| | |
|---|---|
| $g_J$ | Landé factor |
| $\boldsymbol{H}_{app}$ | applied magnetic field (vector) |
| $H_{app}$ | applied magnetic field (magnitude) |
| $H_m$ | molecular field |
| $J$ | exchange integral |
| $\boldsymbol{J}$ | total angular momentum |
| $\boldsymbol{k}_0$ | propagation vector |
| $l$ | orbital quantum number |
| $\boldsymbol{l}$ | orbital momentum |
| $L$ | orbital momentum |
| $\mathscr{L}$ | Langevin function |
| $m$ | magnetic quantum number |
| $m_0$ | measured magnetic moment at 0 K |
| $\boldsymbol{m}$ | magnetic moment |
| $\boldsymbol{m}_l$ | orbital moment |
| $\boldsymbol{m}_s$ | spin moment |
| $\boldsymbol{m}_z$ | projection of $m$ along $H_{app}$ |
| $M$ | magnetization |
| $M_s$ | spontaneous magnetization |
| $M_{s,0}$ | magnetization at absolute saturation |
| $n$ | molecular field coefficient |
| $N$ | number of moments per unit volume |
| $N_D$ | demagnetizing field coefficient |
| $N_T$ | total number of moments |
| $S$ | spin or spin angular momentum |
| $T$ | temperature |
| $T_c$ | critical temperature |
| $T_C$ | Curie temperature |
| $T_N$ | Néel temperature |
| $v_{at}$ | atom volume |
| $x$ | argument of the Langevin or Brillouin function |
| z | number of first neighbors |
| $\chi$ | magnetic susceptibility |
| $\mu_B$ | Bohr magneton |
| $\mu_{eff}$ | effective moment |
| $\mu_0$ | permittivity of vacuum |

# Magnetic Point Groups and Space Groups

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## Introduction

Magnetic groups – also known as antisymmetry groups, Shubnikov groups, Heesch groups, Opechowski–Guccione (OG) groups, as well as dichromatic, 2-color, or simply black-and-white groups – are the simplest extension to standard point group and space group theory. They allow directly to describe, classify, and study the consequences of the symmetry of crystals, characterized by having a certain property, associated with each crystal site, that can take one of two possible values. This is done by introducing a single external operation of order two that interchanges the two possible values everywhere throughout the crystal. This operation can be applied to the crystal along with any of the standard point group or space group operations, and is denoted by adding a prime to the original operation. Thus, any rotation $g$ followed by this external operation is denoted by $g'$.

To start with, a few typical examples of this two-valued property are given, some of which are illustrated in **Figure 1**. In the section "Magnetic point groups" the notion of a magnetic point group is discussed, followed by a discussion on magnetic space groups in the section "Magnetic space groups". The section "Extinctions in neutron diffraction of antiferromagnetic crystals" describes one of the most

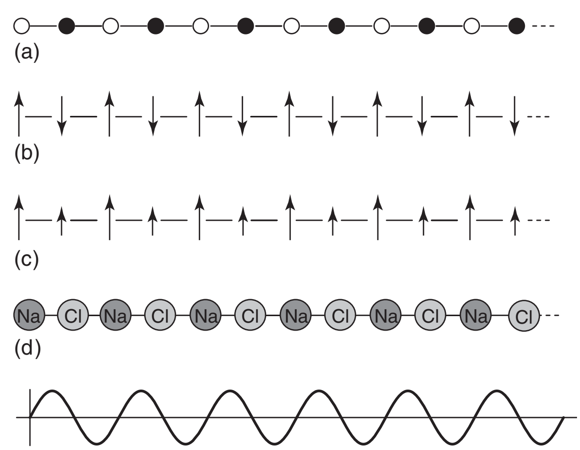



**Figure 1** Several realizations of the simple 1D magnetic space group $p_p\bar{1}$. Note that the number of symmetry translations is doubled if one introduces an operation $e'$ that interchanges the two possible values of the property, associated with each crystal site. Also note that spatial inversion $\bar{1}$ can be performed without a prime on each crystal site, and with a prime ($\bar{1}'$) between every two sites. (a) An abstract representation of the two possible values as the two colors – black and white. The operation $e'$ is the nontrivial permutation of the two colors. (b) A simple antiferromagnetic arrangement of spins. The operation $e'$ is time inversion which reverses the signs of the spins. (c) A ferromagnetic arrangement of two types of spins, where $e'$ exchanges them as in the case of two colors. (d) A 1D version of salt. $e'$ exchanges the chemical identities of the two atomic species. (e) A function $f(x)$ whose overall sign changes by application of the operation $e'$.

direct consequences of having magnetic symmetry in crystals which is the extinction of magnetic Bragg peaks in neutron diffraction patterns. A conclusion is given in the section "Generalizations of magnetic groups" by mentioning the generalization of magnetic groups to cases where the property associated with each crystal site is not limited to having only one of two possible values.

