Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Received 12 June 2003
Accepted 5 January 2004

Magnetically ordered quasicrystals: enumeration of spin groups and calculation of magnetic selection rules

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Details are given of the theory of magnetic symmetry in quasicrystals, which has previously only been outlined. A practical formalism is developed for the enumeration of spin point groups and spin space groups, and for the calculation of selection rules for neutron scattering experiments. The formalism is demonstrated using the simple, yet non-trivial, example of magnetically ordered octagonal quasicrystals in two dimensions. In a companion paper [Even-Dar Mandel & Lifshitz (2004). *Acta Cryst.* A**60**, 179–194], complete results are provided for octagonal quasicrystals in three dimensions.

1. Introduction

The discovery of Zn–Mg–RE icosahedral quasicrystals, where RE stands for one of the rare-earth metals Y, Gd, Tb, Dy, Ho and Er (Niikura *et al.*, 1994; Tsai *et al.*, 1994), and initial indications that some of these quasicrystals may possess long-range antiferromagnetic order (Charrier *et al.*, 1997, 1998), have generated increased interest in the nature of magnetic order in quasicrystals (Fukamichi, 1999, and references therein). Subsequent measurements (Islam *et al.*, 1998; Sato *et al.*, 1998), followed by ongoing vigorous research (Fisher *et al.*, 1999; Sato *et al.*, 1999; Fisher *et al.*, 2000; Sato, Takakura, Tsai, Ohoyama *et al.*, 2000; Sato, Takakura, Tsai, Shibata *et al.*, 2000; Dolinšek *et al.*, 2001; Kramer *et al.*, 2002), have shown that only short-range spin correlations exist in these particular quasicrystals, and therefore the existence of long-range magnetic order in real quasicrystals remains an unresolved question of great interest. The recent discovery of cadmium-based quasicrystals (Guo *et al.*, 2000*a*,*b*; Tsai *et al.*, 2000) and initial studies of magnetic order in the Cd–Mg–Tb icosahedral quasicrystal (Sato *et al.*, 2002) may provide some insight into this question. Theoretical models that deal with magnetism on quasicrystals—purely geometrical models (Niizeki, 1990*a*,*b*; Lifshitz, 1995, 2000) as well as physical ones, such as the Ising model (Grimm & Baake, 1997; Matsuo *et al.*, 2000, 2002), the XY model (Hermisson, 2000), the Heisenberg model (Wessel *et al.*, 2003) and the Hubbard model (Jagannathan & Schulz, 1997; Hida, 2001)—are known to exhibit long-range magnetic order. This is despite initial intuition that aperiodicity necessarily induces geometrical frustration and is therefore inconsistent with having magnetic order.

It is therefore clear—from both a theoretical and an experimental standpoint—that there is a need for a theoretical classification of all types of quasiperiodic long-range magnetic order that are allowed by symmetry. Such a symmetry-based classification of quasiperiodic magnetic structures, combined with a calculation of the selection rules, imposed by magnetic symmetry, will be of great assistance in the study of real magnetic quasicrystals, if and when they are discovered. It will also offer valuable guidance in the search for these novel materials (Lifshitz, 2000). In this paper, we provide the details of the extension to quasicrystals (Lifshitz, 1998) of Litvin & Opechowski's theory of spin groups (Litvin, 1973; Litvin & Opechowski, 1974; Litvin, 1977). In §2, we explain how spin groups are used to describe the magnetic symmetry of periodic as well as quasiperiodic crystals. In §3, we give the group theoretic details of the classification of the different groups into appropriate equivalence classes. In §4, we develop the formalism required for the actual enumeration of spin groups and, in §5, we derive the relations between the magnetic symmetry of a crystal and the selection rules it imposes on neutron diffraction experiments. In §6, we treat the case of octagonal symmetry in two dimensions as a pedagogical example. In a companion paper (Even-Dar Mandel & Lifshitz, 2004), we perform the actual detailed enumeration of three-dimensional octagonal spin groups, which turns out to be surprisingly rich. Complete enumeration for the other common quasicrystals without explicit details will follow in future publications.

2. Using spin groups to describe the symmetry of magnetically ordered crystals

A d-dimensional magnetically ordered crystal, whether periodic or aperiodic, is most directly described by its spin density field $\mathbf{S}(\mathbf{r})$. This field is a three-component real-valued function, transforming like an axial vector under $O(3)$ and changing sign under time inversion. One may think of this function as defining a set of classical magnetic moments, or spins, on the atomic sites of the material.[1] For quasiperiodic crystals, the spin density field may be expressed as a Fourier sum with a countable infinity of wavevectors,

$$\mathbf{S}(\mathbf{r}) = \sum_{\mathbf{k}\in L} \mathbf{S}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{1}$$

The set L of all integral linear combinations of the wavevectors in (1) is called the *magnetic lattice*, and is characterized among other things by a rank D and by a lattice point group G_L: its *rank D* is the smallest number of wavevectors needed to generate it by integral linear combinations. For quasiperiodic crystals, by definition, the rank is finite. For the special case of periodic crystals, the rank is equal to the dimension d of physical space. The set of (proper or improper) rotations, which when applied to the origin of Fourier space leave the magnetic lattice invariant, is the *lattice point group* G_L, also called the *holohedry*.

The theory of magnetic symmetry in quasiperiodic crystals (Lifshitz, 1998) is a reformulation of Litvin & Opechowski's theory of spin space groups (Litvin, 1973; Litvin & Opechowski, 1974; Litvin, 1977). Their theory, which is applicable to periodic crystals, is extended to quasiperiodic crystals by following the ideas of Rokhsar, Wright & Mermin's 'Fourier-space approach' to crystallography (Rokhsar *et al.*, 1988*a*,*b*).[2] At the heart of this approach is a redefinition of the concept of point-group symmetry, which enables one to treat quasicrystals directly in physical space, as opposed to the alternative 'superspace approach' (Janssen *et al.*, 1992). The key to this redefinition is the observation that point-group rotations (proper or improper), when applied to a quasiperiodic crystal, do not leave the crystal invariant but rather take it into one that contains the same spatial distributions of bounded structures of arbitrary size.

This generalized notion of symmetry, termed *indistinguishability*, is captured by requiring that any symmetry operation of the magnetic crystal leaves invariant all spatially averaged autocorrelation functions of its spin density field $\mathbf{S}(\mathbf{r})$, for any order n and for any choice of components $\alpha_i \in \{x, y, z\}$,

$$C^{(n)}_{\alpha_1\ldots\alpha_n}(\mathbf{r}_1, \ldots, \mathbf{r}_n) = \lim_{V\to\infty} \frac{1}{V} \int_V \mathrm{d}\mathbf{r}\, S_{\alpha_1}(\mathbf{r}_1 - \mathbf{r}) \ldots S_{\alpha_n}(\mathbf{r}_n - \mathbf{r}). \tag{2}$$

It has been shown (Lifshitz, 1997, in the Appendix) that an equivalent statement for the indistinguishability of any two quasiperiodic spin density fields, $\mathbf{S}(\mathbf{r})$ and $\mathbf{S}'(\mathbf{r})$, is that their Fourier coefficients are related by

$$\mathbf{S}'(\mathbf{k}) = e^{2\pi i \chi(\mathbf{k})} \mathbf{S}(\mathbf{k}), \tag{3}$$

where χ, called a *gauge function*, is a real-valued scalar function that is linear (modulo integers) on the magnetic lattice L. This simply means that

$$\forall\, \mathbf{k}_1, \mathbf{k}_2 \in L: \quad \chi(\mathbf{k}_1 + \mathbf{k}_2) \equiv \chi(\mathbf{k}_1) + \chi(\mathbf{k}_2), \tag{4}$$

where $\equiv$ denotes equality modulo integers.

With this in mind, we define the *point group G* of a d-dimensional magnetic crystal to be the set of operations g in $O(d)$ that leave it indistinguishable to within rotations γ in spin space, possibly combined with time inversion.[3] Accordingly, for every pair (g, γ), there exists a gauge function, $\Phi^\gamma_g(\mathbf{k})$, called a *phase function*, which satisfies

$$\mathbf{S}(g\mathbf{k}) = e^{2\pi i \Phi^\gamma_g(\mathbf{k})} \gamma \mathbf{S}(\mathbf{k}). \tag{5}$$

In general, as we shall see later, there may be many spin-space operations γ that, when combined with a given physical-space rotation g, satisfy the point-group condition (5). We denote physical-space rotations by Latin letters and spin-space operations by Greek letters. We use a primed Greek letter to explicitly denote the fact that a spin-space rotation is followed by time inversion. Thus, the identity rotation in physical space is e, the identity rotation in spin space is ε, and time inversion is ε'. Also note that we use the same symbol γ to denote an abstract spin-space operation and to denote the 3×3 matrix, operating on the field $\mathbf{S}$, representing this operation.

If (g, γ) and (h, η) both satisfy the point-group condition (5), then it follows from the equality

$$\mathbf{S}([gh]\mathbf{k}) = \mathbf{S}(g[h\mathbf{k}]) \tag{6}$$

that so does $(gh, \gamma\eta)$. This establishes that the set Γ of all transformations γ forms a group, and the set G_S of all pairs (g, γ), satisfying the point-group condition (5), also forms a group. The latter is a subgroup of $G \times \Gamma$, called the *spin point group*. We shall consider here only finite groups G and Γ, although in general this need not be the case. The equality (6) further implies that the corresponding phase functions, one for each pair in G_S, must satisfy the *group compatibility condition*,

$$\forall\, (g, \gamma), (h, \eta) \in G_S: \quad \Phi^{\gamma\eta}_{gh}(\mathbf{k}) \equiv \Phi^\gamma_g(h\mathbf{k}) + \Phi^\eta_h(\mathbf{k}). \tag{7}$$

Note that successive application of the group compatibility condition (7) reveals a relatively simple relation between the phase functions of two conjugate elements (g, γ) and $(hgh^{-1}, \eta\gamma\eta^{-1})$ of G_S,

$$\forall\, (g, \gamma), (h, \eta) \in G_S: \quad \Phi^{\eta\gamma\eta^{-1}}_{hgh^{-1}}(h\mathbf{k}) \equiv \Phi^\gamma_g(\mathbf{k}) + \Phi^\eta_h(g\mathbf{k} - \mathbf{k}). \tag{8}$$

A *spin space group*, describing the symmetry of a magnetic crystal, whether periodic or aperiodic, is thus given by a magnetic lattice L, a spin point group G_S and a set of phase functions $\Phi^\gamma_g(\mathbf{k})$, satisfying the group compatibility condition (7). We continue to call this a spin space group even though its physical-space part is no longer a subgroup of the Euclidean group $E(d)$. Nevertheless, the spin space group may be given an algebraic structure of a group of ordered triplets $(g, \gamma, \Phi^\gamma_g)$

[1] We usually consider three-dimensional magnetic moments, or spins, in a d-dimensional crystal, where $d = 2$ or 3, and therefore take $\mathbf{S}(\mathbf{r})$ to be a three-component field. If necessary, one can generalize to spins of arbitrary dimension.

