trivial vector system corresponds to a grey group. We again apply the group to a point in general position which yields the point pattern displayed in Fig. 2. Note how the black points surround the lattice points while the white points fill the gaps in between. In fact, if instead to a point in general position we applied the group to a point of the underlying lattice (*i.e.* a point of maximal symmetry) we would obtain the points of an octagonal black-and-white Bravais lattice as described in [9].

Acknowledgments. Valuable comments and suggestions by the referee are gratefully acknowledged.

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