Consider first the structure of crystals of the cesium chloride type. In these crystals the atoms are located on the sites of a body-centered cubic (b.c.c.) lattice. Atoms of one type are located on the simple cubic lattice formed by the corners of the cubic cells, and atoms of the other type are located on the simple cubic lattice formed by the body centers of the cubic cells. The parent b.c.c. lattice is partitioned in this way into two identical sublattices, related by a body-diagonal translation. One may describe the symmetry of the cesium chloride structure as having a simple cubic lattice of ordinary translations, with a basis containing one cesium and one chlorine atom. Alternatively, one may describe the symmetry of the crystal as having twice as many translations, forming a b.c.c. lattice, half of which are primed to indicate that they are followed by the external operation that exchanges the chemical identities of the two types of atoms. A similar situation occurs in crystals whose structure is of the sodium chloride type, in which a simple cubic lattice is partitioned into two identical face-centered cubic (f.c.c.) sublattices.

Another typical example is the orientational ordering of magnetic moments (spins), electric dipole moments, or any other tensorial property associated with each site in a crystal. Adopting the language of spins, if these can take only one of two possible orientations – "up" and "down" – as in simple antiferromagnets, the same situation as above is seen, with the two spin orientations replacing the two chemical species of atoms. In the case of spins, the external prime operation is a so-called antisymmetry operation that reverses the signs of the spins. Physically, one may think of using the operation of time inversion to reverse the directions of all the spins without affecting anything else in the crystal.

Finally, consider a periodic or quasiperiodic scalar function of space $f(\mathbf{r})$, as in **Figure 1e**, whose average value is zero. It might be possible to extend the point group or the space group describing the symmetry of the function $f(\mathbf{r})$ by introducing an external prime operation that changes the sign of $f(\mathbf{r})$.

For the sake of clarity, the picture of up-and-down spins, and the use of time inversion to exchange them shall be adopted for the remaining of the discussion. It should be emphasized, though, that most of what is said here (except for the discussion of extinctions) applies equally to all the other two-valued properties. The magnetic crystal is described using a scalar spin density field $S(\mathbf{r})$ whose magnitude gives the magnitude of an atomic magnetic moment, or some coarse-grained value of the magnetic moment, at position $\mathbf{r}$. The sign of $S(\mathbf{r})$ gives the direction of the spin – a positive sign for up spins and a negative sign for down spins. Thus, the function $S(\mathbf{r})$ can be a discrete set of delta functions defined on the crystal sites as in **Figure 1b**, or a continuous spin density field as in **Figure 1e**.

## Magnetic Point Groups

A $d$-dimensional magnetic point group $G_M$ is a subgroup of $O(d) \times 1'$, where $O(d)$ is the group of $d$-dimensional rotations, and $1'$ is the time inversion group containing the identity $e$ and the time inversion operation $e'$. Note that the term "rotation" is used to refer to proper as well as improper rotations such as mirrors.

Three cases exist: (1) all rotations in $G_M$ appear with and without time inversion; (2) half of the rotations in $G_M$ are followed by time inversion and the other half are not; and (3) no rotation in $G_M$ is followed by time inversion. More formally, if $G$ is any subgroup of $O(d)$, it can be used to form at most three types of magnetic point groups, as follows:

1. $G_M = G \times 1'$. Thus, each rotation in $G$ appears in $G_M$ once by itself, and once followed by time inversion. Note that in this case $e' \in G_M$.
2. $G_M = H + g'H$, where $G = H + gH$, and $g \notin H$. Thus, exactly half of the rotations in $G$, which belong to its subgroup $H$, appear in $G_M$ by themselves, and the other half, belonging to the coset $gH$, are followed by time inversion. Note that in this case $e' \notin G_M$.
3. $G_M = G$. Thus, $G_M$ contains rotations, none of which are followed by time inversion.

Enumeration of magnetic point groups is thus straightforward. Any ordinary point group $G$ (i.e., any subgroup, usually finite, of $O(d)$) is trivially a magnetic point group of type 3, and along with the time inversion group gives another magnetic point group of type 1, denoted as $G1'$. One then lists all distinct subgroups $H$ of index 2 in $G$, if there are any, to construct additional magnetic point groups of type 2. These are denoted either by the group–subgroup pair $G(H)$, or by using the International (Hermann–Mauguin) symbol for $G$ and adding a prime to those elements in the symbol that do not belong to the subgroup $H$ (and are therefore followed by time inversion). The set of magnetic groups (here magnetic point groups $G_M$), formed in this way from a single ordinary group (here an ordinary point group $G$), is sometimes called the magnetic superfamily of the group $G$. For example, the orthorhombic point group $G = mm2 = \{e, m_x, m_y, 2_z\}$ has three subgroups of index 2 ($H_1 = \{e, m_x\}$, $H_2 = \{e, m_y\}$, and $H_3 = \{e, 2_z\}$), of which the first two are equivalent through a relabeling of the $x$ and $y$ axes. This yields a total of four magnetic point groups: $mm2$, $mm21'$, $m'm2'$ (equivalently expressed as $mm'2'$), and $m'm'2$.