[2] For a review, see Mermin (1992*b*) or Mermin (1999), for an elementary introduction, see Lifshitz (1996*b*).

[3] Note that since $\mathbf{S}(\mathbf{r})$ is an axial vector field we can restrict γ to be a proper rotation without any loss of generality.

in a manner similar to the one shown originally by Rabson *et al.* (1988), and more recently again by Dräger & Mermin (1996), in the context of ordinary space groups for nonmagnetic crystals.

In the case of periodic crystals, one can show [Mermin, 1992*b*, equation (2.18)] that any gauge function $2\pi\chi(\mathbf{k})$, relating two indistinguishable spin density fields as in equation (3), is necessarily of the form $\mathbf{k}\cdot\mathbf{t}$ for some constant translation vector $\mathbf{t}$ independent of $\mathbf{k}$, so that $\mathbf{S}'(\mathbf{r}) = \mathbf{S}(\mathbf{r}+\mathbf{t})$ and indistinguishability reduces to identity to within a translation. One can then combine rotations in physical space and in spin space with translations to recover the traditional spin space groups of periodic crystals, containing operations that satisfy

$$\mathbf{S}(g\mathbf{r}) = \gamma\mathbf{S}(\mathbf{r}+\mathbf{t}_g^\gamma), \tag{9}$$

leaving the spin density field *identical* to what it was. In the quasiperiodic case, one must retain the general form of $\Phi_g^\gamma(\mathbf{k})$, which is defined only on the magnetic lattice and cannot be linearly extended to arbitrary $\mathbf{k}$.

3. Classification of spin groups

The common symmetry properties of different magnetic structures become clear only after they are classified into properly chosen equivalence classes. We are concerned here with the classification of magnetic crystals into Bravais classes (§3.1), spin geometric crystal classes (§3.2), spin arithmetic crystal classes (§3.3) and spin-space-group types (§3.4).

3.1. Bravais classes

Magnetic crystals, as well as nonmagnetic crystals, are classified into Bravais classes according to their lattices of wavevectors. Intuitively, two magnetic lattices are in the same Bravais class if they have the same rank D and point group G_L (to within a spatial reorientation) and if one can 'interpolate' between them with a sequence of lattices, all with the same point group and rank. Stated more formally, as presented by Dräger & Mermin (1996), we say that two magnetic lattices L and L' belong to the same *Bravais class* if:

1. the two lattices are isomorphic as abelian groups, *i.e* there is a one-to-one mapping, denoted by a prime ($'$), from L onto L':

$$\begin{array}{cccc} ': & L & \longrightarrow & L' \\ & \mathbf{k} & \longrightarrow & \mathbf{k}' \end{array} \tag{10}$$

satisfying

$$(\mathbf{k}_1+\mathbf{k}_2)' = \mathbf{k}_1'+\mathbf{k}_2'; \tag{11}$$

2. the corresponding lattice point groups G_L and G_L' are conjugate subgroups of $O(d)$,

$$G_L' = rG_Lr^{-1}, \tag{12}$$

for some proper d-dimensional rotation r; and

3. the isomorphism (10) between the lattices preserves the actions of their point groups, namely

$$(g\mathbf{k})' = g'\mathbf{k}', \tag{13}$$

where $g' = rgr^{-1}$.

Since the classification of magnetic lattices for magnetic crystals is the same as the classification of ordinary lattices for nonmagnetic crystals, we shall not expand on this issue further but rather refer the interested reader to previous discussions on the matter (Rokhsar *et al.*, 1987; Mermin *et al.*, 1987, 1990; Mermin, 1992*a*,*b*; Mermin & Lifshitz, 1992; Lifshitz, 1996*b*; Dräger & Mermin, 1996).

3.2. Spin geometric crystal classes

When we say that two magnetic crystals 'have the same spin point group', we normally mean that they belong to the same equivalence class of spin point groups, called a spin geometric crystal class. We say that two spin point groups G_S and G_S' are in the same *spin geometric crystal class* if they are conjugate subgroups of $O(d)\times[SO(3)\times 1']$, where $1'$ is the time inversion group, containing the identity ε and the time inversion operation ε'. This simply means that

$$G_S' = (r,\sigma)G_S(r,\sigma)^{-1}, \tag{14}$$

for some physical-space rotation $r\in O(d)$, and some spin-space operation $\sigma\in SO(3)\times 1'$. The effect of these rotations on the spin point group G_S is to reorient its symmetry axes both in physical space and in spin space.

3.3. Spin arithmetic crystal classes

The concept of a spin arithmetic crystal class is used to distinguish between magnetic crystals that have equivalent magnetic lattices and equivalent spin point groups but differ in the manner in which the lattice and the spin point group are combined. Two magnetic crystals belong to the same *spin arithmetic crystal class* if their magnetic lattices are in the same Bravais class, their spin point groups are in the same spin geometric crystal class, and it is possible to choose the lattice isomorphism (10) such that the proper rotation r used in (12) to establish the lattice equivalence is the same rotation used in (14) to establish the spin-point-group equivalence.

3.4. Spin-space-group types

The finer classification of crystals in a given spin arithmetic crystal class into *spin-space-group types* is an organization of sets of phase functions into equivalence classes according to two criteria:

1. Two *indistinguishable* magnetic crystals $\mathbf{S}$ and $\mathbf{S}'$, related as in (3) by a gauge function χ, should clearly belong to the same spin-space-group type. Such crystals are necessarily in the same spin arithmetic crystal class but the sets of phase functions Φ and Φ' used to describe their space groups may, in general, be different. It follows directly from (3) and from the point-group condition (5) that two such sets of phase functions are related by

$$\Phi'^\gamma_g(\mathbf{k}) \equiv \Phi_g^\gamma(\mathbf{k}) + \chi(g\mathbf{k}-\mathbf{k}), \tag{15}$$

for every (g, γ) in the spin point group and every $\mathbf{k}$ in the magnetic lattice. We call two sets of phase functions that describe indistinguishable spin density fields *gauge-equivalent* and equation (15), converting Φ into Φ', a *gauge* transformation. The freedom to choose a gauge χ by which to transform the Fourier coefficients $\mathbf{S}(\mathbf{k})$ of the spin density field and all the phase functions Φ, describing a given magnetic crystal, is associated in the case of periodic magnetic crystals with the freedom one has in choosing the real-space origin about which all the point-group operations are applied.

2. Two *distinguishable* magnetic crystals $\mathbf{S}$ and $\mathbf{S}'$, whose spin space groups are given by magnetic lattices L and L', spin point groups G_S and G_S', and sets of phase functions Φ and Φ' have the same spin-space-group type if they are in the same spin arithmetic crystal class and if, to within a gauge transformation (15), the lattice isomorphism (10) taking every $\mathbf{k} \in L$ into a $\mathbf{k}' \in L'$ preserves the values of all the phase functions

$$\Phi'^{\gamma'}_{g'}(\mathbf{k}') \equiv \Phi^{\gamma}_{g}(\mathbf{k}), \qquad (16)$$

where $g' = rgr^{-1}$ and $\gamma' = \sigma\gamma\sigma^{-1}$. Two sets of phase functions that are related in this way are called *scale-equivalent*. This nomenclature reflects the fact that the lattice isomorphism (10) used to relate the two magnetic lattices may often be achieved by rescaling the wavevectors of one lattice into those of the other.

4. Enumeration of spin groups

The task of enumerating spin groups is limited to the enumeration of the distinct types of spin point groups and spin space groups. This is because the classification of magnetic lattices into Bravais classes, as well as the determination of all distinct relative orientations of point groups G with respect to these lattices, giving rise to different arithmetic crystal classes, are the same as for nonmagnetic crystals, and therefore need not be enumerated again. The enumeration of possible spin point groups and spin space groups is greatly simplified if one first lists all the general constraints these groups must obey owing to their algebraic structure. We list below the general constraints on the spin point group G_S (§4.1), discuss the consequences of these constraints on the group of spin-space operations Γ (§4.2), describe a particularly interesting connection between a certain subgroup of Γ and the magnetic lattice L (§4.3) and then outline the sequence of steps taken in the enumeration of spin groups (§4.4).

4.1. Structure of the spin point group G_S

The algebraic structure of the spin point group G_S is severely constrained by the point-group condition (5) as described by the five statements below. Proofs for the first four statements can be found in the review on color symmetry (Lifshitz, 1997, Section IV.A) as they apply equally to the structure of the *color* point group of a colored crystal.

1. The set of real-space operations associated with the spin-space identity ε forms a normal subgroup of G, called G_ε. Note that as a special case of equation (8) the phase functions of conjugate elements of G_ε are related by

$$\forall g \in G_\varepsilon, (h, \eta) \in G_S: \ \Phi^{\varepsilon}_{hgh^{-1}}(h\mathbf{k}) \equiv \Phi^{\varepsilon}_{g}(\mathbf{k}) + \Phi^{\eta}_{h}(g\mathbf{k} - \mathbf{k}). \qquad (17)$$

2. The set of spin-space operations paired with the real-space identity e forms a normal subgroup of Γ, called the *lattice spin group* Γ_e. In the special case of periodic crystals, the elements of Γ_e are spin-space operations that, when combined with translations, leave the magnetic crystal invariant.
   Again, as a special case of equation (8), the phase functions of conjugate elements of Γ_e are related by

$$\forall\, \gamma \in \Gamma_e, (h, \eta) \in G_S: \quad \Phi^{\eta\gamma\eta^{-1}}_{e}(h\mathbf{k}) \equiv \Phi^{\gamma}_{e}(\mathbf{k}). \qquad (18)$$

3. The lattice spin group Γ_e is abelian.
4. The pairs in G_S associate all the elements of each coset of G_ε with all the elements of a single corresponding coset of Γ_e. This correspondence between cosets is an isomorphism between the quotient groups G/G_ε and Γ/Γ_e.
5. If two phase functions $\Phi^{\gamma_1}_e(\mathbf{k})$ and $\Phi^{\gamma_2}_e(\mathbf{k})$, associated with the lattice spin group Γ_e, are identical on all wavevectors then $\gamma_1 = \gamma_2$.
   <u>*Proof*</u>
   From the point-group condition (5), we obtain

$$\forall\, \mathbf{k} \in L: \quad \gamma_1\mathbf{S}(\mathbf{k}) = \gamma_2\mathbf{S}(\mathbf{k}), \qquad (19)$$

   implying that the two operations have the same effect on all the spin density fields whose symmetry is described by this particular spin-space-group type, and are therefore identical.

4.2. Consequences for Γ and Γ_e

The lattice spin group Γ_e is severely constrained by being an abelian subgroup of $SO(3) \times 1'$. That is, it can have no more than a single axis of n-fold symmetry with $n > 2$. This implies that the possible lattice spin groups Γ_e are the ones listed in the first column of Table 1.

The fact that the lattice spin group Γ_e is a normal subgroup of Γ implies that Γ cannot contain any rotation $\sigma \in SO(3)$ for which $\sigma\Gamma_e\sigma^{-1} \neq \Gamma_e$. One can easily verify that the possible supergroups Γ for each lattice spin group Γ_e are the ones listed in the second column of Table 1.

