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Symmetry of magnetically ordered three-dimensional octagonal quasicrystals

Shahar Even-Dar Mandel and Ron Lifshitz*

School of Physics and Astronomy, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University, Tel Aviv 69978, Israel. Correspondence e-mail: ronlif@post.tau.ac.il

The theory of magnetic symmetry in quasicrystals, described in a companion paper [Lifshitz & Even-Dar Mandel (2004). *Acta Cryst.* A**60**, 167–178], is used to enumerate all three-dimensional octagonal spin point groups and spin-space-group types and calculate the resulting selection rules for neutron diffraction experiments.

1. Introduction

We enumerate here all three-dimensional octagonal spin groups and calculate their selection rules for neutron scattering, based on the theory developed in a companion paper (Lifshitz & Even-Dar Mandel, 2004) where we have provided the details for the extension to quasicrystals (Lifshitz, 1998) of Litvin & Opechowski's theory of spin groups (Litvin, 1973; Litvin & Opechowski, 1974; Litvin, 1977). We assume the reader is familiar with the companion paper, where we have also given experimental and theoretical motivation for carrying out a systematic enumeration of spin groups for quasicrystals. This is the first complete and rigorous enumeration of spin groups and calculation of selection rules for any three-dimensional quasicrystal. Other than the pedagogical example of two-dimensional octagonal spin groups given in the companion paper, past calculations are scarce. 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 by Lifshitz (1998) along with the selection rules that they impose, but a complete enumeration of icosahedral spin groups was not given. We intend to continue the systematic enumeration of spin groups in future publications by treating all the other common quasiperiodic crystal systems (pentagonal, decagonal, dodecagonal and icosahedral), although we shall not provide complete details of the calculations as we do here.

Although the enumeration in three dimensions is more elaborate, it proceeds along the same lines as the two-dimensional example given in the companion paper (Lifshitz & Even-Dar Mandel, 2004). Familiarity with the calculation of ordinary (nonmagnetic) octagonal space groups (Rabson *et al.*, 1991) may also assist the reader in following the calculations performed here, although knowledge of that calculation is not assumed. We begin in §2 with a description of the two rank-5 octagonal Bravais classes, a reminder of the octagonal point groups in three dimensions (summarized in Table 1), and a summary of the effect of the different point-group operations on the generating vectors of the two lattice types (Table 2). In §3, we enumerate the octagonal spin point groups by noting the restrictions (summarized in Table 3) imposed on their generators owing to the isomorphism between G/G_ε and Γ/Γ_e. We then proceed to calculate the phase functions associated with the generators of the spin point groups by making use of the group compatibility condition

$$\forall (g,\gamma),(h,\eta)\in G_{\mathbf{S}}:\ \ \Phi^{\gamma\eta}_{gh}(\mathbf{k})\equiv\Phi^{\gamma}_{g}(h\mathbf{k})+\Phi^{\eta}_{h}(\mathbf{k}). \qquad (1)$$

We begin this in §4 by calculating the gauge-invariant phase functions $\Phi^{\gamma}_{e}(\mathbf{k})$ associated with the lattice spin group Γ_e. To save space, proofs for some of the results of this section appear in Appendix *A*. We then choose a gauge by a sequence of gauge transformations which we describe in §5. We complete the calculation of the remaining phase functions, separately for each octagonal point group—in §6, we provide detailed calculations for point groups 8 and 8*mm*, and in Appendix *B* for all remaining octagonal point groups. The resulting spin-space-group types for point group 8*mm* are listed, for both types of lattice, in Tables 4 and 5 using a generalized format in which we do not explicitly identify the spin-space operations that are paired with the generators of the point group. The spin-space-group types for the remaining octagonal point groups are listed by point group and lattice type in Tables B-1 to B-16 of Appendix *B*. In §7, we complete the enumeration by making this explicit identification and introduce the notation used for octagonal spin space groups. The actual identification of spin-space operations for point group 8*mm* is given in Tables 6 and 7, and for the remaining octagonal point groups in Appendix *C*. We conclude in §8 by calculating the selection rules for neutron diffraction experiments, imposed by the different octagonal spin space groups, which are summarized in Tables 8–12.[1]

[1] Appendices *A*, *B* and *C* are not included in this publication but are available from the IUCr electronic archives (Reference: PZ5003). Services for accessing these data are described at the back of the journal.

Table 1
Three-dimensional octagonal point groups.

There are seven octagonal point groups (geometric crystal classes) in three dimensions, one of which ($\bar{8}m2$) has two distinct orientations with respect to both types of octagonal lattices, giving the eight octagonal arithmetic crystal classes, listed in the first column. The set of generators for each point group, used throughout the paper, are listed in the second column along with the symbols used to denote the spin-space operations with which they are paired in the spin point groups.

Point group	Generators
8	(r_8, δ)
$\bar{8}$	$(\bar{r}_8, \delta)$
$8mm$	$(r_8, \delta), (m, \mu)$
$\bar{8}m2$	$(\bar{r}_8, \delta), (m, \mu)$
822	$(r_8, \delta), (d, \alpha)$
$\bar{8}2m$	$(\bar{r}_8, \delta), (d, \alpha)$
$8/m$	$(r_8, \delta), (h, \eta)$
$8/mmm$	$(r_8, \delta), (m, \mu), (h, \eta)$

Table 2
Effect of the point-group generators on the lattice-generating vectors.

The horizontal shift $\mathbf{h}$ associated with the staggered stacking vector is defined in equation (2).

	$\mathbf{b}^{(1)}$	$\mathbf{b}^{(2)}$	$\mathbf{b}^{(3)}$	$\mathbf{b}^{(4)}$	$\mathbf{z}$	$\mathbf{z}+\mathbf{h}$
r_8	$\mathbf{b}^{(2)}$	$\mathbf{b}^{(3)}$	$\mathbf{b}^{(4)}$	$-\mathbf{b}^{(1)}$	$\mathbf{z}$	$(\mathbf{z}+\mathbf{h})+\mathbf{b}^{(4)}$
$\bar{r}_8$	$-\mathbf{b}^{(2)}$	$-\mathbf{b}^{(3)}$	$-\mathbf{b}^{(4)}$	$\mathbf{b}^{(1)}$	$-\mathbf{z}$	$-(\mathbf{z}+\mathbf{h})-\mathbf{b}^{(4)}$
m	$\mathbf{b}^{(1)}$	$-\mathbf{b}^{(4)}$	$-\mathbf{b}^{(3)}$	$-\mathbf{b}^{(2)}$	$\mathbf{z}$	$(\mathbf{z}+\mathbf{h})-\mathbf{b}^{(3)}$
d	$\mathbf{b}^{(1)}$	$-\mathbf{b}^{(4)}$	$-\mathbf{b}^{(3)}$	$-\mathbf{b}^{(2)}$	$-\mathbf{z}$	$-(\mathbf{z}+\mathbf{h})+2\mathbf{h}-\mathbf{b}^{(3)}$
h	$\mathbf{b}^{(1)}$	$\mathbf{b}^{(2)}$	$\mathbf{b}^{(3)}$	$\mathbf{b}^{(4)}$	$-\mathbf{z}$	$-(\mathbf{z}+\mathbf{h})+2\mathbf{h}$

2. Background for the enumeration

2.1. Three-dimensional octagonal Bravais classes

Recall that all rank-5 octagonal lattices in three dimensions fall into two Bravais classes (Mermin *et al.*, 1990). Lattices of both types contain a two-dimensional rank-4 *horizontal* sublattice in the plane perpendicular to the unique *vertical* eightfold axis. The horizontal sublattice can be generated by four wavevectors $\mathbf{b}^{(1)}, \ldots, \mathbf{b}^{(4)}$ of equal length, separated by angles of $\pi/4$ (as shown in Fig. 1). Throughout the paper, we denote horizontal generating vectors and their negatives by $\mathbf{b}^{(i)}$, where the index i is taken modulo 8, and $\mathbf{b}^{(i)} = -\mathbf{b}^{(i-4)}$ if $i = 5, 6, 7$ or 8.

If the fifth generating vector $\mathbf{c}$—which must be out of the horizontal plane—is parallel to the eightfold axis, the lattice is called a *vertical lattice* or V lattice (also called a primitive or P lattice). In this case, we write $\mathbf{c} = \mathbf{z}$, to emphasize that it is parallel to the eightfold axis, and call $\mathbf{c}$ a *vertical stacking vector*, since the V lattice can be viewed as a vertical stacking of horizontal planes containing two-dimensional rank-4 octagonal lattices.

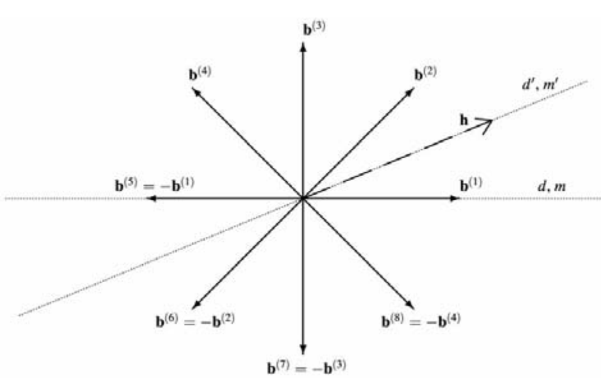

Figure 1
The eightfold star containing the horizontal generating vectors and their negatives $\pm\mathbf{b}^{(1)}, \ldots, \pm\mathbf{b}^{(4)}$ is given by solid arrows. The horizontal shift $\mathbf{h}$ [equation (2)] of the staggered stacking vector is denoted by a dashed arrow. The dotted lines indicate the orientations of the two types of vertical mirrors and dihedral axes, as described in the text.

If the fifth generating vector $\mathbf{c}$ contains both a vertical component $\mathbf{z}$ and a nonzero horizontal component $\mathbf{h}$, then it is called a *staggered stacking vector*, and the lattice is called a *staggered lattice*, or S lattice. One can show (Mermin *et al.*, 1990) that to within a rotation of the lattice, or the addition of a horizontal lattice vector, the horizontal shift can be taken to have the form

$$\mathbf{h} = \tfrac{1}{2}(\mathbf{b}^{(1)} + \mathbf{b}^{(2)} + \mathbf{b}^{(3)} - \mathbf{b}^{(4)}). \qquad (2)$$

As shown in Fig. 1, $\mathbf{h}$ lies halfway between the generating vectors $\mathbf{b}^{(1)}$ and $\mathbf{b}^{(2)}$. Both lattice types are periodic along the vertical axis—with a period of one layer for V lattices and two layers for S lattices.