Magnetic point groups of type 3 are equivalent to ordinary nonmagnetic point groups and are listed here only for the sake of completeness. Strictly speaking, they can be said to describe the symmetry of ferromagnetic structures with no spin–orbit coupling. Groups of this type are not considered here any further. Magnetic point groups of type 2 can be used to describe the point symmetry of finite objects, as described in the next section, as well as that of infinite crystals, as described in the section "Magnetic point groups of crystals." Magnetic point groups of type 1 can be used to describe the point symmetry of infinite crystals, but because they include $e'$ as a symmetry element they cannot be used to describe the symmetry of finite objects, as is now defined.

### Magnetic Point Groups of Finite Objects

The magnetic symmetry of a finite object, such as a molecule or a cluster containing an equal number of two types of spins, can be described by a magnetic point group. One can say that a primed or unprimed rotation from $O(d) \times 1'$ is in the magnetic point group $G_M$ of a finite object in $d$ dimensions, if it leaves the object invariant. Clearly, only magnetic point groups of type 2, listed above, can describe the symmetry of finite magnetically ordered structures. This is because time inversion $e'$ changes the orientations of all the spins, and therefore cannot leave the object invariant unless it is accompanied by a nontrivial rotation. It should be mentioned that in this context, point groups of type 1 are sometimes called "gray" groups, as they describe the symmetry of "gray" objects which stay invariant under the exchange of black and white.

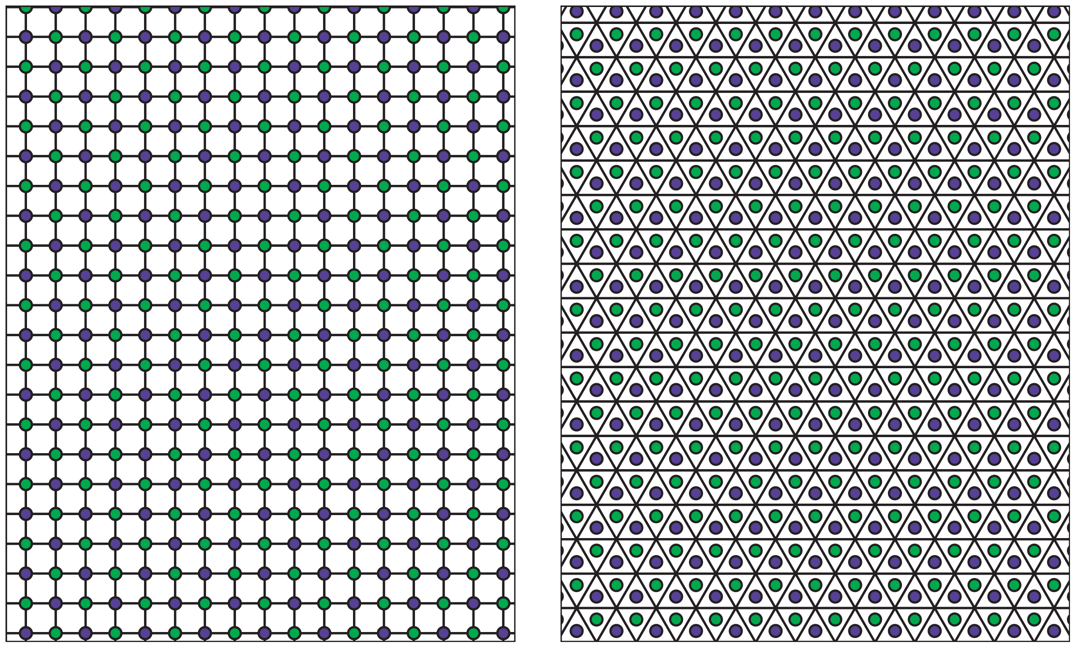
### Magnetic Point Groups of Crystals

The magnetic point group of a $d$-dimensional magnetically ordered "periodic crystal", containing an equal number of up and down spins, is defined as the set of primed or unprimed rotations from $O(d) \times 1'$ that leave the crystal "invariant to within a translation". The magnetic point group of a crystal can be either of the first or of the second type listed above. It is of type 1 if time inversion by itself leaves the crystal invariant to within a translation. Recall that in this case, any rotation in the magnetic point group can be performed either with or without time inversion. If time inversion cannot be combined with a translation to leave the crystal invariant, the magnetic point group is of type 2, in which case half the rotations are performed without time inversion and the other half with time inversion.

**Figure 2a** shows an example of a magnetically ordered crystal whose magnetic point group is of type 1. This is a square crystal with magnetic point group $G_M = 4mm1'$ where time inversion can be followed by a translation to leave the crystal invariant. **Figure 2b** shows an example of a crystal whose magnetic point group is of type 2. This is a hexagonal crystal with point group $G_M = 6'mm'$. Note that all right-side-up triangles contain a blue circle (spin up), and all up-side-down triangles contain a green circle (spin down). Time inversion, exchanging the two types of spins, cannot be combined with a translation to recover the original crystal. Time inversion must be combined with an operation, such as the sixfold rotation or the horizontal mirror that interchanges the two types of triangles, to recover the original crystal. Note that the vertical mirror (the first $m$ in the International symbol) leaves the crystal invariant without requiring time inversion, and is therefore unprimed in the symbol.