4.3. Relation between the magnetic lattice L and the lattice spin group Γ_e

We have already mentioned that, in the special case of periodic crystals, the lattice spin group Γ_e is the set of all spin-space operations that, when combined with real-space translations, leave the magnetic crystal invariant. It should be of no surprise then that in the quasiperiodic case there should remain an intimate relation between the lattice spin group Γ_e

Table 1
Possible lattice spin groups Γ_e and their extensions into the full groups Γ of spin-space operations.

All possible Γ_e's are listed in the first column. The second column shows the constraints on Γ imposed by the fact that Γ_e is a normal subgroup of Γ. The integer k is arbitrary.

Γ_e	Γ
1; $1'$	$\Gamma \subseteq SO(3) \times 1'$
n; n'; $n1'$	$\Gamma \subseteq (kn)221'$
222; $2'2'2'$	$\Gamma \subseteq 4321'$
$2_{\bar{z}}2'2'$	$\Gamma \subseteq 4221'$

and the magnetic lattice L. We describe this relation here without proof, which can be found in the review on color symmetry (Lifshitz, 1997, Section IV.C), where a similar relation exists between the lattice L and lattice *color* group of a colored crystal.

Recalling that the lattice L is itself an abelian group under the addition of wavevectors, one can show that it necessarily contains a sublattice L_0, invariant under the point group G, for which the quotient group L/L_0 is isomorphic to the lattice spin group Γ_e. This isomorphism is established through the properties of the phase functions $\Phi_e^\gamma(\mathbf{k})$ associated with all elements γ of the lattice spin group. In particular, the sublattice L_0 is defined as the set of wavevectors $\mathbf{k}$ for which the phases $\Phi_e^\gamma(\mathbf{k}) \equiv 0$, for all elements γ of the lattice spin group. Furthermore, the relation (18) between phase functions of conjugate elements of Γ_e ensures that the isomorphism between L/L_0 and Γ_e is invariant under all elements (h, η) of the spin point group. In other words, if the isomorphism maps a particular wavevector $\mathbf{k}$ to a particular spin operation γ, then, for every (h, η) in G_S, the wavevector $h\mathbf{k}$ is mapped to $\eta\gamma\eta^{-1}$.

This relation between the lattice spin group and the magnetic lattice not only imposes a severe constraint on the possible lattice spin groups but also provides an additional method to calculate the phase functions $\Phi_e^\gamma(\mathbf{k})$. One of two alternative approaches can be taken to enumerate the allowed combinations of Γ_e and Γ:

1. For each type of lattice spin group Γ_e, listed in Table 1, see whether there exists an invariant sublattice L_0 of L giving a modular lattice L/L_0 isomorphic to Γ_e *and* whether the possible extensions of Γ_e into supergroups Γ, also listed in Table 1, allow the isomorphism to be invariant under the spin point group.

2. For each type of lattice spin group Γ_e and its possible extensions into supergroups Γ, listed in Table 1, simply try to solve all the group compatibility conditions (7) imposed on the phase functions $\Phi_e^\gamma(\mathbf{k})$, associated with the elements of Γ_e and the wavevectors of L. If a solution exists, then Γ_e is a possible lattice spin group, otherwise it is not.

It should be emphasized that, either way, the possible combinations of Γ_e and Γ, and therefore the possible types of spin point groups, cannot be determined independently of the choice of magnetic lattice L.

4.4. Enumeration steps

The enumeration of spin point groups and spin space groups consists of a sequence of steps that are listed schematically in the flow chart of Fig. 1. We shall illustrate the whole process in §6 by enumerating, as an example, all the two-dimensional octagonal spin point groups and spin space groups.

One begins by choosing a lattice L from any of the known Bravais classes. One then picks any point group G, compatible with L, and lists all its normal subgroups G_ε along with the corresponding quotient groups G/G_ε. One then chooses one of the normal subgroups G_ε and calculates, using one of the two approaches described in the previous section, all allowed combinations of Γ and Γ_e such that the quotient group Γ/Γ_e is isomorphic to G/G_ε. One then pairs the cosets of G_ε in G with the cosets of Γ_e in Γ in all distinct ways. After checking for equivalence, as described in §3.2, one arrives at a list of the distinct types of spin point groups.

For each spin point group, one then looks for all solutions to the group compatibility conditions (7) not already considered above. These solutions are organized into gauge-equivalence and scale-equivalence classes, as described in §3.4, yielding the distinct spin-space-group types. Because phase functions are linear on the lattice L [equation (4)], it is sufficient to specify their values on a chosen set of D wavevectors that primitively generate the lattice. Also, it is sufficient to specify the phase functions only for a small set of operations (g, γ) that generate the spin point group. All other phase functions can be determined through the group compatibility condition. Furthermore, one can greatly simplify the calculation of phase functions by making a judicious choice of gauge prior to solving the group compatibility conditions, rather than solving

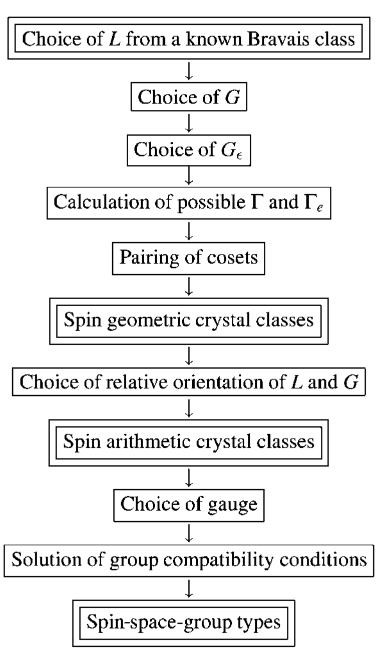

Figure 1
Flow chart describing the steps required for the enumeration of spin point groups and spin space groups. Double boxes indicate the classification into equivalence classes as described in §3.

the group compatibility conditions and only then organizing the solutions into gauge-equivalence classes.

5. Calculation of magnetic selection rules

Magnetic selection rules, or symmetry-imposed constraints on the form of the spin density field, offer one of the most direct experimental observations of the detailed magnetic symmetry of a magnetic crystal. In elastic neutron scattering experiments, every wavevector $\mathbf{k}$ in L is a candidate for a magnetic Bragg peak, whose intensity is given by (Izyumov & Ozerov, 1970)

$$I(\mathbf{k}) \propto |\mathbf{S}(\mathbf{k})|^2 - |\hat{\mathbf{k}} \cdot \mathbf{S}(\mathbf{k})|^2, \tag{20}$$

where $\mathbf{k}$ is the scattering wavevector and $\hat{\mathbf{k}}$ is a unit vector in its direction. It has been shown [Lifshitz (1996*a*); for a sketch of the argument see Lifshitz (1996*c*)] that, under generic circumstances, there can be only three reasons for not observing a magnetic Bragg peak at $\mathbf{k}$ even though $\mathbf{k}$ is in L: (*a*) the intensity $I(\mathbf{k}) \neq 0$ but is too weak to be detected in the actual experiment; (*b*) the intensity $I(\mathbf{k}) = 0$ because $\mathbf{S}(\mathbf{k})$ is parallel to $\mathbf{k}$; and (*c*) the intensity $I(\mathbf{k}) = 0$ because magnetic selection rules require the Fourier coefficient $\mathbf{S}(\mathbf{k})$ to vanish. Selection rules that lead to a full extinction of a Bragg peak are the most dramatic and easiest to observe experimentally. Other types of selection rules [*e.g.* that lead to an extinction of one of the components of $\mathbf{S}(\mathbf{k})$, or to a nontrivial relation between the components of $\mathbf{S}(\mathbf{k})$] are harder to observe.

We calculate the symmetry-imposed constraints on $\mathbf{S}(\mathbf{k})$, for any given wavevector $\mathbf{k} \in L$, by examining all spin-point-group operations (g, γ) for which $g\mathbf{k} = \mathbf{k}$. These elements form a subgroup of the spin point group which we call the *little spin group* of $\mathbf{k}$, $G_S^{\mathbf{k}}$. For elements (g, γ) of $G_S^{\mathbf{k}}$, the point-group condition (5) can be rewritten as

$$\gamma \mathbf{S}(\mathbf{k}) = e^{-2\pi i \Phi_g^{\gamma}(\mathbf{k})} \mathbf{S}(\mathbf{k}). \tag{21}$$

This implies that every Fourier coefficient $\mathbf{S}(\mathbf{k})$ is required to be a simultaneous eigenvector of all spin-space operations γ in the little spin group of $\mathbf{k}$, with the eigenvalues given by the corresponding phase functions. If a non-trivial three-dimensional vector satisfying (21) does not exist, then $\mathbf{S}(\mathbf{k})$ will necessarily vanish. It should be noted that the phase values in (21) are independent of the choice of gauge (15), and are therefore uniquely determined by the spin-space-group type of the crystal.

The process of determining the form of the simultaneous eigenvector $\mathbf{S}(\mathbf{k})$ is greatly simplified if one makes the following observation. Owing to the group compatibility condition (7), the set of eigenvalues in (21) for all the elements $(g, \gamma) \in G_S^{\mathbf{k}}$ forms a one-dimensional representation of that group. Spin-space-group symmetry thus requires the Fourier coefficient $\mathbf{S}(\mathbf{k})$ to transform under a particular one-dimensional representation of the spin-space operations in the little spin group of $\mathbf{k}$. We also independently know that $\mathbf{S}(\mathbf{k})$ transforms under spin-space rotations as a three-dimensional axial vector, changing its sign under time inversion. It is therefore enough to check whether the particular one-dimensional representation, dictated by the spin space group, is contained within the three-dimensional axial-vector representation. If it is not, then $\mathbf{S}(\mathbf{k})$ must vanish; if it is, then $\mathbf{S}(\mathbf{k})$ must lie in the subspace of spin space transforming under this one-dimensional representation.

6. Octagonal spin groups in two dimensions—an example

To demonstrate the ideas presented in this paper, we enumerate the octagonal spin groups in two dimensions and calculate the magnetic selection rules that arise for each spin-space-group type. We choose to treat the octagonal crystal system because it is the most interesting example for a magnetic quasicrystal in two dimensions. The reason for this is twofold: firstly, as for nonmagnetic two-dimensional crystals, only when the order of symmetry is a power of 2 is it possible to have space groups with nonsymmorphic operations; secondly, only when the order of symmetry is a power of 2 is it possible to have simple antiferromagnetic order (Niizeki, 1990*a*,*b*; Lifshitz, 1997, 2000).

Only partial enumerations of spin groups on quasicrystals exist to date. Decagonal spin point groups and spin-space-group types in two dimensions have been listed by Lifshitz (1995) without providing much detail regarding the enumeration process. All possible lattice spin groups Γ_e for icosahedral quasicrystals have been tabulated (Lifshitz, 1998) along with the selection rules that they impose, but a complete enumeration of all icosahedral spin groups was not given. This is therefore the first complete and rigorous enumeration of spin groups and selection rules for a quasiperiodic crystal system in any dimension. In a companion paper (Even-Dar Mandel & Lifshitz, 2004), we enumerate the octagonal spin groups in three dimensions and, in future publications, we intend to treat all the other common quasiperiodic crystal systems, although we shall probably not include the full details of the calculation.