2.2. Three-dimensional octagonal point groups and their generators

There are seven octagonal point groups (geometric crystal classes) in three dimensions, one of which ($\bar{8}m2$) has two distinct orientations with respect to both types of octagonal lattices, giving rise to the eight octagonal arithmetic crystal classes, listed in the first column of Table 1. The point-group generators, listed in the second column of the table, are an eightfold rotation r_8, an eightfold roto-inversion $\bar{r}_8 = ir_8$ (where i is the three-dimensional inversion), a horizontal mirror h whose invariant plane is perpendicular to the eightfold axis, a vertical mirror m whose invariant plane includes the eightfold axis, and a twofold (dihedral) axis d perpendicular to the eightfold axis. The effects of these point-group operations on the generating vectors of the two lattice types are summarized in Table 2.

As shown in Fig. 1, the invariant planes of the vertical mirrors and the axes of the twofold rotations can be oriented either along (labeled m and d) or between (labeled m' and d') the generating vectors of the octagonal horizontal sublattice and their negatives. The point group $\bar{8}m2$ has four mirrors and four twofold axes. If the mirrors are of type m (along the star vectors) and the dihedral axes are of type d' (between them), it is denoted by $\bar{8}m2$. If the mirrors are of type m' (between the star vectors) and the dihedral axes are of type d (along the star vectors), the point group is denoted by $\bar{8}2m$.

Table 3
Normal subgroups G_ε of the seven octagonal point groups.

The resulting quotient group G/G_ε is represented in the seventh column by a point group isomorphic to it. Isomorphic groups G are listed in the same section of the table. Constraints on the spin-space operations δ, μ, α and η, paired with the generators r_8, m, d and h of G are listed in the last column. In each line, the first power of δ that is in Γ_e is given. μ^2, α^2 and η^2 are always in Γ_e, therefore we only note whether μ, α and η are themselves in Γ_e. If a spin-space operation is in Γ_e, it is taken to be ε.

G	G_ε	G	G_ε	G	G_ε	G/G_ε	Constraints
		8	8	$\bar{8}$	$\bar{8}$	1	$\delta = \varepsilon$
			4		4	2	$\delta^2 \in \Gamma_e$
			2		2	4	$\delta^4 \in \Gamma_e$
			1		1	8	$\delta^8 \in \Gamma_e$
$8mm$	$8mm$	822	822	$\bar{8}m2$	$\bar{8}m2$	1	$\delta = \varepsilon, \mu = \varepsilon$
	8		8		$\bar{8}$	2	$\delta = \varepsilon, \mu \notin \Gamma_e$
	$4mm$		422		$4mm$	2	$\delta^2 \in \Gamma_e, \mu = \varepsilon$
	$4m'm'$		$42'2'$		$42'2'$	2	$\delta = \mu \notin \Gamma_e$
	4		4		4	222	$\delta^2 \in \Gamma_e, \mu \notin \Gamma_e, \delta\Gamma_e \neq \mu\Gamma_e$
	2		2		2	422	$\delta^4 \in \Gamma_e, \mu \notin \Gamma_e, \delta^2\Gamma_e \neq \mu\Gamma_e$
	1		1		1	822	$\delta^8 \in \Gamma_e, \mu \notin \Gamma_e, \delta^4\Gamma_e \neq \mu\Gamma_e$
				$8/m$	$8/m$	1	$\delta = \varepsilon, \eta = \varepsilon$
					8	2	$\delta = \varepsilon, \eta \notin \Gamma_e$
					$\bar{8}$	2	$\delta = \eta \notin \Gamma_e$
					$4/m$	2	$\delta^2 \in \Gamma_e, \eta = \varepsilon$
					4	$2/m$	$\delta^2 \in \Gamma_e, \eta \notin \Gamma_e, \delta \notin \eta\Gamma_e$
					$\bar{4}$	4	$\delta^4 \in \Gamma_e, \eta \in \delta^2\Gamma_e$
					$2/m$	4	$\delta^4 \in \Gamma_e, \eta = \varepsilon$
					2	$4/m$	$\delta^4 \in \Gamma_e, \eta \notin \Gamma_e, \eta \notin \delta^2\Gamma_e$
					m	8	$\delta^8 \in \Gamma_e, \eta = \varepsilon$
					$\bar{1}$	8	$\delta^8 \in \Gamma_e, \eta \in \delta^4\Gamma_e$
					1	$8/m$	$\delta^8 \in \Gamma_e, \eta \notin \Gamma_e, \eta \notin \delta^4\Gamma_e$
				$8/mmm$	$8/mmm$	1	$\delta = \mu = \eta = \varepsilon$
					$8mm$	2	$\delta = \mu = \varepsilon, \eta \notin \Gamma_e$
					822	2	$\delta = \varepsilon, \eta = \mu \notin \Gamma_e$
					$8/m$	2	$\delta = \eta = \varepsilon, \mu \notin \Gamma_e$
					$\bar{8}m2$	2	$\delta = \eta \notin \Gamma_e, \mu = \varepsilon$
					$\bar{8}2m$	2	$\delta = \mu = \eta \notin \Gamma_e$
					$4/mmm$	2	$\delta^2 \in \Gamma_e, \eta = \mu = \varepsilon$
					$4/mm'm'$	2	$\delta = \mu \notin \Gamma_e, \eta = \varepsilon$
					8	222	$\delta = \varepsilon, \eta \notin \Gamma_e, \mu \notin \Gamma_e, \eta \notin \mu\Gamma_e$
					$\bar{8}$	222	$\delta = \eta \notin \Gamma_e, \mu \notin \Gamma_e, \mu \notin \eta\Gamma_e$
					$4mm$	222	$\delta^2 \in \Gamma_e, \mu = \varepsilon, \eta \notin \Gamma_e, \eta \notin \delta\Gamma_e$
					$4m'm'$	222	$\delta = \mu \notin \Gamma_e, \eta \notin \Gamma_e, \eta \notin \mu\Gamma_e$
					422	222	$\delta^2 \in \Gamma_e, \mu = \eta \notin \Gamma_e, \eta \notin \delta\Gamma_e$
					$42'2'$	222	$\delta^2 \in \Gamma_e, \mu \notin \Gamma_e, \eta \notin \Gamma_e, \eta \in \delta\mu\Gamma_e$
					$4/m$	222	$\delta^2 \in \Gamma_e, m \notin \Gamma_e, m \notin \delta\Gamma_e, \eta = \varepsilon$
					4	mmm	$\delta^2 \in \Gamma_e, \mu \notin \Gamma_e, \eta \notin \Gamma_e, \delta\Gamma_e \neq \eta\Gamma_e \neq \mu\Gamma_e$
					$\bar{4}$	422	$\delta^4 \in \Gamma_e, \mu \notin \Gamma_e, \mu \notin \delta\Gamma_e, \eta \in \delta^2\Gamma_e$
					$2/m$	422	$\delta^4 \in \Gamma_e, \mu \notin \Gamma_e, \mu \notin \delta\Gamma_e, \eta = \varepsilon$
					2	$4/mmm$	$\delta^4 \in \Gamma_e, \mu \notin \Gamma_e, \eta \notin \Gamma_e, \delta^2\Gamma_e \neq \eta\Gamma_e \neq \mu\Gamma_e$
					m	822	$\delta^8 \in \Gamma_e, \mu \notin \Gamma_e, \mu \notin \delta^4\Gamma_e, \eta = \varepsilon$
					$\bar{1}$	822	$\delta^8 \in \Gamma_e, \mu \notin \Gamma_e, \mu \notin \delta^4\Gamma_e, \eta \in \delta^4\Gamma_e$
					1	$8/mmm$	$\delta^8 \in \Gamma_e, \mu \notin \Gamma_e, \eta \notin \Gamma_e, \delta^4\Gamma_e \neq \mu\Gamma_e \neq \eta\Gamma_e$

3. Enumeration of spin point groups

As generators of the spin point group $G_{\mathbf{S}}$, we take the generators of the point group G and combine each one with a representative spin-space operation from the coset of Γ_e with which it is paired, as listed in the second column of Table 1. The spin-space operation paired in the spin point group with the eightfold generator r_8 or $\bar{r}_8$ is denoted by δ, the operation paired with the vertical mirror m by μ, the operation paired with the horizontal mirror h by η and the spin-space operation paired with the dihedral rotation d is denoted by α. To these generators, 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).

We begin by listing in Table 3 all the normal subgroups G_ε of the seven octagonal point groups, along with the resulting quotient groups G/G_ε. The constraints on the operations δ, μ, η, and α owing to the isomorphism between G/G_ε and Γ/Γ_e are summarized in the last column of Table 3. The actual identification of these spin-space operations is done at the last step of the enumeration process, as described in §7.

4. Phase functions of Γ_e

We calculate the phase functions $\Phi_e^\gamma(\mathbf{k})$, associated with elements in the lattice spin group Γ_e—keeping in mind that Γ_e is abelian and that no two phase functions $\Phi_e^\gamma(\mathbf{k})$ are identical—by finding the solutions to the constraints imposed on these phase functions by all the other elements $\sigma \in \Gamma$,

$$\forall \gamma \in \Gamma_e, (g, \sigma) \in G_S: \quad \Phi_e^\gamma(\mathbf{k}) \equiv \Phi_e^{\sigma\gamma\sigma^{-1}}(g\mathbf{k}), \tag{3}$$

by applying the group compatibility condition (1) to the relation $geg^{-1} = e$, where g is one of the point-group generators r_8, $\bar{r}_8$, m, h and d. In this way, we also find the possible combinations of Γ and Γ_e that are compatible with a given lattice L and point group G. In all that follows, we write $\Phi_g^\gamma(\mathbf{b}^{(i)}) \equiv abcd$ instead of fully writing $\Phi_g^\gamma(\mathbf{b}^{(1)}) \equiv a$, $\Phi_g^\gamma(\mathbf{b}^{(2)}) \equiv b$, $\Phi_g^\gamma(\mathbf{b}^{(3)}) \equiv c$ and $\Phi_g^\gamma(\mathbf{b}^{(4)}) \equiv d$; we write $\Phi_g^\gamma(\mathbf{b}^{(i)}\mathbf{c}) \equiv abcde$ to indicate in addition that $\Phi_g^\gamma(\mathbf{c}) \equiv e$; and occasionally, if the four phases on the horizontal generating vectors are equal to a, we write $\Phi_g^\gamma(\mathbf{b}^{(i)}) \equiv a$ or $\Phi_g^\gamma(\mathbf{b}^{(i)}\mathbf{c}) \equiv ae$.