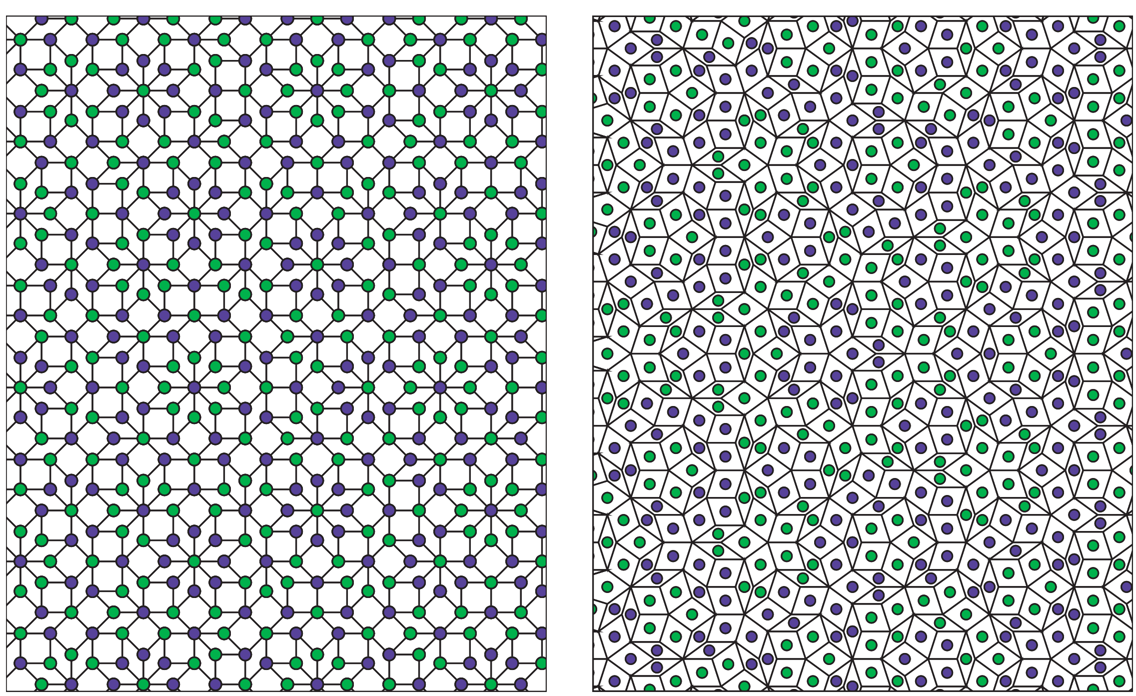
More generally, the magnetic point group of a $d$-dimensional magnetically ordered "quasiperiodic crystal (quasicrystal)," is defined as the set of primed or unprimed rotations from $O(d) \times 1'$ that leave the crystal "indistinguishable." This means that the rotated and unrotated crystals contain the same spatial distributions of finite clusters of spins of arbitrary size. The two are statistically the same though not necessarily identical. For the special case of periodic crystals, the requirement of indistinguishability reduces to the requirement of invariance to within a translation.

**Figure 3** shows two quasiperiodic examples, analogous to the two periodic examples of **Figure 2**. **Figure 3a** shows an octagonal crystal with magnetic point group $G_M = 8mm1'$. One can see that time inversion rearranges the spin clusters in the crystal, but they all still appear in the crystal with the same spatial distribution. This is because any finite spin cluster and its time-reversed image appear in the crystal with the same spatial distribution. **Figure 3b** shows a decagonal crystal with magnetic point group $G_M = 10'm'm$. In this case, time inversion does not leave the crystal indistinguishable. It must be combined either with odd powers of the tenfold rotation, or with mirrors of the vertical type.



(a) (b)

**Figure 2** Periodic antiferromagnets. (a) A square crystal with magnetic point group $G_{\mathrm{M}} = 4mm1'$ and magnetic space group $p_p4mm$ (also denoted $p_c4mm$), (b) A hexagonal crystal with magnetic point group $G_{\mathrm{M}} = 6'mm'$ and magnetic space group $p6'mm'$.



(a) (b)

**Figure 3** Quasiperiodic antiferromagnets. (a) An octagonal quasicrystal with magnetic point group $G_{\mathrm{M}} = 8mm1'$ and magnetic space group $p_p8mm$, first appeared in an article by Niizeki (1990) *Journal of Physics A: Mathematical and General* 23: 5011. (b) A decagonal quasicrystal with magnetic point group $G_{\mathrm{M}} = 10'm'm$ and magnetic space group $p10'm'm$ based on the tiling of Li, Dubois, and Kuo (1994) *Philosophical Magazine Letters* 69: 93.

## Magnetic Space Groups

The full symmetry of a magnetically ordered crystal, described by a scalar spin density field $S(\boldsymbol{r})$, is given by its magnetic space group $\mathcal{G}_{\mathrm{M}}$. It was mentioned earlier that the magnetic point group $G_{\mathrm{M}}$ is the set of primed or unprimed rotations that leave a periodic crystal invariant to within a translation, or more generally, leave a quasiperiodic crystal indistinguishable. One still needs to specify the distinct sets of translations $\boldsymbol{t}_g$ or $\boldsymbol{t}_{g'}$ that can accompany the rotations $g$ or $g'$ in a periodic crystal to leave it invariant, or provide the more general characterization of the nature of the indistinguishability in the case of quasicrystals.