6.1. Two-dimensional octagonal point groups and Bravais classes

The lowest rank D that a two-dimensional octagonal lattice can have is 4. There is just a single Bravais class of two-dimensional rank-4 octagonal lattices (Mermin *et al.*, 1987). All lattices in this two-dimensional Bravais class contain an eightfold star of wavevectors of equal length, separated by angles of $\pi/4$ (as shown in Fig. 2), of which four, labeled $\mathbf{b}^{(1)} \ldots \mathbf{b}^{(4)}$, can be taken as integrally independent lattice-generating vectors. The lattice point group G_L is $8mm$, generated by an eightfold rotation r_8 and either a mirror of type m, which contains one of the generating vectors and its negative, or a mirror of type m', which lies between two of the generating vectors. The two-dimensional point groups G to be considered in the enumeration are $8mm$ and its subgroup 8. There is only a single way to orient the two point groups with respect to the lattice, so there is just a single spin arithmetic crystal class for each spin geometric crystal class.

Table 2
Normal subgroups G_ε of the point groups $G = 8mm$ and 8.

The resulting quotient group G/G_ε is represented in the third column by a point group, isomorphic to it. Constraints on the spin-space operations δ and μ, paired with the generators r_8 and m of G are listed in the fourth column. In each line, the first power of δ that is in Γ_e is given. μ^2 is always in Γ_e, therefore we only note whether $\mu \in \Gamma_e$. If δ or μ are in Γ_e, they are chosen as ε.

G	G_ε	G/G_ε	Constraints
$8mm$	$8mm$	1	$\delta = \varepsilon, \mu = \varepsilon$
	8	m	$\delta = \varepsilon, \mu \notin \Gamma_e$
	$4mm$	2	$\delta^2 \in \Gamma_e, \mu = \varepsilon$
	$4m'm'$	2	$\delta = \mu \notin \Gamma_e$
	4	$2mm$	$\delta^2 \in \Gamma_e, \mu \notin \Gamma_e, \delta\Gamma_e \neq \mu\Gamma_e$
	2	$4mm$	$\delta^4 \in \Gamma_e, \mu \notin \Gamma_e, \delta^2\Gamma_e \neq \mu\Gamma_e$
	1	$8mm$	$\delta^8 \in \Gamma_e, \mu \notin \Gamma_e, \delta^4\Gamma_e \neq \mu\Gamma_e$
8	8	1	$\delta = \varepsilon$
	4	2	$\delta^2 \in \Gamma_e$
	2	4	$\delta^4 \in \Gamma_e$
	1	8	$\delta^8 \in \Gamma_e$

6.2. Enumeration of spin point groups

We begin by listing in the first columns of Table 2 all normal subgroups G_ε of the point groups $G = 8mm$ and 8, and the resulting quotient groups G/G_ε. Note that the two subgroups $2mm$ and m of the point group $8mm$ are not normal and therefore do not appear in the table.

As generators of the spin point groups, we take the generators of G (r_8 and m for $G = 8mm$, and r_8 alone for $G = 8$) and combine each one with a representative spin-space operation from the coset of Γ_e with which it is paired. We denote the spin-space operation paired with r_8 by δ and the operation paired with m by μ. When r_8 (or m) are in G_ε, we take δ (or μ) to be ε. The constraints on the operations δ and μ, owing to the isomorphism between G/G_ε and Γ/Γ_e, are summarized in the fourth column of Table 2. To the generators (r_8, δ) and (m, μ), we add as many generators of the form (e, γ_i) as required, where γ_i are the generators of Γ_e (three at the most). Although this set of spin-point-group generators may, in general, be overcomplete, it is the most convenient set to take.

6.3. Calculation of possible Γ and Γ_e

We use the group compatibility conditions (7) on the phase functions $\Phi_e^\gamma(\mathbf{k})$, associated with elements in the lattice spin group Γ_e, in order to calculate the possible combinations of Γ and Γ_e.

We first note, from inspection of Table 2, that no quotient group G/G_ε contains an operation of order 3. This implies, among other things, that Γ/Γ_e cannot contain such an operation and therefore the extensions of the orthorhombic lattice spin groups Γ_e, listed in the third row of Table 1, into supergroups Γ cannot be cubic—they can be tetragonal at most. This then implies that, for any possible combination of Γ and Γ_e,

$$\forall \gamma \in \Gamma_e, \delta \in \Gamma: \quad \delta^2\gamma\delta^{-2} = \gamma. \tag{22}$$

With this relation at hand, we can proceed to prove the following short lemmas:

1. The lattice spin group Γ_e contains no more than three elements $\gamma \neq \varepsilon$, all of which are of order 2.

Proof

Let $\delta \in \Gamma$ be the operation paired with r_8 in the spin point group. The relation (22) together with equation (18), relating phase functions of conjugate elements in Γ_e, yields

$$\Phi_e^\gamma(\mathbf{b}^{(i)}) \equiv \Phi_e^{\delta^2\gamma\delta^{-2}}({r_8}^2\mathbf{b}^{(i)}) \equiv \Phi_e^\gamma({r_8}^2\mathbf{b}^{(i)}). \tag{23}$$

Thus, for any $\gamma \in \Gamma_e$,

$$\Phi_e^\gamma(\mathbf{b}^{(1)}) \equiv \Phi_e^\gamma(\mathbf{b}^{(3)}) \equiv \alpha; \quad \Phi_e^\gamma(\mathbf{b}^{(2)}) \equiv \Phi_e^\gamma(\mathbf{b}^{(4)}) \equiv \beta; \tag{24}$$

and

$$\Phi_e^\gamma(-\mathbf{b}^{(i)}) \equiv \Phi_e^\gamma(\mathbf{b}^{(i)}) \Rightarrow \Phi_e^\gamma(\mathbf{b}^{(i)}) \equiv 0 \text{ or } \tfrac{1}{2}. \tag{25}$$

The last result (owing to the linearity of the phase function) implies through the group compatibility condition that $\Phi_e^{\gamma^2}(\mathbf{b}^{(i)}) \equiv 0$ and, therefore, that $\gamma^2 = \varepsilon$ or that γ is an operation of order 2. It also implies that each of the phases α and β in (24) can be either 0 or 1/2, but they cannot both be 0 if $\gamma \neq \varepsilon$. Thus, there can be no more than three operations in Γ_e other than the identity.

2. Only a single element $\gamma \neq \varepsilon$ in the lattice spin group Γ_e commutes with the operation $\delta \in \Gamma$, paired with r_8 in the spin point group.

Proof

If $\gamma \neq \varepsilon$ in Γ_e commutes with δ, then the relation (18) between phase functions of conjugate elements of γ_e implies that

$$\Phi_e^\gamma(\mathbf{b}^{(i)}) \equiv \Phi_e^{\delta\gamma\delta^{-1}}(r_8\mathbf{b}^{(i)}) \equiv \Phi_e^\gamma(r_8\mathbf{b}^{(i)}). \tag{26}$$

Thus, γ is necessarily the operation whose phase function is given by (24) with $\alpha \equiv \beta \equiv 1/2$.

These lemmas, together with the facts that G/G_ε can be no bigger than a group isomorphic to $8mm$, and that the order of the operation δ paired with r_8 is no bigger than 8 (proven in §6.4.1 below), narrow the possible combinations of Γ and Γ_e, listed in Table 1, to the ones listed in Table 3.

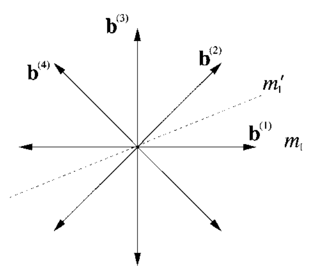

Figure 2
Generating vectors and mirror lines for two-dimensional octagonal lattices. The solid arrows are the star of generating vectors and their negatives $\pm\mathbf{b}^{(1)} \ldots \pm\mathbf{b}^{(4)}$. The dashed lines show the two types of mirrors in the $8mm$ point group, as described in the text.

6.4. Enumeration of spin-space-group types

We now turn to the enumeration of spin-space-group types by calculating the possible values of the phase functions for

Table 3
Possible lattice spin groups Γ_e and their extensions into the full groups Γ of spin-space operations, compatible with the two-dimensional rank-4 octagonal lattice.

All possible Γ_e's are listed in the first column and constraints on the possible supergroups Γ are listed in the second column. The phase functions for the generators of Γ_e are listed in the third column.

Γ_e	Constraints on Γ	Phase functions for generators of Γ_e
1	$\Gamma_e \subseteq \Gamma \subset 8221'$	N/A
$1'$	$\Gamma_e \subseteq \Gamma \subseteq 8221'$	$\Phi_e^{\varepsilon'}(\mathbf{b}^{(i)}) \equiv \frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$
2	$\Gamma_e \subseteq \Gamma \subset 8221'$	$\Phi_e^{2_{\bar z}}(\mathbf{b}^{(i)}) \equiv \frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$
$2'$	$\Gamma_e \subseteq \Gamma \subseteq 8221'$	$\Phi_e^{2'_{\bar z}}(\mathbf{b}^{(i)}) \equiv \frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$
222	$422 \subseteq \Gamma \subseteq 4221'$	$\Phi_e^{2_{\bar x}}(\mathbf{b}^{(i)}) \equiv 0\frac{1}{2}0\frac{1}{2}$; $\Phi_e^{2_{\bar y}}(\mathbf{b}^{(i)}) \equiv \frac{1}{2}0\frac{1}{2}0$
$2_{\bar z}2'2'$	$42'2' \subseteq \Gamma \subseteq 4221'$	$\Phi_e^{2'_{\bar x}}(\mathbf{b}^{(i)}) \equiv 0\frac{1}{2}0\frac{1}{2}$; $\Phi_e^{2'_{\bar y}}(\mathbf{b}^{(i)}) \equiv \frac{1}{2}0\frac{1}{2}0$

Table 4
Two-dimensional octagonal spin point groups and spin-space-group types with point group $G = 8$.

The phase function Φ_ε^γ is zero everywhere by choice of gauge. The values of the phase function Φ_e^γ for $\gamma \in \Gamma_e$ on the lattice-generating vectors are listed in Table 3. The symbols for the spin space groups are listed in the rightmost column using the notation described in §6.5.