Before starting, we note from inspection of Table 3 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 that Γ cannot be cubic. This then implies that, for any possible combination of Γ and Γ_e,

$$\forall \gamma \in \Gamma_e, \delta \in \Gamma: \quad \delta^2\gamma\delta^{-2} = \gamma. \tag{4}$$

This relation, together with equation (3) for $\sigma = \delta^2$, yields the following basic result:

R0. For any $\gamma \in \Gamma_e$, the in-plane phases of Φ_e^γ are

$$\Phi_e^\gamma(\mathbf{b}^{(i)}) \equiv \begin{cases} abab & V \text{ lattice}, \\ aaaa & S \text{ lattice}, \end{cases} \tag{5}$$

where a and b are independently either 0 or 1/2.

Proof

Let g_8 denote the eightfold generator (r_8 or $\bar{r}_8$) and recall that $\delta \in \Gamma$ denotes the operation paired with it in the spin point group. It follows from relation (4) together with equation (3) that

$$\Phi_e^\gamma(\mathbf{b}^{(i)}) \equiv \Phi_e^{\delta^2\gamma\delta^{-2}}(g_8^2\mathbf{b}^{(i)}) \equiv \Phi_e^\gamma(g_8^2\mathbf{b}^{(i)}). \tag{6}$$

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

$$\Phi_e^\gamma(\mathbf{b}^{(1)}) \equiv \Phi_e^\gamma(\mathbf{b}^{(3)}) \equiv a; \quad \Phi_e^\gamma(\mathbf{b}^{(2)}) \equiv \Phi_e^\gamma(\mathbf{b}^{(4)}) \equiv b; \tag{7}$$

and

$$\Phi_e^\gamma(-\mathbf{b}^{(i)}) \equiv \Phi_e^\gamma(\mathbf{b}^{(i)}) \Longrightarrow \Phi_e^\gamma(\mathbf{b}^{(i)}) \equiv 0 \text{ or } \tfrac{1}{2}. \tag{8}$$

The last result (owing to the linearity of the phase function) implies that each of the phases a and b in (7) can be either 0 or 1/2. No further constraints arise from application of (3) to the vertical stacking vector. On the other hand, for the staggered stacking vector, using the fact (Table 2) that $g_8^2(\mathbf{z}+\mathbf{h}) = (\mathbf{z}+\mathbf{h}) + \mathbf{b}^{(4)} - \mathbf{b}^{(1)}$, we obtain

$$\Phi_e^\gamma(\mathbf{z}+\mathbf{h}) \equiv \Phi_e^\gamma(\mathbf{z}+\mathbf{h}) + b - a, \tag{9}$$

implying that $a \equiv b$. □

Note that as a consequence of R0 along with the fact that for twofold operations all phases are either 0 or 1/2, and the fact that no two phase functions Φ_e^γ can be the same—on S lattices there can be no more than three operations of order 2 in Γ_e.

Relation (4) implies that one of three conditions must be satisfied:

1. $\delta\gamma\delta^{-1} = \gamma$, or simply δ and γ commute.
2. $\delta\gamma\delta^{-1} = \gamma^{-1}$, where $\gamma^{-1} \neq \gamma$. This may happen if γ is an n-fold rotation ($n > 2$), possibly followed by time-inversion, and δ is a perpendicular twofold rotation.
3. γ is one of a pair of operations in Γ_e satisfying $\delta\gamma\delta^{-1} = \gamma'$ and $\delta\gamma'\delta^{-1} = \gamma$. This may happen if the two operations are $2_{\bar{x}}$ and $2_{\bar{y}}$, or $2'_{\bar{x}}$ and $2'_{\bar{y}}$, and δ is either a fourfold rotation about the $\bar{z}$ axis or a twofold rotation about the plane diagonal.

We shall use relation (4), and the three possibilities for satisfying it, in order to calculate the constraints imposed on $\Phi_e^\gamma(\mathbf{k})$ by the spin-space operations, paired with the generators of the different octagonal point groups. In the following subsections, we quote the results of these calculations. The proofs can be found in Appendix A.

4.1. Additional constraints imposed by δ (all point groups)

In addition to result R0, we find that

R1. For any $\gamma \in \Gamma_e$, if δ commutes with γ ($\delta\gamma\delta^{-1} = \gamma$) and the eightfold generator is r_8, then the in-plane phases of Φ_e^γ are

$$\Phi_e^\gamma(\mathbf{b}^{(i)}) \equiv \begin{cases} aaaa & V \text{ lattice}, \\ 0000 & S \text{ lattice}, \end{cases} \tag{10}$$

where a is either 0 or 1/2.

If the eightfold generator is $\bar{r}_8$, the in-plane phases of Φ_e^γ are

$$\Phi_e^\gamma(\mathbf{b}^{(i)}) \equiv aaaa \tag{11a}$$

regardless of the lattice type, and the phase on the stacking vector is

$$\Phi_e^\gamma(\mathbf{c}) \equiv \begin{cases} c & V \text{ lattice}, \\ \frac{a}{2} + c & S \text{ lattice}, \end{cases} \tag{11b}$$

where a is the in-plane phase in (11a), $c \equiv 0$ or 1/2, but a and c cannot both be 0. As a consequence, on vertical lattices, γ is an operation of order 2 and, on staggered lattices, γ is of order 2 or 4 depending on whether $a \equiv 0$ or 1/2.

R2. If $\gamma \in \Gamma_e$ is an operation of order $n > 2$, $\delta\gamma\delta^{-1} = \gamma^{-1}$ and the eightfold generator is r_8, then the lattice must be staggered, n must be 4 and the phases of Φ_e^γ are

$$\Phi_e^\gamma(\mathbf{b}^{(i)}) \equiv \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}, \quad \Phi_e^\gamma(\mathbf{z}+\mathbf{h}) \equiv \tfrac{1}{4} \text{ or } \tfrac{3}{4}. \tag{12}$$

If the eightfold generator is $\bar{r}_8$, the in-plane phases of Φ_e^γ are

$$\Phi_e^\gamma(\mathbf{b}^{(i)}) \equiv \begin{cases} aaaa & V \text{ lattice}, \\ 0000 & S \text{ lattice}, \end{cases} \tag{13}$$

where a is either 0 or 1/2.

R3. If $2^*_{\bar{x}}, 2^*_{\bar{y}} \in \Gamma_e$, where the asterisk denotes an optional prime, and $\delta 2^*_{\bar{x}}\delta^{-1} = 2^*_{\bar{y}}$, the directions of the $\bar{x}$ and $\bar{y}$ axes in spin space can be chosen so that the in-plane phases of $\Phi_e^{2^*_{\bar{x}}}$ and $\Phi_e^{2^*_{\bar{y}}}$ are

$$\begin{cases} \Phi_e^{2_{\bar{x}}^*}(\mathbf{b}^{(i)}) \equiv 0\tfrac{1}{2}0\tfrac{1}{2},\ \ \Phi_e^{2_{\bar{y}}^*}(\mathbf{b}^{(i)}) \equiv \tfrac{1}{2}0\tfrac{1}{2}0 & V \text{ lattice}, \\ \Phi_e^{2_{\bar{x}}^*}(\mathbf{b}^{(i)}) \equiv \Phi_e^{2_{\bar{y}}^*}(\mathbf{b}^{(i)}) \equiv \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2} & S \text{ lattice}, \end{cases} \tag{14a}$$

and the phases on the stacking vector are

$$\begin{cases} \Phi_e^{2_{\bar{x}}^*}(\mathbf{z}) \equiv \Phi_e^{2_{\bar{y}}^*}(\mathbf{z}) \equiv 0 \text{ or } \tfrac{1}{2} & V \text{ lattice}, \\ \Phi_e^{2_{\bar{x}}^*}(\mathbf{z}+\mathbf{h}) \equiv 0,\ \ \Phi_e^{2_{\bar{y}}^*}(\mathbf{z}+\mathbf{h}) \equiv \tfrac{1}{2} & S \text{ lattice}. \end{cases} \tag{14b}$$

4.2. Constraints imposed by μ (point groups $8mm$, $\bar{8}m2$ and $8/mmm$)

M1. For any $\gamma \in \Gamma_e$, if μ commutes with γ, the in-plane phases of Φ_e^γ are

$$\Phi_e^\gamma(\mathbf{b}^{(i)}) \equiv \begin{cases} abab & V \text{ lattice}, \\ 0000 & S \text{ lattice}, \end{cases} \tag{15}$$

where a and b are independently either 0 or 1/2.

M2. If $\gamma \in \Gamma_e$ is an operation of order $n > 2$ and $\mu\gamma\mu^{-1} = \gamma^{-1}$, then the lattice must be staggered, n must be 4 and the phases of Φ_e^γ are

$$\Phi_e^\gamma(\mathbf{b}^{(i)}) \equiv \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}, \quad \Phi_e^\gamma(\mathbf{z}+\mathbf{h}) \equiv \tfrac{1}{4} \text{ or } \tfrac{3}{4}. \tag{16}$$

M3. If $2_{\bar{x}}^*, 2_{\bar{y}}^* \in \Gamma_e$, where the asterisk denotes an optional prime, $\mu 2_{\bar{x}}^* \mu^{-1} = 2_{\bar{y}}^*$ and the mirror is of type m, then the lattice must be staggered, the in-plane phases of $\Phi_e^{2_{\bar{x}}^*}$ and $\Phi_e^{2_{\bar{y}}^*}$ are

$$\Phi_e^{2_{\bar{x}}^*}(\mathbf{b}^{(i)}) \equiv \Phi_e^{2_{\bar{y}}^*}(\mathbf{b}^{(i)}) \equiv \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}, \tag{17a}$$

and the directions of the $\bar{x}$ and $\bar{y}$ axes in spin space can be chosen so that the phases on the staggered stacking vector are

$$\Phi_e^{2_{\bar{x}}^*}(\mathbf{z}+\mathbf{h}) \equiv 0,\ \ \Phi_e^{2_{\bar{y}}^*}(\mathbf{z}+\mathbf{h}) \equiv \tfrac{1}{2}. \tag{17b}$$

4.3. Constraints imposed by α (point groups 822 and $\bar{8}2m$)

D1. For any $\gamma \in \Gamma_e$, if α commutes with γ, the in-plane phases are the general ones given in result R0 [equation (5)]. If the lattice is vertical, the phase of $\Phi_e^\gamma(\mathbf{z})$ is independently 0 or 1/2, implying that γ is an operation of order 2. If the lattice is staggered, the phase on the stacking vector is

$$\Phi_e^\gamma(\mathbf{z}+\mathbf{h}) \equiv \tfrac{a}{2} + c, \tag{18}$$

where a is the in-plane phase in (5) and $c \equiv 0$ or 1/2 but a and c cannot both be 0. Consequently, γ is an operation of order 2 or 4, depending on whether $a \equiv 0$ or 1/2.