### Periodic Crystals

As in the case of point groups, one can take any space group $\mathcal{G}$ of a periodic crystal and form its magnetic superfamily, consisting of one trivial group $\mathcal{G}_{\mathrm{M}} = \mathcal{G}$, one gray group $\mathcal{G}_{\mathrm{M}} = \mathcal{G}1'$, and possibly nontrivial magnetic groups of the form $\mathcal{G}_{\mathrm{M}} = \mathcal{H} + (g'|\boldsymbol{t}_{g'})\mathcal{H}$, where $\mathcal{H}$ is a subgroup of index 2 of $\mathcal{G}$. Only the latter, nontrivial groups are relevant as magnetic space groups consisting of operations that leave the magnetically ordered crystal "invariant." These nontrivial magnetic space groups are divided into two types depending on their magnetic point groups $G_{\mathrm{M}}$:

1. *Class-equivalent magnetic space groups*. The magnetic point group $G_{\mathrm{M}}$ is of type 1, and therefore all rotations in $G$ appear with and without time inversion. In this case the point groups of $\mathcal{G}$ and $\mathcal{H}$ are the same, but the Bravais lattice of $\mathcal{H}$ contains exactly half of the translations that are in the Bravais lattice of $\mathcal{G}$.
2. *Translation-equivalent magnetic space groups*. The magnetic point group $G_{\mathrm{M}}$ is of type 2. Here the Bravais lattices of $\mathcal{G}$ and $\mathcal{H}$ are the same, but the point group $H$ of $\mathcal{H}$ is a subgroup of index 2 of the point group $G$ of $\mathcal{G}$.

Enumeration of translation-equivalent magnetic space group types is very simple. Given a space group $\mathcal{G}$, all that one needs to do is to consider all subgroups $H$ of index 2 of the point group $G$ of $\mathcal{G}$, as explained earlier. The only additional consideration is that with an underlying Bravais lattice, there may be more than one way to orient the subgroup $H$ relative to the lattice. For example, consider the magnetic point group $m'm2'$ which, as noted earlier, is equivalent to $mm'2'$. If the lattice is an $A$-centered orthorhombic lattice, then the $x$- and $y$-axes are no longer equivalent, and one needs to consider both options as distinct groups. It can be said that $Am'm2'$ and $Amm'2'$ belong to the same "magnetic geometric crystal class" (i.e., have the same magnetic point group), but to two distinct "magnetic arithmetic crystal classes." Translation-equivalent magnetic space groups are denoted by taking the International symbol for $\mathcal{G}$, and adding a prime to those elements in the symbol that do not belong to $\mathcal{H}$ and are therefore followed by time inversion.

Enumeration of class-equivalent magnetic space group types can proceed in two alternative ways. Given a space group $\mathcal{G}$, one may consider all distinct sublattices of index 2 of the Bravais lattice of $\mathcal{G}$. Alternatively, given a space group $\mathcal{H}$, one may consider all distinct superlattices of index 2 of the Bravais lattice of $\mathcal{H}$. It is also to be noted that if one prefers to look at the reciprocal lattices in Fourier space, instead of the lattices of real-space translations, the roles of superlattice and sublattice are exchanged. Although the lattice of $\mathcal{G}$ contains twice as many points as the lattice of $\mathcal{H}$, the reciprocal lattice of $\mathcal{G}$ contains exactly half of the points of the reciprocal lattice of $\mathcal{H}$.

Because of the different enumeration methods, there are conflicting notations in the literature for class-equivalent magnetic space groups. The OG notation follows the first approach (sublattices of $\mathcal{G}$), taking the International symbol for the space group $\mathcal{G}$ with a subscript on the Bravais class symbol denoting the Bravais lattice of $\mathcal{H}$. The Belov notation follows the second approach (superlattices of $\mathcal{H}$), taking the International symbol for the space group $\mathcal{H}$ with a subscript on the Bravais class symbol denoting one or more of the primed translations $\boldsymbol{t}_{e'}$ in the coset $(e'|\boldsymbol{t}_{e'})\mathcal{H}$. The Lifshitz notation, which follows a third approach (sublattices of $\mathcal{H}$ in Fourier space), resembles that of Belov but generalizes more easily to quasiperiodic crystals.

There is an additional discrepancy in the different notations which has been the cause of some confusion over the years. It is due to the fact that when $e' \in G_{\mathrm{M}}$, ordinary mirrors or rotations when unprimed may become glide planes or screw axes when primed, and vice versa. The only consistent way to avoid this confusion is to use only unprimed elements for the symbols of class-equivalent magnetic space group types. This is the approach adopted by both the Belov and the Lifshitz notations, but unfortunately not by the OG notation, having introduced errors into their list of magnetic space group types. In any case, there is no need to leave the $1'$ at the end of the symbol, as it is clear from the existence of a subscript on the lattice symbol that the magnetic point group $G_{\mathrm{M}}$ contains $e'$.