Γ_e	G_ε	G/G_ε	Γ	Generators	Space groups
1	8	1	1	(r_8, ε)	$P8$
	4	2	2^*	$(r_8, 2^*_{\bar z})$	$P8^{2^*}$
			$1'$	(r_8, ε')	$P8'$
	2	4	4^*	$(r_8, 4^*_{\bar z})$	$P8^{4^*}$
	1	8	8^*	$(r_8, 8^*_{\bar z})$	$P8^{8^*}$
				$(r_8, 8^{3*}_{\bar z})$	$P8^{8^{3*}}$
2	8	1	2	$(r_8, \varepsilon), (e, 2_{\bar z})$	$P8(2)$
	4	2	4^*	$(r_8, 4^*_{\bar z}), (e, 2_{\bar z})$	$P8^{4^*}(2)$
			2^*2^*2	$(r_8, 2^*_{\bar x})(e, 2_{\bar z})$	$P8^{2^*_{\bar x}}(2)$
			$21'$	$(r_8, \varepsilon')(e, 2_{\bar z})$	$P8'(2)$
	2	4	8^*	$(r_8, 8^*_{\bar z})(e, 2_{\bar z})$	$P8^{8^*}(2)$
$2'$	8	1	$2'$	$(r_8, \varepsilon)(e, 2'_{\bar z})$	$P8(2')$
	4	2	$2'2'2$	$(r_8, 2^*_{\bar x})(e, 2'_{\bar z})$	$P8^{2^*_{\bar x}}(2')$
			$21'$	$(r_8, \varepsilon')(e, 2'_{\bar z})$	$P8'(2')$
	2	4	$41'$	$(r_8, 4_{\bar z})(e, 2'_{\bar z})$	$P8^4(2')$
	1	8	$81'$	$(r_8, 8_{\bar z})(e, 2'_{\bar z})$	$P8^8(2')$
$1'$	8	1	$1'$	$(r_8, \varepsilon)(e, \varepsilon')$	$P8(1')$
	4	2	$21'$	$(r_8, 2_{\bar z})(e, \varepsilon')$	$P8^2(1')$
	2	4	$41'$	$(r_8, 4_{\bar z})(e, \varepsilon')$	$P8^4(1')$
	1	8	$81'$	$(r_8, 8_{\bar z})(e, \varepsilon')$	$P8^8(1')$
				$(r_8, 8^3_{\bar z})(m, \varepsilon')$	$P8^{8^3}(1')$
222	4	2	4^*22^*	$(r_8, 4^*_{\bar z})(e, 2_{\bar x})(e, 2_{\bar y})$	$P8^{4^*}(222)$

the generators (r_8, δ) and (m, μ) on the star of generating vectors $\mathbf{b}^{(i)}$.

6.4.1. The phase function for (r_8, δ). As in the case of regular space groups for nonmagnetic crystals (Rokhsar *et al.*, 1988*b*; Rabson *et al.*, 1991), there is a gauge in which the phase function $\Phi_{r_8}^\delta(\mathbf{k}) \equiv 0$ on the whole lattice. This can be shown by starting with arbitrary values for the phase function $\Phi_{r_8}^\delta$ and performing a gauge transformation (15) with the gauge function

$$\chi(\mathbf{b}^{(i)}) = \tfrac{1}{2}\,\Phi_{r_8}^\delta\left(\sum_{j=i}^{i+3}\mathbf{b}^{(j)}\right), \qquad i = 1, \ldots, 4, \tag{27}$$

where $\mathbf{b}^{(j)} = -\mathbf{b}^{(j-4)}$ for $j = 5, 6, 7, 8$. The change to $\Phi_{r_8}^\delta$ caused by this gauge transformation exactly cancels it:

$$\begin{aligned}\Delta\Phi_{r_8}^\delta(\mathbf{b}^{(i)}) &\equiv \chi(r_8\mathbf{b}^{(i)} - \mathbf{b}^{(i)})\\ &\equiv \tfrac{1}{2}\,\Phi_{r_8}^\delta(\mathbf{b}^{(i+4)} - \mathbf{b}^{(i)})\\ &\equiv -\Phi_{r_8}^\delta(\mathbf{b}^{(i)}),\end{aligned} \tag{28}$$

so that after the gauge transformation $\Phi_{r_8}^\delta(\mathbf{k}) \equiv 0$ for all wavevectors $\mathbf{k}$. Note that this implies, through the group compatibility condition (7), that $\Phi_e^{\delta^8}(\mathbf{k}) \equiv 0$, so that $\delta^8 = \varepsilon$, imposing an additional restriction on the group Γ, as indicated in Table 3.

6.4.2. The phase function for (m, μ). When $G = 8mm$, we need to calculate the additional phase function $\Phi_m^\mu(\mathbf{k})$, associated with the second point-group generator (m, μ). The generating relations that contribute to the determination of this phase function are $(m, \mu)^2 = (e, \mu^2)$ and $(r_8, \delta)(m, \mu)(r_8, \delta) = (m, \delta\mu\delta)$. Applying the group compatibility condition (7) to these relations, in the gauge where $\Phi_{r_8}^\delta(\mathbf{k}) \equiv 0$, yields

$$\Phi_e^{\mu^2}(\mathbf{b}^{(i)}) \equiv \Phi_m^\mu(m\mathbf{b}^{(i)} + \mathbf{b}^{(i)}), \tag{29}$$

$$\Phi_m^{\delta\mu\delta}(\mathbf{b}^{(i)}) \equiv \Phi_m^\mu(r_8\mathbf{b}^{(i)}). \tag{30}$$

We shall first determine the value of the phase $\Phi_m^\mu(\mathbf{b}^{(1)})$ using equation (29), and then use equation (30) to infer the values of Φ_m^μ on the remaining three generating vectors. We start by noting that μ^2 is an operation in Γ_e that is the square of an operation in Γ. Inspection of all the possibilities, listed in Table 3, reveals that only two operations, $2_{\bar z}$ and ε, satisfy this condition. Furthermore, if m is the mirror that leaves $\mathbf{b}^{(1)}$ invariant, then application of equation (29) to $\mathbf{b}^{(3)}$, which is perpendicular to m ($m\mathbf{b}^{(3)} = -\mathbf{b}^{(3)}$) yields

$$\Phi_e^{\mu^2}(\mathbf{b}^{(3)}) \equiv \Phi_m^\mu(m\mathbf{b}^{(3)} + \mathbf{b}^{(3)}) \equiv 0. \tag{31}$$

This implies that μ^2 cannot be $2_{\bar z}$ because $\Phi_e^{2_{\bar z}}$ has the value $\frac{1}{2}$ on all lattice generating vectors. Therefore, μ^2 must be equal to ε. Application of equation (29) to $\mathbf{b}^{(1)}$ now yields

$$0 \equiv 2\Phi_m^\mu(\mathbf{b}^{(1)}) \;\Rightarrow\; \Phi_m^\mu(\mathbf{b}^{(1)}) \equiv 0 \text{ or } \tfrac{1}{2}, \tag{32}$$

and application of equation (29) to $\mathbf{b}^{(2)}$ and $\mathbf{b}^{(4)}$ shows that $\Phi_m^\mu(\mathbf{b}^{(2)}) \equiv \Phi_m^\mu(\mathbf{b}^{(4)})$, but provides no further information regarding the actual values of these phases.

Next, we examine equation (30), which can be rephrased [using the group compatibility condition (7)] as

$$\Phi_m^\mu(\mathbf{b}^{(i)}) + \Phi_e^{\mu^{-1}\delta\mu\delta}(\mathbf{b}^{(i)}) \equiv \Phi_m^\mu(r_8\mathbf{b}^{(i)}). \tag{33}$$

The value of Φ_m^μ on $\mathbf{b}^{(1)}$ determines the values of Φ_m^μ on the remaining generating vectors through some phase function, associated with an element of Γ_e. Note that $\mu^{-1}\delta\mu\delta$ is an operation in Γ_e, which is the product of two operations, $\mu^{-1}\delta\mu$ and δ, that are conjugate in Γ. Inspection of Table 3 shows that, if the product of any two conjugate operations in Γ is in Γ_e, then this product is necessarily either $2_{\bar z}$ or the identity ε. Substituting the values $\Phi_e^\varepsilon(\mathbf{b}^{(i)}) \equiv 0000$ and $\Phi_e^{2_{\bar z}}(\mathbf{b}^{(i)}) \equiv \frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$, we conclude that

$$\Phi_m^\mu(\mathbf{b}^{(i)}) \equiv \begin{cases} 0000 \text{ or } \frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2} & \text{if } \delta\mu\delta = \mu,\\ 0\frac{1}{2}0\frac{1}{2} \text{ or } \frac{1}{2}0\frac{1}{2}0 & \text{if } \delta\mu\delta = \mu 2_{\bar z}.\end{cases} \tag{34}$$

Table 5
Two-dimensional octagonal spin point groups and spin-space-group types with point group $G = 8mm$.

The phase function $\Phi^{\delta}_{r_8}$ is zero everywhere by choice of gauge. The values of the phase function Φ^{γ}_{e} for $\gamma \in \Gamma_e$ on the lattice-generating vectors are listed in Table 3. The possible values of the phase function Φ^{μ}_{m} are listed in the sixth column using the notation described in §6.5. The symbols for the spin space groups are listed in the rightmost column using the notation that is also described in §6.5.