D2. If $\gamma \in \Gamma_e$ is an operation of order $n > 2$, $\alpha\gamma\alpha^{-1} = \gamma^{-1}$ and the lattice is vertical, there are no additional constraints on the phase function Φ_e^γ. If the lattice is staggered, then the in-plane phases of Φ_e^γ are all 0.

D3. If $2_{\bar{x}}^*, 2_{\bar{y}}^* \in \Gamma_e$, where the asterisk denotes an optional prime, and $\alpha 2_{\bar{x}}^* \alpha^{-1} = 2_{\bar{y}}^*$, then the lattice must be staggered, the in-plane phases of $\Phi_e^{2_{\bar{x}}^*}$ and $\Phi_e^{2_{\bar{y}}^*}$ are

$$\Phi_e^{2_{\bar{x}}^*}(\mathbf{b}^{(i)}) \equiv \Phi_e^{2_{\bar{y}}^*}(\mathbf{b}^{(i)}) \equiv \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}, \tag{19}$$

and the directions of the $\bar{x}$ and $\bar{y}$ axes in spin space can be chosen so that the phases on the staggered stacking vector are

$$\Phi_e^{2_{\bar{x}}^*}(\mathbf{c}) \equiv 0,\ \ \Phi_e^{2_{\bar{y}}^*}(\mathbf{c}) \equiv \tfrac{1}{2}. \tag{20}$$

4.4. Constraints imposed by η (point groups $8/m$ and $8/mmm$)

H1. For any $\gamma \in \Gamma_e$, if η commutes with γ, then the phase of Φ_e^γ on the stacking vector is

$$\Phi_e^\gamma(\mathbf{c}) \equiv 0 \text{ or } \tfrac{1}{2}, \tag{21}$$

which implies that γ is an operation of order 2.

H2. If $\gamma \in \Gamma_e$ is an operation of order $n > 2$ and $\eta\gamma\eta^{-1} = \gamma^{-1}$, there are no additional constraints on the phase function Φ_e^γ.

H3. If $2_{\bar{x}}^*, 2_{\bar{y}}^* \in \Gamma_e$, where the asterisk denotes an optional prime, then they must both commute with η and their phase functions are only constrained by results R0 and H1.

4.5. Enumeration of lattice spin groups Γ_e

We shall now use the results of the previous sections to enumerate the lattice spin groups and calculate their phase functions. We also introduce a notation—to be used in the final spin-space-group symbol—that encodes the values of these phase functions. In this notation, the symbol of the lattice spin group Γ_e is added as a superscript over the lattice symbol (unless Γ_e is 1 or $1'$). In addition, for each spin-space operation γ in the symbol for Γ_e (with one exception when these operations are $2_{\bar{x}}^*$ and $2_{\bar{y}}^*$, as noted below), we add a subscript to the lattice symbol describing the sublattice L_γ, defined by all wavevectors $\mathbf{k}$ for which $\Phi_e^\gamma(\mathbf{k}) \equiv 0$, with an additional index whenever this sublattice does not uniquely describe the phase function. The results of this section are summarized in the left-hand sides of Tables 8–11 and in the headings of Table 12.

There are a few cases in which the zeros of the phase functions, associated with the operations $2_{\bar{x}}^*$ and $2_{\bar{y}}^*$, define a pair of rank-5 *tetragonal* sublattices related by an eightfold rotation. Each wavevector in these tetragonal sublattices can be decomposed into the sum of two vectors, one belonging to a three-dimensional rank-3 tetragonal lattice of type P or I, and the second belonging to a two-dimensional rank-2 square lattice. If the squares of the rank-2 lattice are aligned along the same directions as the squares of the rank-3 lattice, then we denote the combined rank-5 lattice by $P + p$ or $I + p$; if they are aligned along the diagonals of the rank-3 lattice, we denote the combined rank-5 lattice by $P \times p$ (a lattice that does not occur here) or $I \times p$. This is somewhat of an *ad hoc* notation for some of the rank-5 tetragonal lattices as compared, for example, with the notation used by Lifshitz & Mermin (1994) in their enumeration of the analogous hexagonal and trigonal lattices of arbitrary finite rank. Nevertheless, it is more compact and sufficient for our current purpose. Since the pair of sublattices, associated with the operations $2_{\bar{x}}^*$ and $2_{\bar{y}}^*$, are identical (to within an eightfold rotation), and the different assignments of the two sublattices to the two operations are scale equivalent, we denote their symbol only once.

4.5.1. $\Gamma_e = 1$. The trivial lattice spin group is always possible. In this case, every operation in G is paired with a single operation in Γ. The lattice symbol remains the same as for nonmagnetic space groups: P for vertical lattices and S for staggered lattices.

4.5.2. $\Gamma_e = 2, 2', 1'$. Let γ denote the single generator ($2, 2'$ or ε') of Γ_e. Since γ commutes with all elements of Γ, we can infer the possible values of the phase function Φ_e^γ from results R1, M1, D1 and H1. We find that for all point groups G

$$\Phi_e^\gamma(\mathbf{b}^{(i)}\mathbf{c}) \equiv \begin{cases} 0\tfrac{1}{2};\ \tfrac{1}{2}0;\ \text{ or } \tfrac{1}{2}\tfrac{1}{2} & V \text{ lattice,} \\ 0\tfrac{1}{2} & S \text{ lattice.} \end{cases} \qquad (22)$$

Because γ is an operation of order 2, the zeros of its phase function define a sublattice of index 2 in L. Let us express an arbitrary wavevector in L as $\mathbf{k} = \sum_{i=1}^4 n_i\mathbf{b}^{(i)} + l\mathbf{c}$. The zeros of the first solution $\Phi_e^\gamma(\mathbf{b}^{(i)}\mathbf{c}) \equiv 0\frac{1}{2}$ define a vertical octagonal sublattice, containing all wavevectors with even l, or simply all the even layers of L, whether L is a V lattice or an S lattice. This solution is denoted on the two lattice types by P_{2c}^γ and S_P^γ, respectively. The second solution $\Phi_e^\gamma(\mathbf{b}^{(i)}\mathbf{c}) \equiv \frac{1}{2}0$ on the V lattice defines a vertical octagonal sublattice, containing all vectors with even $\sum_i n_i$ and is denoted by P_P^γ. The third solution $\Phi_e^\gamma(\mathbf{b}^{(i)}\mathbf{c}) \equiv \frac{1}{2}\frac{1}{2}$ on the V lattice defines a staggered octagonal sublattice, containing all vectors with even $\sum_i n_i + l$, and is denoted by P_S^γ. If $\gamma = \varepsilon'$, it is omitted from the symbols, yielding the same symbols used for the so-called magnetic (or black-and-white) space groups (Lifshitz, 1997). The possible phase functions for $\Gamma_e = 2, 2', 1'$ are summarized in the left-hand side of Table 8.

4.5.3. $\Gamma_e = 21'$. Here, Γ_e contains three operations of order 2 that commute with all the elements of Γ. For V lattices, there are $3! = 6$ distinct ways of assigning the three different solutions (22) to the three phase functions of these operations. These are denoted by $P_{2c,P}^{21'}$, $P_{P,S}^{21'}$, $P_{S,2c}^{21'}$, $P_{P,2c}^{21'}$, $P_{S,P}^{21'}$ and $P_{2c,S}^{21'}$, where the first subscript denotes the sublattice defined by the phase function Φ_e^2 and the second subscript denotes that of $\Phi_e^{\varepsilon'}$. These solutions are summarized in the left-hand side of Table 9.

For S lattices, Γ_e cannot be $21'$ because there is only one solution in (22), and therefore there can be only one operation in Γ_e that commutes with all elements of Γ.

4.5.4. $\Gamma_e = 222, 2'2'2$. We generate Γ_e by $2_{\bar{x}}^*$ ($2_{\bar{x}}$ or $2_{\bar{x}}'$) and $2_{\bar{y}}^*$ ($2_{\bar{y}}$ or $2_{\bar{y}}'$), noting that in the case of $\Gamma_e = 2'2'2$ the unprimed twofold rotation defines the direction of the $\bar{z}$ axis in spin space. For vertical lattices, we see from results M3, D3 and H3 that the operations μ, α and η, paired with m, d and h if they are in the point group, must all commute with $2_{\bar{x}}^*$ and $2_{\bar{y}}^*$. It only remains to check whether δ, paired with the eightfold generator, commutes with the generators of Γ_e.

If δ commutes with $2_{\bar{x}}^*$ and $2_{\bar{y}}^*$, then again, as in the previous section, we have three operations in Γ_e that commute with all the elements of Γ, implying that Γ is orthorhombic and not tetragonal. The difference between this case and that of the previous section is that here different solutions can be related by scale transformations that reorient the directions of the spin-space axes. For $\Gamma_e = 222$, all three operations are equivalent so we can define the directions of the spin-space axes such that

$$\Phi_e^{2_{\bar{x}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv 0\tfrac{1}{2}, \quad \Phi_e^{2_{\bar{y}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}0, \quad \Phi_e^{2_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}\tfrac{1}{2} \qquad (23)$$

and denote the lattice spin group and its associated phase functions by $P_{2c,P,S}^{222}$. Any permutation of the three subscripts in the symbol yields an alternative setting for the same scale-equivalence class of solutions.