Consider, for example, all the class-equivalent magnetic space group types with point group 432. In the cubic system there are two lattice–sublattice pairs: (1) The simple cubic lattice $P$ has a face-centered sublattice $F$ of index 2, and (2) The b.c.c. lattice $I$ has a simple cubic sublattice $P$ of index 2. Recall that the reciprocal of $F$ is a b.c.c. lattice in Fourier space, denoted by $I^*$, and the reciprocal of $I$ is an f.c.c. lattice, denoted by $F^*$. In the Belov notation one has $F_s432$, $F_s4_j32$, $P_I432$, and $P_I4_j32$ with $j = 1, 2, 3$. The subscript $s$ is for "simple". In the Lifshitz notation, using Fourier space lattices, these groups become $I^*_P432$, $I^*_P4_j32$, $P_{F^*}432$, and $P_{F^*}4_j32$. In the OG notation these groups should become $P_F432$, $P_F4_j32$, $I_P432$, and $I_P4_j32$. Instead, they list $P_F432$, $P_F4_232$, $I_P432$, $I_P4_132$, $I_P4'32'$, and $I_P4'_132'$, using primes inconsistently and clearly missing two groups. It is therefore recommended that one refrains from using primes when denoting class-equivalent magnetic space groups.

The reader is referred to the "Further reading" section for complete lists of magnetic space group types. However, some statistics are summarized. Starting from the 17 space group types in two dimensions, also known as the 17 plane groups, one can form a total of 80 magnetic space group types as follows: 17 trivial groups, 17 gray groups, and 46 nontrivial groups of which 18 are class-equivalent and 28 are translation equivalent. Starting from the 230 space group types in three dimensions, one can form a total of 1651 magnetic space group types as follows: 230 trivial groups, 230 gray groups, and 1191 nontrivial groups of which 517 are class-equivalent and 674 are translation equivalent. These numbers have no particular significance other than the fact that they are surprisingly large.

### Quasiperiodic Crystals

**Lattices and Bravais classes** Magnetically-ordered quasiperiodic crystals, in general, possess no lattices of real space translations that leave them invariant, but they do have reciprocal lattices (or Fourier modules) $L$ that can be inferred directly from their neutron diffraction diagrams. To be a bit more specific, consider spin density fields with well-defined Fourier transforms

$$S(\boldsymbol{r}) = \sum_{\boldsymbol{k}\in L} S(\boldsymbol{k}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \qquad [1]$$

in which the set $L$ contains, at most, a countable infinity of plane waves. In fact, the "reciprocal lattice" $L$ of a magnetic crystal can be defined as the set of all integral linear combinations of wave vectors $\boldsymbol{k}$ determined from its neutron diffraction diagram, as one expects to see a magnetic Bragg peak at every linear combination of observed peaks, unless it is forbidden by symmetry, as explained in the next section. The "rank" $D$ of $L$ is the smallest number of vectors needed to generate $L$ by integral linear combinations. If $D$ is finite the crystal is quasiperiodic. If, in particular, $D$ is equal to the number $d$ of spatial dimensions, and $L$ extends in all $d$ directions, the crystal is periodic. In this special case, the magnetic lattice $L$ is reciprocal to a lattice of translations in real space that leave the magnetic crystal invariant. The reciprocal lattices $L$ of magnetic crystals are classified into Bravais classes, just like those of ordinary nonmagnetic crystals.

**Phase functions and space group types** The precise mathematical statement of indistinguishability, used earlier to define the magnetic point group, is the requirement that any symmetry operation of the magnetic crystal leaves invariant all spatially averaged $n$th-order autocorrelation functions of its spin-density field,

$$C^{(n)}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_n) = \lim_{V\to\infty} \frac{1}{V} \int_V d\boldsymbol{r} S(\boldsymbol{r}_1 - \boldsymbol{r}) \cdots S(\boldsymbol{r}_n - \boldsymbol{r}) \qquad [2]$$

One can prove that two quasiperiodic spin density fields $S(\boldsymbol{r})$ and $\hat{S}(\boldsymbol{r})$ are indistinguishable in this way, if their Fourier coefficients, defined in eqn [1], are related by

$$\hat{S}(\boldsymbol{k}) = e^{2\pi i\chi(\mathbf{k})} S(\boldsymbol{k}) \qquad [3]$$

where $\chi$ is a real-valued linear function (modulo integers) on $L$, called a "gauge function". By this it is meant that for every pair of wave vectors $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ in the magnetic lattice $L$,

$$\chi(\boldsymbol{k}_1 + \boldsymbol{k}_2) \equiv \chi(\boldsymbol{k}_1) + \chi(\boldsymbol{k}_2) \qquad [4]$$

where "$\equiv$" means equal to within adding an integer. Thus, for each element $g$ or $g'$ in the magnetic point group $G_M$ of the crystal, that by definition leaves the crystal indistinguishable, there exists such a gauge function $\Phi_g(\boldsymbol{k})$ or $\Phi_{g'}(\boldsymbol{k})$, called a "phase function", satisfying

$$S(g\boldsymbol{k}) = \begin{cases} e^{2\pi i\Phi_g(\boldsymbol{k})} S(\boldsymbol{k}), & g \in G_M \\ -e^{2\pi i\Phi_{g'}(\boldsymbol{k})} S(\boldsymbol{k}), & g' \in G_M \end{cases} \qquad [5]$$