Γ_e	G_ε	G/G_ε	Γ	Generators	Φ^{μ}_{m}	Spin-space-group types	
1	$8mm$	1	1	$(r_8, \varepsilon)(m, \varepsilon)$	$0; \frac{1}{2}$	$P8mm$;	$P8bm$
	8	2	2^*	$(r_8, \varepsilon)(m, 2^*_{\bar z})$	$0; \frac{1}{2}$	$P8m^{2^*}m$;	$P8b^{2^*}m$
			$1'$	$(r_8, \varepsilon)(m, \varepsilon')$	$0; \frac{1}{2}$	$P8m'm$;	$P8b'm$
	$4mm$	2	2^*	$(r_8, 2^*_{\bar z})(m, \varepsilon)$	$0; \frac{1}{2}$	$P8^{2^*}mm$;	$P8^{2^*}bm$
			$1'$	$(r_8, \varepsilon')(m, \varepsilon)$	$0; \frac{1}{2}$	$P8'mm$;	$P8'bm$
	$4m'm'$	2	2^*	$(r_8, 2^*_{\bar z})(m, 2^*_{\bar z})$	$0; \frac{1}{2}$	$P8^{2^*}m^{2^*}m$;	$P8^{2^*}b^{2^*}m$
			$1'$	$(r_8, \varepsilon')(m, \varepsilon')$	$0; \frac{1}{2}$	$P8'm'm$;	$P8'b'm$
	4	$2mm$	$2^*2^{\dagger}2^{*\dagger}$	$(r_8, 2^*_{\bar z})(m, 2^{\dagger}_{\bar x})$	$0; \frac{1}{2}$	$P8^{2^*}m^{2^{\dagger}_{\bar x}}m$;	$P8^{2^*}b^{2^{\dagger}_{\bar x}}m$
			$21'$	$(r_8, 2^*_{\bar z})(m, 2'^*_{\bar z})$	$0; \frac{1}{2}$	$P8^{2^*}m^{2'^*}m$;	$P8^{2^*}b^{2'^*}m$
				$(r_8, 2^*_{\bar z})(m, \varepsilon')$	$0; \frac{1}{2}$	$P8^{2^*}m'm$;	$P8^{2^*}b'm$
				$(r_8, \varepsilon')(m, 2^*_{\bar z})$	$0; \frac{1}{2}$	$P8'm^{2^*}m$;	$P8'b^{2^*}m$
	2	$4mm$	$4^*2^{\dagger}2^{*\dagger}$	$(r_8, 4^*_{\bar z})(m, 2^{\dagger}_{\bar x})$	$0; \frac{1}{2}$	$P8^{4^*}m^{2^{\dagger}}m$;	$P8^{4^*}b^{2^{\dagger}}m$
	1	$8mm$	$8^*2^{\dagger}2^{*\dagger}$	$(r_8, 8^*_{\bar z})(m, 2^{\dagger}_{\bar x})$	$0; \frac{1}{2}$	$P8^{8^*}m^{2^{\dagger}_{\bar x}}2$;	$P8^{8^*}b^{2^{\dagger}_{\bar x}}m$
				$(r_8, 8^{3*}_{\bar z})(m, 2^{\dagger}_{\bar x})$	$0; \frac{1}{2}$	$P8^{8^{3*}}m^{2^{\dagger}_{\bar x}}2$;	$P8^{8^{3*}}b^{2^{\dagger}_{\bar x}}m$
2	$8mm$	1	2	$(r_8, \varepsilon), (m, \varepsilon)(e, 2_{\bar z})$	$0; \frac{1}{2}$	$P8mm(2)$;	$P8bm(2)$
	8	m	2^*2^*2	$(r_8, \varepsilon)(m, 2^*_{\bar x})(e, 2_{\bar z})$	$0; \frac{1}{2}$	$P8m^{2^*_{\bar x}}m(2)$;	$P8b^{2^*_{\bar x}}m(2)$
			$21'$	$(r_8, \varepsilon)(m, \varepsilon')(e, 2_{\bar z})$	$0; \frac{1}{2}$	$P8m'm(2)$;	$P8b'm(2)$
	$4mm$	2	2^*2^*2	$(r_8, 2^*_{\bar x})(m, \varepsilon)(e, 2_{\bar z})$	$0; \frac{1}{2}$	$P8^{2^*_{\bar x}}mm(2)$;	$P8^{2^*_{\bar x}}bm(2)$
			$21'$	$(r_8, \varepsilon')(m, \varepsilon)(e, 2_{\bar z})$	$0; \frac{1}{2}$	$P8'mm(2)$;	$P8'bm(2)$
			4^*	$(r_8, 4^*_{\bar z})(m, \varepsilon)(e, 2_{\bar z})$	A	$P8^{4^*}m_am(2)$;	$P8^{4^*}b_am(2)$
	$4m'm'$	2	2^*2^*2	$(r_8, 2^*_{\bar x})(m, 2^*_{\bar x})(e, 2_{\bar z})$	$0; \frac{1}{2}$	$P8^{2^*_{\bar x}}m^{2^*_{\bar x}}m(2)$;	$P8^{2^*_{\bar x}}b^{2^*_{\bar x}}m(2)$
			$21'$	$(r_8, \varepsilon')(m, \varepsilon')(e, 2_{\bar z})$	$0; \frac{1}{2}$	$P8'm'm(2)$;	$P8'b'm(2)$
	4	$2mm$	$4^*2^{\dagger}2^{*\dagger}$	$(r_8, 4^*_{\bar z})(m, 2^{\dagger}_{\bar x})(e, 2_{\bar z})$	$0; \frac{1}{2}$	$P8^{4^*}m^{2^{\dagger}_{\bar x}}m(2)$;	$P8^{4^*}b^{2^{\dagger}_{\bar x}}m(2)$
				$(r_8, 2^{\dagger}_{\bar x})(m, 2^*_{\overline{xy}})(e, 2_{\bar z})$	A	$P8^{2^{\dagger}_{\bar x}}m_a^{2^*_{\overline{xy}}}m(2)$;	$P8^{2^{\dagger}_{\bar x}}b_a^{2^*_{\overline{xy}}}m(2)$
			$2221'$	$(r_8, \varepsilon')(m, 2^*_{\bar x})(e, 2_{\bar z})$	$0; \frac{1}{2}$	$P8'm^{2^*_{\bar x}}m(2)$;	$P8'b^{2^*_{\bar x}}m(2)$
				$(r_8, 2^*_{\bar x})(m, \varepsilon')(e, 2_{\bar z})$	$0; \frac{1}{2}$	$P8^{2^*_{\bar x}}m'm(2)$;	$P8^{2^*_{\bar x}}b'm(2)$
				$(r_8, 2^*_{\bar x})(m, 2^{*'}_{\bar x})(e, 2_{\bar z})$	$0; \frac{1}{2}$	$P8^{2^*_{\bar x}}m^{2'^*_{\bar x}}m(2)$;	$P8^{2^*_{\bar x}}b^{2'^*_{\bar x}}m(2)$
	2	$4mm$	$8^*2^{\dagger}2^{*\dagger}$	$(r_8, 8^*_{\bar z})(m, 2^{\dagger}_{\bar x})(e, 2_{\bar z})$	$0; \frac{1}{2}$	$P8^{8^*}m^{2^{\dagger}_{\bar x}}m(2)$;	$P8^{8^*}b^{2^{\dagger}_{\bar x}}m(2)$
$2'$	$8mm$	1	$2'$	$(r_8, \varepsilon)(m, \varepsilon)(e, 2'_{\bar z})$	$0; \frac{1}{2}$	$P8mm(2')$;	$P8bm(2')$
	8	m	$2'22'$	$(r_8, \varepsilon)(m, 2_{\bar x})(e, 2'_{\bar z})$	$0; \frac{1}{2}$	$P8m^{2_{\bar x}}m(2')$;	$P8b^{2_{\bar x}}m(2')$
			$21'$	$(r_8, \varepsilon)(m, \varepsilon')(e, 2'_{\bar z})$	$0; \frac{1}{2}$	$P8m'm(2')$;	$P8b'm(2')$
	$4mm$	2	$2'22'$	$(r_8, 2_{\bar x})(m, \varepsilon)(e, 2'_{\bar z})$	$0; \frac{1}{2}$	$P8^{2_{\bar x}}mm(2')$;	$P8^{2_{\bar x}}bm(2')$
			$21'$	$(r_8, \varepsilon')(m, \varepsilon)(e, 2'_{\bar z})$	$0; \frac{1}{2}$	$P8'mm(2')$;	$P8'bm(2')$
	$4m'm'$	2	$2'22'$	$(r_8, 2^*_{\bar x})(m, 2_{\bar x})(e, 2'_{\bar z})$	$0; \frac{1}{2}$	$P8m^{2^*_{\bar x}}m^{2^*_{\bar x}}m(2')$;	$P8m^{2^*_{\bar x}}b^{2^*_{\bar x}}m(2')$
			$21'$	$(r_8, \varepsilon')(m, \varepsilon')(e, 2'_{\bar z})$	$0; \frac{1}{2}$	$P8'm'm(2')$;	$P8'b'm(2')$
	4	$2mm$	$2221'$	$(r_8, \varepsilon')(m, 2^*_{\bar x})(e, 2'_{\bar z})$	$0; \frac{1}{2}$	$P8'm^{2_{\bar x}}m(2')$;	$P8'b^{2_{\bar x}}m(2')$
				$(r_8, 2^*_{\bar x})(m, \varepsilon')(e, 2'_{\bar z})$	$0; \frac{1}{2}$	$P8^{2_{\bar x}}m'm(2')$;	$P8^{2_{\bar x}}b'm(2')$
	2	$4mm$	$4221'$	$(r_8, 4^*_{\bar z})(m, 2_{\bar x})(e, 2'_{\bar z})$	$0; \frac{1}{2}$	$P8^{4^*}m^{2_{\bar x}}m(2')$;	$P8^{4^*}m^{2_{\bar x}}m(2')$
	1	$8mm$	$8221'$	$(r_8, 8^*_{\bar z})(m, 2_{\bar x})(e, 2'_{\bar z})$	$0; \frac{1}{2}$	$P8^{8^*}m^{2_{\bar x}}m(2')$;	$P8^{8^*}b^{2_{\bar x}}m(2')$
$1'$	$8mm$	1	$1'$	$(r_8, \varepsilon)(m, \varepsilon)(e, \varepsilon')$	$0; \frac{1}{2}$	$P8mm(1')$;	$P8bm(1')$
	8	m	$21'$	$(r_8, \varepsilon)(m, 2_{\bar z})(e, \varepsilon')$	$0; \frac{1}{2}$	$P8m^2m(1')$;	$P8b^2m(1')$
	$4mm$	2	$21'$	$(r_8, 2_{\bar z})(m, \varepsilon)(e, \varepsilon')$	$0; \frac{1}{2}$	$P8^2mm(1')$;	$P8^2bm(1')$
	$4m'm'$	2	$21'$	$(r_8, 2_{\bar z})(m, 2_{\bar z})(e, \varepsilon')$	$0; \frac{1}{2}$	$P8^2m^2m(1')$;	$P8^2b^2m(1')$
	4	$2mm$	$2221'$	$(r_8, 2_{\bar z})(m, 2_{\bar x})(e, \varepsilon')$	$0; \frac{1}{2}$	$P8^2m^{2_{\bar x}}m(1')$;	$P8^2b^{2_{\bar x}}m(1')$
	2	$4mm$	$4221'$	$(r_8, 4_{\bar z})(m, 2_{\bar x})(e, \varepsilon')$	$0; \frac{1}{2}$	$P8^4m^{2_{\bar x}}m(1')$;	$P8^4b^{2_{\bar x}}m(1')$
	1	$8mm$	$8221'$	$(r_8, 8_{\bar z})(m, 2_{\bar x})(e, \varepsilon')$	$0; \frac{1}{2}$	$P8^8m^{2_{\bar x}}m(1')$;	$P8^8b^{2_{\bar x}}m(1')$
				$(r_8, 8^3_{\bar z})(m, 2_{\bar x})(e, \varepsilon')$	$0; \frac{1}{2}$	$P8^{8^3}m^{2_{\bar x}}m(1')$;	$P8^{8^3}b^{2_{\bar x}}m(1')$
222	$4mm$	2	4^*22^*	$(r_8, 4^*_{\bar z})(m, \varepsilon)(e, 2_{\bar x})(e, 2_{\bar y})$	A	$P8^{4^*}m_am(222)$;	$P8^{4^*}b_am(222)$
	4	$2mm$	$4221'$	$(r_8, 4_{\bar z})(m, \varepsilon')(e, 2_{\bar x})(e, 2_{\bar y})$	A	$P8^4m'_am(222)$;	$P8^4b'_am(222)$

Thus, there are two spin space groups for each two-dimensional octagonal spin point group with $G = 8mm$.

6.5. Spin group tables

The resulting two-dimensional octagonal spin point groups and spin space groups are listed in Table 4 for $G = 8$, and in Table 5 for $G = 8mm$, using the following notation:

Each line in the tables represents one or more spin point group and its associated spin space groups. The spin point groups are given by their generators, listed in the fifth column of each table. The first four columns provide the group theoretic structure of the spin point group by listing the lattice spin group Γ_e, the normal subgroup G_ε of G, paired with Γ_e, the quotient group G/G_ε, and the full group of spin-space rotations Γ, satisfying the requirement that $G/G_\varepsilon \simeq \Gamma/\Gamma_e$. We use stars and daggers to denote optional primes on elements of Γ (*i.e.* the application of time inversion after a spin-space rotation). If two operations in Γ can be independently primed or unprimed, we use a star for the first and a dagger for the

Table 6
Restrictions on the form of $\mathbf{S}(\mathbf{k})$ for any wavevector $\mathbf{k}$ in the magnetic lattice when $\Gamma_e = 2, 2'$ or $1'$.