For $\Gamma_e = 2'2'2$, only the two primed rotations are equivalent, so we have three distinct solutions, where we choose the directions of the $\bar{x}$ and $\bar{y}$ axes in spin space such that the phase function associated with $2_{\bar{y}}'$ is $1/2$ on the horizontal generating vectors. These solutions are

$$\begin{aligned} &1.\quad \Phi_e^{2_{\bar{x}}'}(\mathbf{b}^{(i)}\mathbf{c}) \equiv 0\tfrac{1}{2}, \quad \Phi_e^{2_{\bar{y}}'}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}0, \quad \Phi_e^{2_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}\tfrac{1}{2}; \\ &2.\quad \Phi_e^{2_{\bar{x}}'}(\mathbf{b}^{(i)}\mathbf{c}) \equiv 0\tfrac{1}{2}, \quad \Phi_e^{2_{\bar{y}}'}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}\tfrac{1}{2}, \quad \Phi_e^{2_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}0; \\ &3.\quad \Phi_e^{2_{\bar{x}}'}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}0, \quad \Phi_e^{2_{\bar{y}}'}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}\tfrac{1}{2}, \quad \Phi_e^{2_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv 0\tfrac{1}{2}. \end{aligned} \qquad (24)$$

These three solutions are denoted by $P_{2c,P,S}^{2'2'2}$, $P_{2c,S,P}^{2'2'2}$ and $P_{P,S,2c}^{2'2'2}$, respectively. Their scale-equivalent forms are obtained by exchanging the first two subscripts: $P_{P,2c,S}^{2'2'2}$, $P_{S,2c,P}^{2'2'2}$ and $P_{S,P,2c}^{2'2'2}$.

If δ is a fourfold rotation or a twofold diagonal rotation (requiring Γ to be tetragonal) such that $\delta 2_{\bar{x}}^*\delta^{-1} = 2_{\bar{y}}^*$, then according to result R3 there are two solutions for the phase functions:

$$\Phi_e^{2_{\bar{x}}^*}(\mathbf{b}^{(i)}\mathbf{c}) \equiv 0\tfrac{1}{2}0\tfrac{1}{2}c, \quad \Phi_e^{2_{\bar{y}}^*}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}0\tfrac{1}{2}0c, \quad c \equiv 0 \text{ or } \tfrac{1}{2}. \qquad (25)$$

These are interesting solutions in which the horizontal planes of the sublattices, defined by the zeros of the phase functions associated with the operations $2_{\bar{x}}^*$ and $2_{\bar{y}}^*$, contain all vectors $\mathbf{k} = \sum_{i=1}^4 n_i\mathbf{b}^{(i)} + l\mathbf{c}$ from L with even $n_2 + n_4$ and even $n_1 + n_3$, respectively, with both parities being odd if $c \equiv 1/2$ whenever l is also odd. Consequently, the two sublattices are not octagonal but rather a pair of tetragonal lattices of rank 5, related to each other by an eightfold rotation. As described in the introduction to this section, we denote the lattice spin groups in this case by $P_{P+p,P}^{2^*2^*2}$ ($c \equiv 0$) and $P_{I+p,P}^{2^*2^*2}$ ($c \equiv 1/2$). Note that in both cases the sublattice defined by the zeros of the phase function of $2_{\bar{z}}$ is an octagonal V lattice with a thinned-out horizontal plane.

All these solutions on the V lattice are valid for all octagonal point groups because other generators of Γ, if they exist, impose no further restrictions on the phase functions above.

On staggered lattices (from results R1, M1 and D1), only a single twofold operation can commute with δ, μ or α which are paired with the eightfold generator, the mirror m and the dihedral rotation d, respectively. These operations therefore necessarily exchange the two generators of Γ_e, requiring Γ to be tetragonal. On the other hand (from result H3), η which is paired with h necessarily commutes with the two generators of Γ_e. If these conditions are satisfied then for all point groups the directions of the $\bar{x}$ and $\bar{y}$ axes in spin space can be chosen so that there is a single solution for the phase functions,

$$\Phi_e^{2^*_{\bar{x}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}0, \quad \Phi_e^{2^*_{\bar{y}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}\tfrac{1}{2}. \tag{26}$$

The sublattices defined by the zeros of these two phase functions are rank-5 tetragonal lattices of type $I \times p$. One has the rank-3 I lattice oriented in the directions of the x and y axes and the other has the rank-3 I lattice oriented along the diagonal directions. The sublattice defined by the zeros of the phase function of $2_{\bar{z}}$ is an octagonal V lattice. The lattice spin group is therefore denoted by $S^{2^*2^*2}_{I\times p,P}$.

The possible phase functions for $\Gamma_e = 222, 2'2'2$ are summarized in the left-hand side of Table 10.

4.5.5. $\Gamma_e = 2'2'2' = 2221'$. We choose to generate Γ_e using the three primed rotations and note that, since Γ_e has three twofold operations ($2_{\bar{z}}$, $2'_{\bar{z}}$ and ε') that commute with all elements of Γ, the lattice must be vertical. Furthermore, since there can be no more than three operations that commute with δ, all other twofold operations in $\Gamma_e = 2'2'2'$, including the two generators $2'_{\bar{x}}$ and $2'_{\bar{y}}$, cannot commute with δ (requiring Γ to be tetragonal). The operations μ, η and α must commute with all operations in Γ_e.

If all these conditions are satisfied, then the phase functions for $2'_{\bar{x}}$ and $2'_{\bar{y}}$ have the same two solutions given in equation (25) for $\Gamma_e = 2'2'2$. In both of these solutions, $\Phi_e^{2_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}0$. This leaves two possibilities for the phase function of the third generator of Γ_e,

$$\Phi_e^{2'_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv 0\tfrac{1}{2} \text{ or } \tfrac{1}{2}\tfrac{1}{2}, \tag{27}$$

giving a total of four distinct solutions for the phase functions of $\Gamma_e = 2'2'2'$ on the V lattice, denoted by $P^{2'2'2'}_{P+p,2c}$, $P^{2'2'2'}_{P+p,S}$, $P^{2'2'2'}_{I+p,2c}$ and $P^{2'2'2'}_{I+p,S}$ (and none on the S lattice). These solutions are summarized in the left-hand side of Table 11.

4.5.6. $\Gamma_e = n, n', n1'$ ($n > 2$). These lattice spin groups contain a single generator γ of order $N > 2$, where $N = n$ unless $\Gamma_e = n'$ and n is odd, in which case $N = 2n$. Note that if n is odd then $n1'$ need not be considered because it is the same as n'. For operations of order N, it follows from the group compatibility condition (1) that

$$\Phi_e^{\gamma^N}(\mathbf{k}) \equiv N\Phi_e^{\gamma}(\mathbf{k}) \equiv 0 \Longrightarrow \Phi_e^{\gamma}(\mathbf{k}) \equiv \tfrac{j}{n}, \quad j = 0, 1, \ldots, N-1. \tag{28}$$

For vertical lattices, we find from result R2 that, if the eightfold generator is r_8, then δ, paired with it, must commute with γ and, if it is $\bar{r}_8$, then δ must be a perpendicular twofold rotation taking γ to γ^{-1}. Furthermore, we find from results M2, D2 and H2 that μ (paired with m) must commute with γ, and α and η (paired with d and h) must both be perpendicular twofold rotations. If these conditions are satisfied whenever these operations are in the point group, then

$$\Phi_e^{\gamma}(\mathbf{b}^{(i)}) \equiv \begin{cases} aaaa & N \text{ even}, \\ 0000 & N \text{ odd}, \end{cases} \tag{29}$$

where a is either 0 or 1/2. The only constraint on the phase $\Phi_e^{\gamma}(\mathbf{z})$ comes from the requirement that γ is an operation of order N. If the in-plane phases are 0 then $\Phi_e^{\gamma}(\mathbf{z}) \equiv j/N$, where j and N must be co-prime, otherwise the true denominator is smaller than N, and consequently the order of γ is smaller than N. If the in-plane phase $a \equiv 1/2$ and N is twice an even number, then j and N must still be co-prime, but if N is twice an odd number then j may also be even and γ would still be an operation of order N. This is so because, even though the phase of $\gamma^{N/2}$ is zero on the stacking vector, it is 1/2 on the horizontal generating vector and therefore $\gamma^{N/2} \neq \varepsilon$.

To summarize, for $\Gamma_e = n$ (odd or even n) or $\Gamma_e = n', n1'$ (even n), the possible solutions for the phase function $\Phi_e^{n^*_{\bar{z}}}$ are

$$\Phi_e^{n^*_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \begin{cases} 0\tfrac{j}{n} & n \text{ odd}, \\ 0\tfrac{j}{n}; \tfrac{1}{2}\tfrac{j}{n} & n \text{ twice even}, \\ 0\tfrac{j}{n}; \tfrac{1}{2}\tfrac{j}{n}; \tfrac{1}{2}\tfrac{2j}{n} & n \text{ twice odd}, \end{cases} \tag{30}$$

where in all cases j and n are co-prime. The first subscript in the symbols for the three distinct solutions for $\Phi_e^{n^*_{\bar{z}}}$ are n_jc for $\Phi_e^{n^*_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv 0\tfrac{j}{n}$, n_jS for $\Phi_e^{n^*_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}\tfrac{j}{n}$ and $(\tfrac{n}{2})_jP$ for $\Phi_e^{n^*_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}\tfrac{2j}{n}$. The index j is necessary here because the sublattices defined by the zeros of these phase functions do not depend on j, and therefore it must be specified in addition to specifying the sublattice symbol.