Since for any $g, h \in G$, $S([gh]\boldsymbol{k}) = S(g[h\boldsymbol{k}])$, the corresponding phase functions for elements in $G_M$, whether primed or not, must satisfy the "group compatibility condition",

$$\Phi_{g*h\dagger}(\boldsymbol{k}) \equiv \Phi_{g*}(h\boldsymbol{k}) + \Phi_{h\dagger}(\boldsymbol{k}) \qquad [6]$$

where the asterisk and the dagger denote optional primes. A "magnetic space group," describing the symmetry of a magnetic crystal, whether periodic or aperiodic, is thus given by a lattice $L$, a magnetic point group $G_M$, and a set of phase functions $\Phi_g(\boldsymbol{k})$

and $\Phi_{g'}(\boldsymbol{k})$, satisfying the group compatibility condition [6].

Magnetic space groups are classified in this formalism into magnetic space group types by organizing sets of phase functions satisfying the group compatibility condition [6] into equivalence classes. Two such sets, $\Phi$ and $\hat{\Phi}$, are equivalent if: (1) they describe indistinguishable spin density fields related as in [3] by a gauge function $\chi$; or (2) they correspond to alternative descriptions of the same crystal that differ by their choices of absolute length scales and spatial orientations. In case (1), $\Phi$ and $\hat{\Phi}$ are related by a "gauge transformation,"

$$\hat{\Phi}_{g*}(\boldsymbol{k}) \equiv \Phi_{g*}(\boldsymbol{k}) + \chi(g\boldsymbol{k} - \boldsymbol{k}) \qquad [7]$$

where, again, the asterisk denotes an optional prime.

In the special case that the crystal is periodic ($D = d$), it is possible to replace each gauge function by a corresponding $d$-dimensional translation $\boldsymbol{t}$, satisfying $2\pi\chi(\boldsymbol{k}) = \boldsymbol{k} \cdot \boldsymbol{t}$, thereby reducing the requirement of indistinguishability to that of invariance to within a translation. Only then does the point group condition [5] become

$$S(g\boldsymbol{r}) = \begin{cases} S(\boldsymbol{r} - \boldsymbol{t}_g), & g \in G_M \\ -S(\boldsymbol{r} - \boldsymbol{t}_{g'}), & g' \in G_M \end{cases} \qquad [8]$$

the gauge transformation [7] becomes a mere shift of the origin, and the whole description reduces to that given in the section "Periodic crystals." The reader is referred to references in the "Further reading" section for details regarding the enumeration of magnetic space groups of quasiperiodic crystals and for complete lists of such groups.

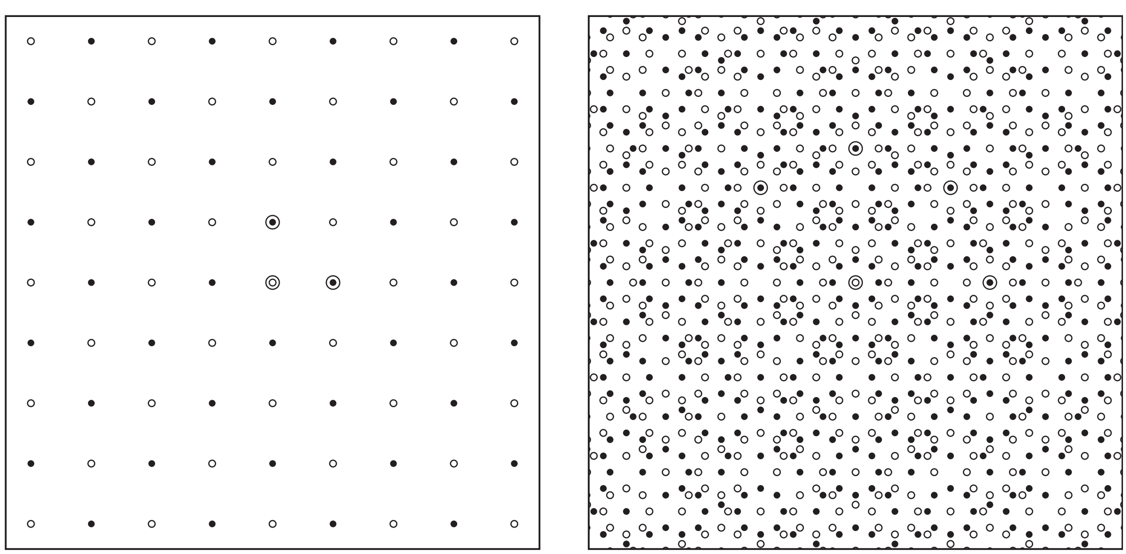
## Extinctions in Neutron Diffraction of Anti-Ferromagnetic Crystals