In each case, the form of $\mathbf{S}(\mathbf{k})$ depends on the parity of $\sum n_i$ where $\mathbf{k} = \sum n_i \mathbf{b}^{(i)}$. Colors refer to the points in Fig. 3.

Γ_e	$\sum n_i$ even Red or black	$\sum n_i$ odd Green or blue
2	$(0, 0, S_z)$	$(S_x, S_y, 0)$
$2'$	$(S_x, S_y, 0)$	$(0, 0, S_z)$
$1'$	$(0, 0, 0)$	(S_x, S_y, S_z)

Table 7
Restrictions on the form of $\mathbf{S}(\mathbf{k})$ for any wavevector $\mathbf{k}$ in the magnetic lattice when $\Gamma_e = 222$ or $22'2'$.

In each case, the form of $\mathbf{S}(\mathbf{k})$ depends on the parities of $n_1 + n_3$ and $n_2 + n_4$, where $\mathbf{k} = \sum n_i \mathbf{b}^{(i)}$. Colors refer to the points in Fig. 3.

Γ_e	$n_1 + n_3$ even $n_2 + n_4$ even Red	$n_1 + n_3$ odd $n_2 + n_4$ odd Black	$n_1 + n_3$ odd $n_2 + n_4$ even Green	$n_1 + n_3$ even $n_2 + n_4$ odd Blue
222	$(0, 0, 0)$	$(0, 0, S_z)$	$(S_x, 0, 0)$	$(0, S_y, 0)$
$22'2'$	$(0, 0, S_z)$	$(0, 0, 0)$	$(0, S_y, 0)$	$(S_x, 0, 0)$

second. For example, the symbol 2*2*2 stands for the two possible groups $\Gamma = 222$ and $2'2'2$, whereas the symbol $4^*2^\dagger 2^{*\dagger}$ stands for four distinct groups, $\Gamma = 422$, $4'22'$, $42'2'$ and $4'2'2$.

To list the spin space groups for each spin point group, we must specify the values of the phase functions for all the spin-point-group generators on the four generating vectors of the lattice. The phase functions Φ_e^γ for generators of the form (e, γ) are already listed in Table 3 and are not repeated in Tables 4 and 5. The phase function $\Phi_{r_8}^\delta$ is zero everywhere owing to the choice of gauge, and is therefore also not listed in Tables 4 and 5. The two possible values of the phase function Φ_m^μ when the point group is $8mm$, which according to equation (34) depend on the value of $\delta\mu\delta$, are listed in the sixth column of Table 5. If $\delta\mu\delta = \mu$, we write $0; \frac{1}{2}$ to indicate that $\Phi_m^\mu(\mathbf{b}^{(i)}) \equiv 0000$ or $\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$. When $\delta\mu\delta \neq \mu$, we write A to indicate that $\Phi_m^\mu(\mathbf{b}^{(i)}) \equiv 0\frac{1}{2}0\frac{1}{2}$ or $\frac{1}{2}0\frac{1}{2}0$, alternating its value from one generating vector to the next.

In the last column of each table, we give a unique symbol for each spin space group, based on the familiar International (Hermann–Mauguin) symbols for the regular (nonmagnetic) space groups. To incorporate all the spin-space-group information, we augment the regular symbol in the following ways: (i) The symbol for the lattice spin group Γ_e is added in parentheses immediately after the regular space-group symbol, unless $\Gamma_e = 1$. (ii) In the case of two-dimensional octagonal spin space groups, the values of the phase functions associated with the elements of Γ_e are unique and therefore need not be listed. In general, one can encode these phase functions by indicating the sublattice L_0 (for which L/L_0 is isomorphic to Γ_e, as described in §4.3) as a subscript of the magnetic lattice symbol P. (iii) To each generator of the point group G, we add a superscript listing an operation from the coset of Γ_e with which it is paired (if that operation is ε, we omit it, if it is ε', we simply add a prime, we use stars and daggers, as described above, to denote multiple groups, and we omit the axis about which rotations are performed if it is the $\bar{z}$ axis). (iv) The value of the phase function Φ_m^μ, when the point group is $8mm$, is encoded by replacing the secondary m by a b (as in the International symbols) when $\Phi_m^\mu(\mathbf{b}^{(i)}) \equiv \frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$, and by adding a subscript a (for alternating) so that m_a indicates that $\Phi_m^\mu(\mathbf{b}^{(i)}) \equiv 0\frac{1}{2}0\frac{1}{2}$ and b_a indicates that $\Phi_m^\mu(\mathbf{b}^{(i)}) \equiv \frac{1}{2}0\frac{1}{2}0$.

6.6. Selection rules due to Γ_e

Operations in G that impose selection rules for neutron diffraction are those that leave some lattice vectors invariant. In two dimensions, these can be the identity e, which leaves all lattice vectors invariant or mirror lines that leave all vectors along them invariant. We first consider the selection rules that arise from operations (e, γ), where $\gamma \in \Gamma_e$, and therefore apply to all lattice vectors, expressed in terms of the four generating vectors as $\mathbf{k} = n_1\mathbf{b}^{(1)} + n_2\mathbf{b}^{(2)} + n_3\mathbf{b}^{(3)} + n_4\mathbf{b}^{(4)}$.

6.6.1. Selection rules for $\Gamma_e = 2, 2', 1'$. If we denote the generator of Γ_e by γ, the phases $\Phi_e^\gamma(\mathbf{b}^{(i)}) \equiv \frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$ in all of these cases. This implies through the eigenvalue relation (21) that

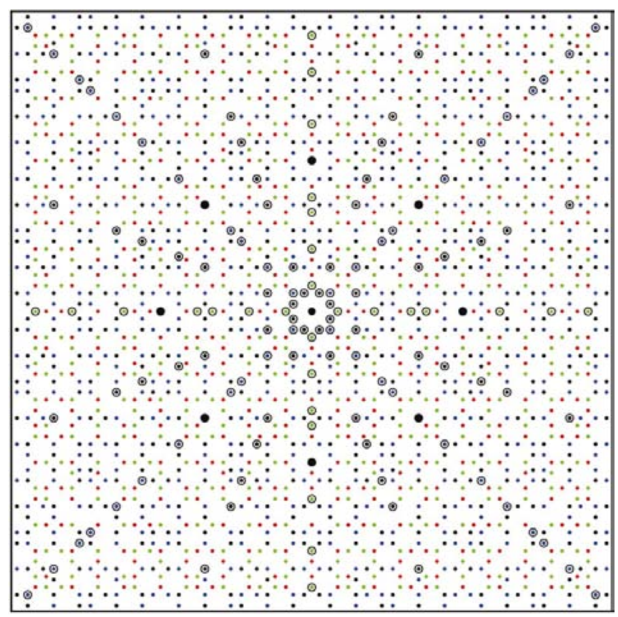

Figure 3
A subset of the wavevectors of the two-dimensional octagonal lattice, exhibiting all possible selection rules. The lattice-generating vectors $\mathbf{b}^{(i)}$ and their negatives, as well as the origin, are denoted by solid black circles. The rest of the points shown are of the form $\mathbf{k} = n_1\mathbf{b}^{(1)} + n_2\mathbf{b}^{(2)} + n_3\mathbf{b}^{(3)} + n_4\mathbf{b}^{(4)}$, with indices running from -6 to 6. Colors encode the parities of the indices of $\mathbf{k}$ at each point as follows. Red: $n_1 + n_3$ and $n_2 + n_4$ both even; black: $n_1 + n_3$ and $n_2 + n_4$ both odd; blue: $n_1 + n_3$ even and $n_2 + n_4$ odd; green: $n_1 + n_3$ odd and $n_2 + n_4$ even. These color codes should be used together with Tables 6 and 7 to determine the selection rules at each wavevector that are due to the lattice spin group Γ_e. Vectors $\mathbf{k}_i = n_i\mathbf{b}^{(i)} + l_i(\mathbf{b}^{(i-1)} + \mathbf{b}^{(i+1)})$ invariant under mirrors m_i with n_i odd, and vectors $\mathbf{k}'_i = n_i(\mathbf{b}^{(i)} + \mathbf{b}^{(i+1)}) + l_i(\mathbf{b}^{(i-1)} + \mathbf{b}^{(i+2)})$ invariant under mirrors m'_i, with $n_i + l_i$ odd, are represented as open circles. These points should be used together with Table 8 in determining the additional selection rules for wavevectors along mirror lines, when the point group is $8mm$.

Table 8
Additional restrictions on the form of $\mathbf{S}(\mathbf{k})$ for special wavevectors that are invariant under mirror reflections when $G = 8mm$.

Note that in most cases the group of spin-space rotations Γ is abelian (except when Γ contains a fourfold or an eightfold rotation, with optional primes), in which case $\delta^{i-1}\mu\delta^{1-i} = \mu$ and $\delta^{i}\mu\delta^{1-i} = \delta\mu$, and the selection rules take a much simpler form. Vectors $\mathbf{k}_i$ along mirrors m_i with n_i odd and vectors $\mathbf{k}'_i$ along mirrors m'_i with $n_i + l_i$ odd are represented as open circles in Fig. 3.

Spin-space-group type	$\mathbf{k}_i = n_i\mathbf{b}^{(i)} + l_i(\mathbf{b}^{(i-1)} + \mathbf{b}^{(i+1)})$ along m_i	$\mathbf{k}'_i = n_i(\mathbf{b}^{(i)} + \mathbf{b}^{(i+1)}) + l_i(\mathbf{b}^{(i-1)} + \mathbf{b}^{(i+2)})$ along m'_i
$P8^{\delta}m^{\mu}m(\Gamma_e)$	$\delta^{i-1}\mu\delta^{1-i}\mathbf{S}(\mathbf{k}_i) = \mathbf{S}(\mathbf{k}_i)$	$\delta^{i}\mu\delta^{1-i}\mathbf{S}(\mathbf{k}'_i) = \mathbf{S}(\mathbf{k}'_i)$
$P8^{\delta}b^{\mu}m(\Gamma_e)$	$\begin{cases}\delta^{i-1}\mu\delta^{1-i}\mathbf{S}(\mathbf{k}_i) = \mathbf{S}(\mathbf{k}_i) & \text{if } n_i \text{ even}\\ \delta^{i-1}\mu\delta^{1-i}\mathbf{S}(\mathbf{k}_i) = -\mathbf{S}(\mathbf{k}_i) & \text{if } n_i \text{ odd}\end{cases}$	$\delta^{i}\mu\delta^{1-i}\mathbf{S}(\mathbf{k}'_i) = \mathbf{S}(\mathbf{k}'_i)$
$P8^{\delta}m_a^{\mu}m(\Gamma_e)$	$\delta^{i-1}\mu\delta^{1-i}\mathbf{S}(\mathbf{k}_i) = \mathbf{S}(\mathbf{k}_i)$	$\begin{cases}\delta^{i}\mu\delta^{1-i}\mathbf{S}(\mathbf{k}'_i) = \mathbf{S}(\mathbf{k}'_i) & \text{if } n_i + l_i \text{ even}\\ \delta^{i}\mu\delta^{1-i}\mathbf{S}(\mathbf{k}'_i) = -\mathbf{S}(\mathbf{k}'_i) & \text{if } n_i + l_i \text{ odd}\end{cases}$
$P8^{\delta}b_a^{\mu}m(\Gamma_e)$	$\begin{cases}\delta^{i-1}\mu\delta^{1-i}\mathbf{S}(\mathbf{k}_i) = \mathbf{S}(\mathbf{k}_i) & \text{if } n_i \text{ even}\\ \delta^{i-1}\mu\delta^{1-i}\mathbf{S}(\mathbf{k}_i) = -\mathbf{S}(\mathbf{k}_i) & \text{if } n_i \text{ odd}\end{cases}$	$\begin{cases}\delta^{i}\mu\delta^{1-i}\mathbf{S}(\mathbf{k}'_i) = \mathbf{S}(\mathbf{k}'_i) & \text{if } n_i + l_i \text{ even}\\ \delta^{i}\mu\delta^{1-i}\mathbf{S}(\mathbf{k}'_i) = -\mathbf{S}(\mathbf{k}'_i) & \text{if } n_i + l_i \text{ odd}\end{cases}$

the form of $\mathbf{S}(\mathbf{k})$ depends on γ and on the parity of $\sum n_i$ as follows:

$$\gamma\mathbf{S}(\mathbf{k}) = e^{-i\pi\sum n_i}\mathbf{S}(\mathbf{k}). \tag{35}$$