For $\Gamma_e = n'$ with odd n, the order of the generator is $2n$ and the possible solutions are

$$\Phi_e^{n'_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv 0\tfrac{j}{2n}; \tfrac{1}{2}\tfrac{j}{2n}; \tfrac{1}{2}\tfrac{j}{n} \quad n \text{ odd}, \tag{31}$$

where j and $2n$ are co-prime. The symbols for these three types of lattice spin group are $P^{n'}_{(2n)_jc}$, $P^{n'}_{(2n)_jS}$ and $P^{n'}_{n_jP}$. Finally, for $\Gamma_e = n1'$ (n necessarily even), we need to find the possible solutions for the phase function associated with the second generator ε'. Since the phase function $\Phi_e^{2_{\bar{z}}}$ is determined by the phase function $\Phi_e^{n_{\bar{z}}}$, we are left with only two possible solutions for the phase function $\Phi_e^{\varepsilon'}$. If n is twice even then we always have

$$\Phi_e^{\varepsilon'}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}0 \text{ or } \tfrac{1}{2}\tfrac{1}{2}, \tag{32}$$

thus obtaining a total of four solutions denoted $P^{n1'}_{n_jc,P}$, $P^{n1'}_{n_jc,S}$, $P^{n1'}_{n_jS,P}$ and $P^{n1'}_{n_jS,S}$. If n is twice odd then the possible solutions depend on $\Phi_e^{n_{\bar{z}}}$ as follows:

$$\Phi_e^{\varepsilon'}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \begin{cases} \tfrac{1}{2}0 \text{ or } \tfrac{1}{2}\tfrac{1}{2} & \Phi_e^{n^*_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv 0\tfrac{j}{n}, \\ 0\tfrac{1}{2} \text{ or } \tfrac{1}{2}0 & \Phi_e^{n^*_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}\tfrac{j}{n}, \\ \tfrac{1}{2}\tfrac{1}{2} \text{ or } 0\tfrac{1}{2} & \Phi_e^{n^*_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}\tfrac{2j}{n}, \end{cases} \tag{33}$$

giving a total of six solutions denoted by $P^{n1'}_{n_jc,P}$, $P^{n1'}_{n_jc,S}$, $P^{n1'}_{n_jS,2c}$, $P^{n1'}_{n_jS,P}$, $P^{n1'}_{(n/2)_jP,S}$ and $P^{n1'}_{(n/2)_jP,2c}$.

On staggered lattices, we first note that Γ_e cannot be $n1'$ which contains three operations of order 2 that commute with all the elements of Γ. Furthermore, we find from the results of the previous sections that η (paired with h if it is in G) must be a twofold rotation perpendicular to the axis of γ and that two possibilities exist for the remaining generators of Γ:

(i) If the eightfold generator is r_8, then δ, paired with it, must commute with γ and, if it is $\bar{r}_8$, then δ must be a perpendicular twofold rotation taking γ to γ^{-1}. The operation μ (paired with m) must commute with γ and α (paired with d) must be a perpendicular twofold rotation. If these conditions are satisfied whenever these operations are in G, then the in-plane phases are all 0. For $\Gamma_e = n$ (either parity) and $\Gamma_e = n'$ (even n), the possible solutions for the phase function $\Phi_e^{n_{\hat z}^*}$ are therefore

$$\Phi_e^{n_{\hat z}^*}(\mathbf{b}^{(i)}\mathbf{c}) \equiv 0\,\tfrac{j}{n}, \tag{34}$$

where j and n are co-prime. These are denoted by $S_{n_j c}^{n^*}$. For $\Gamma_e = n'$ with odd n, the order of the generator is $2n$ and the possible solutions are

$$\Phi_e^{n'_{\hat z}}(\mathbf{b}^{(i)}\mathbf{c}) \equiv 0\,\tfrac{j}{2n}, \tag{35}$$

where j and $2n$ are co-prime. These are denoted by $S_{(2n)_j c}^{n'}$.

(ii) If the eightfold generator is $\bar r_8$ then δ, paired with it, must commute with γ and, if it is r_8, then δ must be a perpendicular twofold rotation taking γ to γ^{-1}. The operation α (paired with d) must commute with γ and μ (paired with m) must be a perpendicular twofold rotation. If these conditions are satisfied whenever these operations are in G, then $n = 4$ and the possible solutions for the phase function $\Phi_e^{4_{\hat z}^*}$ are

$$\Phi_e^{4_{\hat z}^*}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \tfrac{1}{2}\tfrac{1}{4} \text{ or } \tfrac{1}{2}\tfrac{3}{4}, \tag{36}$$

denoted by $S_{4_1 S}^{4^*}$ and $S_{4_3 S}^{4^*}$

The possible phase functions for $\Gamma_e = n, n', n1'$ ($n > 2$) are summarized in the headings of Table 12.

5. Initial choice of gauge

Before starting the actual calculation of phase functions for the generators of the different octagonal point groups, we make an initial choice of gauge that (i) sets the phases $\Phi_{g_8}^{\delta}(\mathbf{b}^{(i)})$ to zero, where g_8 is the eightfold generator—r_8 for point groups 8, $8mm$, 822, $8/m$ and $8/mmm$, or $\bar r_8$ for $\bar 8$, $\bar 8m2$ and $\bar 82m$; and (ii) sets the phase $\Phi_g^{\sigma}(\mathbf{c})$ to zero for one generator satisfying $g\mathbf{z} = -\mathbf{z}$.

5.1. Setting $\Phi_{g_8}^{\delta}(\mathbf{b}^{(i)})$ to zero

We can make $\Phi_{g_8}^{\delta}(\mathbf{b}^{(i)}) \equiv 0$ with a gauge transformation given by

$$\chi_1(\mathbf{b}^{(i)}) \equiv \tfrac{1}{2}\Phi_{g_8}^{\delta}(\mathbf{b}^{(i)} \pm \mathbf{b}^{(i+1)} + \mathbf{b}^{(i+2)} \pm \mathbf{b}^{(i+3)}), \tag{37}$$

where the upper signs are for $g_8 = r_8$ and the lower signs for $g_8 = \bar r_8$, and the value of $\chi_1(\mathbf{c})$ is unimportant. Using this gauge function, we obtain

$$\begin{aligned}\Delta\Phi_{g_8}^{\delta}(\mathbf{b}^{(i)}) &\equiv \chi_1(g_8\mathbf{b}^{(i)} - \mathbf{b}^{(i)})\\ &\equiv \chi_1(\pm\mathbf{b}^{(i+1)} - \mathbf{b}^{(i)})\\ &\equiv \tfrac{1}{2}\Phi_{g_8}^{\delta}(\mathbf{b}^{(i+4)} - \mathbf{b}^{(i)})\\ &\equiv -\Phi_{g_8}^{\delta}(\mathbf{b}^{(i)}),\end{aligned} \tag{38}$$

thereby setting $\Phi_{g_8}^{\delta}(\mathbf{b}^{(i)})$ to zero.

5.2. Setting $\Phi_g^{\sigma}(\mathbf{c})$ to zero when $g\mathbf{z} = -\mathbf{z}$

We apply a second gauge transformation to set $\Phi_g^{\sigma}(\mathbf{c})$ to zero for a single $g \in G$ for which $g\mathbf{z} = -\mathbf{z}$. We use this transformation for the operation $\bar r_8$ when G is $\bar 8$, $\bar 82m$ or $\bar 8m2$, and for the operations d when G is 822 and h when G is $8/m$ or $8/mmm$. For both lattice types, we take

$$\chi_2(\mathbf{b}^{(i)}) \equiv 0, \quad \chi_2(\mathbf{c}) = \tfrac{1}{2}\Phi_g^{\sigma}(\mathbf{c}), \tag{39}$$

from which we get, for vertical lattices,

$$\Delta\Phi_g^{\sigma}(\mathbf{z}) \equiv \chi_2(g\mathbf{z} - \mathbf{z}) \equiv \chi_2(-2\mathbf{z}) \equiv -\Phi_g^{\sigma}(\mathbf{z}) \tag{40}$$

and for staggered lattices

$$\begin{aligned}\Delta\Phi_g^{\sigma}(\mathbf{z}+\mathbf{h}) &\equiv \chi_2(g(\mathbf{z}+\mathbf{h}) - (\mathbf{z}+\mathbf{h}))\\ &\equiv \chi_2((-2(\mathbf{z}+\mathbf{h}) + (g\mathbf{h}+\mathbf{h}))\\ &\equiv -\Phi_g^{\sigma}(\mathbf{z}+\mathbf{h}),\end{aligned} \tag{41}$$

where the last equivalence is because the vector $g\mathbf{h}+\mathbf{h}$ is in the horizontal plane where χ_2 is zero. Also note that since χ_2 is zero on the horizontal sublattice it does not affect the phases that were set to zero in the previous section.

5.3. Remaining gauge freedom

We still remain with some freedom to perform a third gauge transformation without undermining the effect of the previous two gauge transformations. Such a transformation can be performed with a gauge function χ_3 satisfying

$$\Delta\Phi_{g_8}^{\delta}(\mathbf{b}^{(i)}) \equiv \chi_3(g_8\mathbf{b}^{(i)} - \mathbf{b}^{(i)}) \equiv 0 \tag{42}$$

and

$$\Delta\Phi_g^{\sigma}(\mathbf{c}) \equiv \chi_3(g\mathbf{c} - \mathbf{c}) \equiv 0, \tag{43}$$

where g is the operation chosen in the previous section. The first condition, for all point groups and both lattice types, requires χ_3 to have the same value of 0 or 1/2 on all the horizontal generating vectors. For point groups 8 and $8mm$, where the second gauge transformation χ_2 is not used, there is no constraint on the value of $\chi_3(\mathbf{c})$. For the remaining point groups, we must consider the two lattice types separately. For V lattices, $g\mathbf{c}$ in equation (43) is $-\mathbf{c}$ and therefore $\chi_3(\mathbf{c}) \equiv 0$ or 1/2 independently of its value on the horizontal generating vectors. Thus, on V lattices, one must check for gauge equivalence of solutions to the group compatibility conditions using the three non-trivial gauge functions

$$\chi_3(\mathbf{b}^{(i)}\mathbf{c}) \equiv 0\tfrac{1}{2}; \quad \tfrac{1}{2}0; \quad \text{or} \quad \tfrac{1}{2}\tfrac{1}{2}. \tag{44}$$

For S lattices, using Table 2 and the fact that $\chi_3(2\mathbf{h}) \equiv 0$, we find that we may still perform gauge transformations using the gauge functions

$$\chi_3(\mathbf{b}^{(i)}\mathbf{c}) \equiv \begin{cases} 0\tfrac{1}{2}; \quad \tfrac{1}{2}0; \quad \text{or} \quad \tfrac{1}{2}\tfrac{1}{2}; \quad G = 8/m, 8/mmm,\\ 0\tfrac{1}{2}; \quad \tfrac{1}{2}\tfrac{1}{4}; \quad \text{or} \quad \tfrac{1}{2}\tfrac{3}{4}; \quad G = \bar 8, \bar 8m2, \bar 82m, 822.\end{cases} \tag{45}$$

6. Determination of phase functions for the different octagonal point groups

Further calculations of phase functions are carried out for each point group G separately, based on its specific generating relations. Two typical relations appear in most of the point

Table 4
Spin-space-group types on V lattices with $G = 8mm$.