It was said earlier that every wave vector $\boldsymbol{k}$ in the lattice $L$ of a magnetic crystal is a candidate for a diffraction peak unless symmetry forbids it. One can now understand exactly how this happens. Given a wave vector $\boldsymbol{k} \in L$, all magnetic point-group operations $g$ or $g'$ for which $g\boldsymbol{k} = \boldsymbol{k}$ are examined. For such elements, the point-group condition [5] can be rewritten as

$$S(\boldsymbol{k}) = \begin{cases} e^{2\pi i \Phi_g(\boldsymbol{k})} S(\boldsymbol{k}), & g \in G_M \\ -e^{2\pi i \Phi_{g'}(\boldsymbol{k})} S(\boldsymbol{k}), & g' \in G_M \end{cases} \qquad [9]$$

requiring $S(\boldsymbol{k})$ to vanish unless $\Phi_g(\boldsymbol{k}) \equiv 0$, or $\Phi_{g'}(\boldsymbol{k}) \equiv 1/2$, or unless both conditions are satisfied when both $g$ and $g'$ are in $G_M$. It should be noted that the phase values in eqn [9], determining the extinction of $S(\boldsymbol{k})$, are independent of the choice of gauge [7], and are therefore uniquely determined by the magnetic space-group type of the crystal.

Particularly striking are the extinctions when the magnetic point group is of type 1, containing time inversion $e'$. The relation $(e')^2 = e$ implies – through



(a) (b)

**Figure 4** Extinctions of magnetic Bragg peaks in crystals with magnetic point groups of type 1, containing time inversion $e'$. Both figures show the positions of expected magnetic Bragg peaks indexed by integers ranging from –4 to 4. Filled circles indicate observed peaks and open circles indicate positions of extinct peaks. The origin and the $D$ vectors used to generate the patterns are indicated by an additional large circle. (a) corresponds to the square crystal in **Figure 2a** with magnetic space group $p_p4mm$, and (b) corresponds to the octagonal crystal in **Figure 3a** with magnetic space group $p_p8mm$.

the group compatibility condition [6] and the fact that $\Phi_e(\boldsymbol{k}) \equiv 0$ – that $\Phi_{e'}(\boldsymbol{k}) \equiv 0$ or 1/2. It then follows from the linearity of the phase function that on exactly half of the wave vectors in $L$ $\Phi_{e'}(\boldsymbol{k}) \equiv 1/2$, and on the remaining half, which form a sublattice $L_0$ of index 2 in $L$, $\Phi_{e'}(\boldsymbol{k}) \equiv 0$. Thus, in magnetic crystals with magnetic point groups of type 1 at least half of the diffraction peaks are missing. **Figure 4** shows the positions of the expected magnetic Bragg peaks corresponding to the square and octagonal magnetic structures shown in **Figures 2a** and **3a**, illustrating this phenomenon.

## Generalizations of Magnetic Groups

There are two natural generalizations of magnetic groups. One is to color groups with more than two colors, and the other is to spin groups where the spins are viewed as classical axial vectors free to rotate continuously in any direction.

An $n$-color point group $G_C$ is a subgroup of $O(d) \times S_n$, where $S_n$ is the permutation group of $n$ colors. Elements of the color point group are pairs $(g, \gamma)$ where $g$ is a $d$-dimensional (proper or improper) rotation and $\gamma$ is a permutation of the $n$ colors. As before, for $(g, \gamma)$ to be in the color point group of a finite object it must leave it invariant, and for $(g, \gamma)$ to be in the color point group of a crystal it must leave it indistinguishable, which in the special case of a periodic crystal reduces to invariance to within a translation. To each element $(g, \gamma) \in G_C$ corresponds a phase function $\Phi_g^\gamma(\boldsymbol{k})$, satisfying a generalized version of the group compatibility condition [6]. The color point group contains an important subgroup of elements of the form $(e, \gamma)$ containing all the color permutations that leave the crystal indistinguishable without requiring any rotation $g$.

A spin point group $G_S$ is a subgroup of $O(d) \times SO(d_s) \times 1'$, where $SO(d_s)$ is the group of $d_s$-dimensional proper rotations operating on the spins, and $1'$ is the time inversion group as before. Note that the dimension of the spins need not be equal to the dimension of space (e.g., one may consider a planar arrangement of 3D spins). Also note that because the spins are axial vectors there is no loss of generality by restricting their rotations to being proper. Elements of the spin point group are pairs $(g, \gamma)$, where $g$ is a $d$-dimensional (proper or improper) rotation and $\gamma$ is a spin-space rotation possibly followed by time inversion. Here as well, elements of the form $(e, \gamma)$ play a central role in the theory, especially in determining the symmetry constraints imposed by the corresponding phase functions $\Phi_e^\gamma(\boldsymbol{k})$ on the patterns of magnetic Bragg peaks, observed in elastic neutron diffraction experiments.

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*See also:* Crystal Symmetry; Disordered Magnetic Systems; Magnetic Materials and Applications; Magnetoelasticity; Paramagnetism; Periodicity and Lattices; Point Groups; Quasicrystals; Space Groups.

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