Namely, whenever $\sum n_i$ is even the phase in equation (35) vanishes and $\mathbf{S}(\mathbf{k})$ must be invariant under the operation γ; and whenever $\sum n_i$ is odd the phase is $i\pi$ and $\mathbf{S}(\mathbf{k})$ must change its sign under γ. The consequences for the three possible operations γ are summarized in Table 6.

6.6.2. Selection rules for Γ_e = 222, 22′2′. Here Γ_e is generated by $(e, 2^*_{\bar{x}})$ and $(e, 2^*_{\bar{y}})$, with phase functions given by $\Phi_e^{2^*_{\bar{x}}}(\mathbf{b}^{(i)}) \equiv 0\frac{1}{2}0\frac{1}{2}$ and $\Phi_e^{2^*_{\bar{y}}}(\mathbf{b}^{(i)}) \equiv \frac{1}{2}0\frac{1}{2}0$. The eigenvalue relations (21) for the two generators are

$$2^*_{\bar{x}}\mathbf{S}(\mathbf{k}) = e^{-i\pi(n_2+n_4)}\mathbf{S}(\mathbf{k}), \tag{36}$$

$$2^*_{\bar{y}}\mathbf{S}(\mathbf{k}) = e^{-i\pi(n_1+n_3)}\mathbf{S}(\mathbf{k}), \tag{37}$$

so that $\mathbf{S}(\mathbf{k})$ remains invariant (changes its sign) under $2^*_{\bar{x}}$ if $n_2 + n_4$ is even (odd); and remains invariant (changes its sign) under $2^*_{\bar{y}}$ if $n_1 + n_3$ is even (odd). These results are summarized in Table 7 for the two possible Γ_e's.

6.7. Selection rules on mirror lines

In addition to the selection rules arising from Γ_e, there are also selection rules that occur when $\mathbf{k}$ lies on one of the mirror lines and is therefore invariant under reflection through that particular mirror. In this case, the eigenvalue equation (21) imposes further restrictions on the Fourier coefficients of the spin density field.

Vectors lying along the mirror m_i, which leaves the generating vector $\mathbf{b}^{(i)}$ invariant, have the general form

$$\mathbf{k}_i = n_i\mathbf{b}^{(i)} + l_i(\mathbf{b}^{(i-1)} + \mathbf{b}^{(i+1)}), \quad i = 1, 2, 3, 4, \tag{38}$$

where all indices are taken modulo 8, and $\mathbf{b}^{(j)} = -\mathbf{b}^{(j-4)}$ for $j = 5, 6, 7, 8$. Selection rules along m_1, which is the mirror m used to generate the point group (see Fig. 2), are determined by the equation

$$\mu\mathbf{S}(\mathbf{k}_1) = e^{-2i\pi n_1\Phi_m^{\mu}(\mathbf{b}^{(1)})}\mathbf{S}(\mathbf{k}_1), \tag{39}$$

where we have used the fact [equation (34)] that $\Phi_m^{\mu}(\mathbf{b}^{(2)}) - \Phi_m^{\mu}(\mathbf{b}^{(4)}) \equiv 0$. Therefore, the form of $\mathbf{S}(\mathbf{k}_1)$ depends on μ, on the parity of n_1 and on the phase $\Phi_m^{\mu}(\mathbf{b}^{(1)})$ as follows: if n_1 is odd *and* $\Phi_m^{\mu}(\mathbf{b}^{(1)}) \equiv \frac{1}{2}$, then $\mathbf{S}(\mathbf{k}_1)$ must change its sign under μ, otherwise $\mathbf{S}(\mathbf{k}_1)$ must remain invariant under μ.

To obtain the selection rules for vectors lying along the remaining mirrors m_i $(i = 2, 3, 4)$, we use successive applications of the symmetry operation (r, δ) to the result (39) for m_1. Since $m\mathbf{k}_1 = \mathbf{k}_1$, it follows from relation (8), between phase functions of conjugate operations, that

$$\delta^{i-1}\mu\delta^{1-i}\mathbf{S}(\mathbf{k}_i) = e^{-2i\pi n_i\Phi_m^{\mu}(\mathbf{b}^{(1)})}\mathbf{S}(\mathbf{k}_i). \tag{40}$$

Thus, in general, for a vector $\mathbf{k}_i$, given by equation (38) and lying along the mirror m_i, the form of $\mathbf{S}(\mathbf{k}_i)$ must satisfy the following requirement: if n_i is odd *and* $\Phi_m^{\mu}(\mathbf{b}^{(1)}) \equiv \frac{1}{2}$, then $\mathbf{S}(\mathbf{k}_i)$ must change its sign under $\delta^{i-1}\mu\delta^{1-i}$, otherwise $\mathbf{S}(\mathbf{k}_i)$ must remain invariant under $\delta^{i-1}\mu\delta^{1-i}$. Note that $\Phi_m^{\mu}(\mathbf{b}^{(1)}) \equiv 0$ for spin space groups of type $P8^{\delta}m^{\mu}m(\Gamma_e)$ and $P8^{\delta}m_a^{\mu}m(\Gamma_e)$, and that $\Phi_m^{\mu}(\mathbf{b}^{(1)}) \equiv \frac{1}{2}$ for spin space groups of type $P8^{\delta}b^{\mu}m(\Gamma_e)$ and $P8^{\delta}b_a^{\mu}m(\Gamma_e)$. Also note that in most cases Γ is abelian, so $\delta^{i-1}\mu\delta^{1-i} = \mu$ and the selection rules take a much simpler form. These results are summarized in the second column of Table 8.

Vectors lying along the mirror m'_i, which is between the generating vector $\mathbf{b}^{(i)}$ and $\mathbf{b}^{(i+1)}$, have the general form

$$\mathbf{k}'_i = n_i(\mathbf{b}^{(i)} + \mathbf{b}^{(i+1)}) + l_i(\mathbf{b}^{(i-1)} + \mathbf{b}^{(i+2)}), \quad i = 1, 2, 3, 4, \tag{41}$$

again with all indices taken modulo 8, and $\mathbf{b}^{(j)} = -\mathbf{b}^{(j-4)}$ for $j = 5, 6, 7, 8$. Using the group compatibility condition for the relation $m'_1 = r_8 m_1$ (see Fig. 2), in the gauge where $\Phi_{r_8}^{\delta}(\mathbf{k}) \equiv 0$, yields

$$\Phi_{m'_1}^{\delta\mu}(\mathbf{k}'_1) \equiv \Phi_m^{\mu}(\mathbf{k}'_1) \equiv (n_1 + l_1)[\Phi_m^{\mu}(\mathbf{b}^{(1)}) + \Phi_m^{\mu}(\mathbf{b}^{(2)})], \tag{42}$$

where we have used the fact [equation (34)] that $\Phi_m^{\mu}(\mathbf{b}^{(3)}) \equiv \Phi_m^{\mu}(\mathbf{b}^{(1)})$ and $\Phi_m^{\mu}(-\mathbf{b}^{(4)}) \equiv \Phi_m^{\mu}(\mathbf{b}^{(2)})$. Therefore, the selection rules for m'_1 are determined by the equation

$$\delta\mu\mathbf{S}(\mathbf{k}'_1) = e^{-2i\pi(n_1+l_1)[\Phi_m^{\mu}(\mathbf{b}^{(1)})+\Phi_m^{\mu}(\mathbf{b}^{(2)})]}\mathbf{S}(\mathbf{k}'_1), \tag{43}$$

and again, by successive rotations (r, δ), we obtain the selection rules for the remaining mirrors m'_i,

$$\delta^i \mu \delta^{1-i} \mathbf{S}(\mathbf{k}'_i) = e^{-2i\pi(n_i+l_i)[\Phi^\mu_m(\mathbf{b}^{(1)})+\Phi^\mu_m(\mathbf{b}^{(2)})]} \mathbf{S}(\mathbf{k}'_i). \qquad (44)$$

Thus, in general, for a vector $\mathbf{k}'_i$, given by equation (41) and lying along the mirror m'_i, the form of $\mathbf{S}(\mathbf{k}'_i)$ must satisfy the following requirement: if $n_i + l_i$ is odd *and* $\Phi^\mu_m(\mathbf{b}^{(1)}) + \Phi^\mu_m(\mathbf{b}^{(2)}) \equiv \frac{1}{2}$ then $\mathbf{S}(\mathbf{k}'_i)$ must change its sign under $\delta^i \mu \delta^{1-i}$, otherwise $\mathbf{S}(\mathbf{k}'_i)$ must remain invariant under $\delta^i \mu \delta^{1-i}$. Note that $\Phi^\mu_m(\mathbf{b}^{(1)}) + \Phi^\mu_m(\mathbf{b}^{(2)}) \equiv 0$ for spin space groups of type $P8^\delta m^\mu m(\Gamma_e)$ and $P8^\delta b^\mu m(\Gamma_e)$, and that $\Phi^\mu_m(\mathbf{b}^{(1)}) + \Phi^\mu_m(\mathbf{b}^{(2)}) \equiv \frac{1}{2}$ for spin space groups of type $P8^\delta m^\mu_a m(\Gamma_e)$ and $P8^\delta b^\mu_a m(\Gamma_e)$. Also note that in most cases Γ is abelian, so $\delta^i \mu \delta^{1-i} = \delta\mu$, and the selection rules take a much simpler form. These results are summarized in the third column of Table 8.

The authors thank Benji Fisher for his comments on a draft of this manuscript. This research was funded by the Israel Science Foundation through grant No. 278/00.

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