All distinct combinations of phase functions are listed without explicitly identifying the spin-space operations δ and μ. For the sake of abbreviation, a, b, a' and b' each indicate phases that are either 0 or $\frac{1}{2}$, as long as no two elements in Γ_e have identical phase functions. For $\Gamma_e = n, n'$ or $n1'$, the integer j is co-prime with N, where $N = n$ unless $\Gamma_e = n'$ and n is odd, in which case, $N = 2n$. If N is odd, a is necessarily 0. The integer $d = 1$ unless N is twice an odd number and $\Phi_e^{n_{\bar{z}}^*}(\mathbf{b}^{(i)}) \equiv \frac{1}{2}$, in which case $d = 1$ or 2. A_0 denotes the values $0\frac{1}{2}0\frac{1}{2}$ of a phase function on the horizontal generating vectors and A_1 denotes the values $\frac{1}{2}0\frac{1}{2}0$ on the same vectors. Lines 5a and 5b refer to distinct spin-space-group types if $\Gamma_e = 2'2'2$ but are scale equivalent if $\Gamma_e = 222$ or $2'2'2'$, for which line 5a suffices. $\hat{a}$, $\hat{b}$ and $\tilde{a}$ denote either 0 or $\frac{1}{2}$. Spin-space-group symbols are of the form $P^{\Gamma_e}_{...}8^\delta m^\mu m^{\delta\mu}$, where the primary 8^δ is replaced by 8^δ_4 if $\tilde{a} = \frac{1}{2}$ and the secondary m^μ is replaced according to the values of $\hat{a}$ and $\hat{b}$: $\hat{a} = \hat{b} = 0 \Rightarrow m^\mu \to m^\mu$, $\hat{a} = 0, \hat{b} = \frac{1}{2} \Rightarrow m^\mu \to c^\mu$, $\hat{a} = \frac{1}{2}, \hat{b} = 0 \Rightarrow m^\mu \to b^\mu$, $\hat{a} = \hat{b} = \frac{1}{2} \Rightarrow m^\mu \to n^\mu$. The tertiary $m^{\delta\mu}$ is replaced by $c^{\delta\mu}$ if either $\hat{b}$ or $\tilde{a}$ (but not both) is $\frac{1}{2}$. Furthermore, a subscript a is added to the secondary m^μ when $\Phi_m^\mu(\mathbf{b}^{(i)}) \equiv A_0 + \hat{a}$. For example, if $\Gamma_e = 2'2'2$, $G_\varepsilon = 4mm$, $\Gamma = 2'2'2'$, then δ can be chosen to be ε' and the spin space group is described by line 5a or 5b, if $ab = \frac{1}{2}0$, $\hat{a} = \frac{1}{2}$, $\hat{b} = \frac{1}{2}$ and $\tilde{a} = 0$, the spin-space-group symbol will be $P^{2'2'2}_{P,S,2c}8'nc'$.

$\Gamma_e = 1, 1', 2, 2', 21'$								$(\delta^8 = \varepsilon)$
	$\mu^{-1}\delta\mu\delta$	μ^2	$\Phi_e^{2_{\bar{z}}^*}(\mathbf{b}^{(i)}\mathbf{c})$	$\Phi_e^{\varepsilon'}(\mathbf{b}^{(i)}\mathbf{c})$	$\Phi_m^\mu(\mathbf{b}^{(i)})$	$\Phi_m^\mu(\mathbf{z})$	$\Phi_{r_8}^\delta(\mathbf{z})$	
1	ε	ε	ab	$a'b'$	$\hat{a}$	$\hat{b}$	$\tilde{a}$	
2	ε	$2_{\bar{z}}$	$0\frac{1}{2}$	$\frac{1}{2}a$	$\hat{a}$	$\hat{b}$	$\tilde{a}$	
3	$2_{\bar{z}}$	ε	$0\frac{1}{2}$	$\frac{1}{2}a$	$\hat{a}$	$\hat{b}$	$\tilde{a}$	
			$\frac{1}{2}a$	$a'b'$	$\hat{a} + A_0$	$\hat{b}$	$\tilde{a} + \frac{a}{2}$	
4	$2_{\bar{z}}$	$2_{\bar{z}}$	$0\frac{1}{2}$	$\frac{1}{2}b$	$\hat{a}$	$\hat{b} + \frac{1}{4}$	$\tilde{a} + \frac{1}{4}$	
$\Gamma_e = 222, 2'2'2, 2'2'2'$								$(\mu 2_{\bar{x}}\mu^{-1} = 2_{\bar{x}} \Rightarrow \mu^2 = \varepsilon)$
	$\delta 2_{\bar{x}}\delta^{-1}$	$\mu^{-1}\delta\mu\delta$	$\Phi_e^{2_{\bar{x}}^*}(\mathbf{b}^{(i)}\mathbf{c})$	$\Phi_e^{2_{\bar{y}}^*}(\mathbf{b}^{(i)}\mathbf{c})$	$\Phi_e^{2'_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c})$	$\Phi_m^\mu(\mathbf{b}^{(i)})$	$\Phi_m^\mu(\mathbf{z})$	$\Phi_{r_8}^\delta(\mathbf{z})$
5a	$2_{\bar{x}}$	ε	$0\frac{1}{2}$	$\frac{1}{2}0$	–	$\hat{a}$	$\hat{b}$	$\tilde{a}$
5b	$2_{\bar{x}}$	ε	ab	$\frac{1}{2}\frac{1}{2}$	–	$\hat{a}$	$\hat{b}$	$\tilde{a}$
6	$2_{\bar{y}}$	$2_{\bar{z}}$	A_0b	A_1b	$a\frac{1}{2}$	$A_0 + \hat{a}$	$\hat{b}$	$\tilde{a}$
$\Gamma_e = n, n', n1'$								$(\delta n_{\bar{z}}\delta^{-1} = \mu n_{\bar{z}}\mu^{-1} = n_{\bar{z}}, \delta^8 = (\mu^{-1}\delta\mu\delta)^4)$
	$\mu^{-1}\delta\mu\delta$	μ^2	$\Phi_e^{n_{\bar{z}}^*}(\mathbf{b}^{(i)}\mathbf{c})$	$\Phi_e^{\varepsilon'}(\mathbf{b}^{(i)}\mathbf{c})$	$\Phi_m^\mu(\mathbf{b}^{(i)})$	$\Phi_m^\mu(\mathbf{z})$	$\Phi_{r_8}^\delta(\mathbf{z})$	
7	ε	ε	$a\frac{dj}{N}$	$a'b'$	$\hat{a}$	$\hat{b}$	$\tilde{a}$	
8	ε	$n_{\bar{z}}$	$0\frac{j}{n}$	ab	$\hat{a}$	$\hat{b} + \frac{j}{2n}$	$\tilde{a}$	
9	$n_{\bar{z}}$	ε	$0\frac{j}{n}$	ab	$\hat{a}$	$\hat{b}$	$\tilde{a} + \frac{j}{2n}$	
			$\frac{1}{2}\frac{dj}{n}$	ab	$\hat{a} + A_0$	$\hat{b}$	$\tilde{a} + \frac{dj}{2n}$	
10	$n_{\bar{z}}$	$n_{\bar{z}}$	$0\frac{j}{n}$	ab	$\hat{a}$	$\hat{b} + \frac{j}{2n}$	$\tilde{a} + \frac{j}{2n}$	

groups. All twofold generators $(g, \sigma) \in G_S$ satisfy a generating relation of the form $g^2 = e$ and therefore impose, through the group compatibility condition (1), equations of the form

$$\Phi_e^{\sigma^2}(\mathbf{k}) \equiv \Phi_g^\sigma(g\mathbf{k} + \mathbf{k}). \tag{46}$$

In general, σ^2 may be different from ε and therefore the phase $\Phi_e^{\sigma^2}(\mathbf{k})$ is not necessarily zero. But note that for any $\sigma \in \Gamma$ the operation σ^2 is either ε or a pure rotation about the $\bar{z}$ axis in spin space, and therefore $\Phi_e^{\sigma^2}(\mathbf{b}^{(i)}) \equiv 0000$ or $\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$.

Generating relations involving pairs of generators are of the form $ghg = h$, where (g, σ) and (h, τ) are in G_S. Application of the group compatibility condition (1) to these generating relations yields

$$\Phi_h^{\sigma\tau\sigma}(\mathbf{k}) \equiv \Phi_{ghg}^{\sigma\tau\sigma}(\mathbf{k}) \equiv \Phi_g^\sigma(\mathbf{k} + hg\mathbf{k}) + \Phi_h^\tau(g\mathbf{k}). \tag{47}$$

We expand the left-hand side by

$$\Phi_h^{\sigma\tau\sigma}(\mathbf{k}) \equiv \Phi_h^{\tau\tau^{-1}\sigma\tau\sigma}(\mathbf{k}) \equiv \Phi_h^\tau(\mathbf{k}) + \Phi_e^{\tau^{-1}\sigma\tau\sigma}(\mathbf{k}) \tag{48}$$

to obtain

$$\Phi_e^{\tau^{-1}\sigma\tau\sigma}(\mathbf{k}) \equiv \Phi_g^\sigma(\mathbf{k} + hg\mathbf{k}) + \Phi_h^\tau(g\mathbf{k} - \mathbf{k}). \tag{49}$$

This last form, as well as equation (46) for the twofold generators, emphasizes the fact that the new phase functions that are yet to be determined may depend on the phase functions $\Phi_e^\gamma(\mathbf{k})$ that were calculated in §4. Note that $\tau^{-1}\sigma\tau\sigma$ is the product of two conjugate operations in Γ and is therefore either the identity ε or a pure rotation about the $\bar{z}$ axis in spin space, and therefore $\Phi_e^{\tau^{-1}\sigma\tau\sigma}(\mathbf{b}^{(i)}) \equiv 0000$ or $\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$.

Owing to lack of space, detailed calculations leading to the results of this section are given here only for the two point groups 8 and $8mm$ as typical examples. Explicit tables, summarizing the results of the calculations of this section, are given here only for point group $8mm$ (Table 4 for V lattices and Table 5 for S lattices). All other results and calculations are given in Appendix B.

6.1. Point group $G = 8$ (generator r_8)

The only phase to be determined is $\Phi_{r_8}^\delta(\mathbf{c})$ because the in-plane phases of $\Phi_{r_8}^\delta$ were set to zero by the gauge transformation of §5.1. Successive applications of the group compatibility condition to the generating relation $r_8^8 = e$ yield

$$\Phi_e^{\delta^8}(\mathbf{c}) \equiv \Phi_{r_8}^\delta(\mathbf{c} + r_8\mathbf{c} + \ldots + r_8^7\mathbf{c}), \tag{50}$$

where, in general, δ^8 may be different from ε and therefore the phase $\Phi_e^{\delta^8}(\mathbf{c})$ is not necessarily zero. For vertical lattices, $\mathbf{c} = \mathbf{z}$ and equation (50) becomes

$$\Phi_e^{\delta^8}(\mathbf{z}) \equiv 8\Phi_{r_8}^\delta(\mathbf{z}), \tag{51}$$

with gauge-invariant solutions of the form

Table 5
Spin-space-group types on S lattices with $G = 8mm$.

All distinct combinations of phase functions are listed without explicitly identifying the spin-space operations δ and μ. For the sake of abbreviation, $\hat{a}$ and $\tilde{a}$ denote either 0 or $\frac{1}{2}$. For $\Gamma_e = n$ or n', the integer j is co-prime with N, where $N = n$ unless $\Gamma_e = n'$ and n is odd, in which case $N = 2n$. For any choice of spin-space operations, $(\mu^{-1}\delta\mu\delta)^4 = \delta^8$. Spin-space-group symbols are of the form $S^{\Gamma_e}_{\cdots}8^\delta m^\mu m^{\delta\mu}$, where the primary 8^δ is replaced by 8^δ_2 if $\hat{a} = \frac{1}{2}$ and the secondary m^μ is replaced by d^μ if $\hat{a} = \frac{1}{2}$. The tertiary $m^{\delta\mu}$ is replaced by $c^{\delta\mu}$ if $\tilde{a} = \frac{1}{2}$. A subscript a is added to the secondary m if $\Phi^\mu_m(\mathbf{b}^{(i)}) \equiv \hat{a} + A_0$.

$\Gamma_e = 1, 1', 2, 2'$								$(\delta^8 = \varepsilon)$
	$\mu^{-1}\delta\mu\delta$	μ^2	$\Phi^\gamma_e(\mathbf{k})$	$\Phi^\mu_m(\mathbf{b}^{(i)})$	$\Phi^\mu_m(\mathbf{z}+\mathbf{h})$	$\Phi^\delta_{r_8}(\mathbf{z}+\mathbf{h})$		
1	ε	ε	$0\frac{1}{2}$	$\hat{a}$	$\tilde{a}+\frac{1}{2}\hat{a}$	$\frac{1}{2}\hat{a}$		
2	ε	$2_{\bar{z}}$	$0\frac{1}{2}$	$\hat{a}$	$\tilde{a}+\frac{1}{2}\hat{a}+\frac{1}{4}$	$\frac{1}{2}\hat{a}$		
3	$2_{\bar{z}}$	ε	$0\frac{1}{2}$	$\hat{a}$	$\tilde{a}+\frac{1}{2}\hat{a}$	$\frac{1}{2}\hat{a}+\frac{1}{4}$		
4	$2_{\bar{z}}$	$2_{\bar{z}}$	$0\frac{1}{2}$	$\hat{a}$	$\tilde{a}+\frac{1}{2}\hat{a}+\frac{1}{4}$	$\frac{1}{2}\hat{a}+\frac{1}{4}$		
$\Gamma_e = 222, 2'2'2$								$(\mu 2_{\bar{x}}\mu^{-1} = 2_{\bar{y}} \Rightarrow \mu^2 = 2_{\bar{z}})$
	$\delta 2_{\bar{x}}\delta^{-1}$	$\mu^{-1}\delta\mu\delta$	$\Phi^{2^*_{\bar{x}}}_e(\mathbf{b}^{(i)}\mathbf{c})$	$\Phi^{2^*_{\bar{y}}}_e(\mathbf{b}^{(i)}\mathbf{c})$	$\Phi^\mu_m(\mathbf{b}^{(i)})$	$\Phi^\mu_m(\mathbf{z}+\mathbf{h})$	$\Phi^\delta_{r_8}(\mathbf{z}+\mathbf{h})$	
5	$2_{\bar{y}}$	$2_{\bar{z}}$	$\frac{1}{2}0$	$\frac{1}{2}\frac{1}{2}$	$\hat{a}$	$\tilde{a}+\frac{1}{2}\hat{a}+\frac{1}{4}$	$\frac{1}{2}\hat{a}+\frac{1}{4}$	
$\Gamma_e = n, n'$								$(\delta n_{\bar{z}}\delta^{-1} = \mu n_{\bar{z}}\mu^{-1})$
	$\delta n_{\bar{z}}\delta^{-1}$	$\mu^{-1}\delta\mu\delta$	μ^2	δ^8	$\Phi^{n^*_{\bar{z}}}_e(\mathbf{b}^{(i)}\mathbf{c})$	$\Phi^\mu_m(\mathbf{b}^{(i)})$	$\Phi^\mu_m(\mathbf{z}+\mathbf{h})$	$\Phi^\delta_{r_8}(\mathbf{z}+\mathbf{h})$
6	$n_{\bar{z}}$	ε	ε	ε	$0\frac{j}{n}$	$\hat{a}$	$\tilde{a}+\frac{1}{2}\hat{a}$	$\frac{1}{2}\hat{a}$
7	$n_{\bar{z}}$	ε	$n_{\bar{z}}$	ε	$0\frac{j}{n}$	$\hat{a}$	$\tilde{a}+\frac{1}{2}\hat{a}+\frac{j}{2n}$	$\frac{1}{2}\hat{a}$
8	$n_{\bar{z}}$	$n_{\bar{z}}$	ε	$n^4_{\bar{z}}$	$0\frac{j}{n}$	$\hat{a}$	$\tilde{a}+\frac{1}{2}\hat{a}$	$\frac{1}{2}\hat{a}+\frac{j}{2n}$
9	$n_{\bar{z}}$	$n_{\bar{z}}$	$n_{\bar{z}}$	$n^4_{\bar{z}}$	$0\frac{j}{n}$	$\hat{a}$	$\tilde{a}+\frac{1}{2}\hat{a}+\frac{j}{2n}$	$\frac{1}{2}\hat{a}+\frac{j}{2n}$
10	$n^{-1}_{\bar{z}}$	ε	ε	ε	$\frac{1}{2}\frac{j}{n}(n=4)$	$\hat{a}$	$\tilde{a}+\frac{1}{2}\hat{a}$	$\frac{1}{2}\hat{a}$
11	$n^{-1}_{\bar{z}}$	$n^{-1}_{\bar{z}}$	ε	ε	$\frac{1}{2}\frac{j}{n}(n=4)$	$\hat{a}+A_0$	$\tilde{a}+\frac{1}{2}\hat{a}$	$\frac{1}{2}(\frac{1}{2}-\hat{a})-\frac{j}{8}$

$$\Phi^\delta_{r_8}(\mathbf{z}) \equiv \tfrac{1}{8}\Phi^{\delta^8}_e(\mathbf{z}) + \tfrac{c}{8}, \quad c = 0, \ldots, 7. \tag{52}$$

For staggered lattices, $\mathbf{c} = \mathbf{z} + \mathbf{h}$ and equation (50) becomes

$$\Phi^{\delta^8}_e(\mathbf{z}+\mathbf{h}) \equiv \Phi^\delta_{r_8}(8\mathbf{z}) \equiv 8\Phi^\delta_{r_8}(\mathbf{z}+\mathbf{h}), \tag{53}$$

where the second equality follows from the fact that $8\mathbf{h}$ is a lattice vector in the horizontal plane for which $\Phi^\delta_{r_8}(8\mathbf{h}) \equiv 0$. The solutions of equation (53) are

$$\Phi^\delta_{r_8}(\mathbf{z}+\mathbf{h}) \equiv \tfrac{1}{8}\Phi^{\delta^8}_e(\mathbf{z}+\mathbf{h}) + \tfrac{c}{8}, \qquad c = 0, \ldots, 7, \tag{54}$$

just as for the vertical stacking vector but, unlike the vertical stacking vector, the phase $\Phi^\delta_{r_8}(\mathbf{z}+\mathbf{h})$ is not gauge invariant because $r_8(\mathbf{z}+\mathbf{h}) \neq (\mathbf{z}+\mathbf{h})$. We need to check whether any of the solutions are gauge equivalent through the remaining gauge freedom given by one of the gauge functions (45). Taking $\chi_3(\mathbf{b}^{(i)}) \equiv 1/2$ changes the phase $\Phi^\delta_{r_8}(\mathbf{z}+\mathbf{h})$ by

$$\Delta\Phi^\delta_{r_8}(\mathbf{z}+\mathbf{h}) \equiv \chi_3(r_8(\mathbf{z}+\mathbf{h}) - (\mathbf{z}+\mathbf{h})) \equiv \chi_3(\mathbf{b}^{(4)}) \equiv \tfrac{1}{2}. \tag{55}$$

Therefore, on the S lattice two solutions differing by $1/2$ are gauge equivalent, so the distinct solutions are

$$\Phi^\delta_{r_8}(\mathbf{z}+\mathbf{h}) \equiv \tfrac{1}{8}\Phi^{\delta^8}_e(\mathbf{z}+\mathbf{h}) + \tfrac{c'}{8}, \quad c' = 0, \ldots, 3. \tag{56}$$

The phase functions for point group $G = 8$ are summarized in Appendix B in Table B-1 for V lattices and Table B-2 for S lattices.

6.2. Point group $G = 8mm$ (generators r_8 and m)

We need to determine the phase $\Phi^\delta_{r_8}(\mathbf{c})$ and the phase function $\Phi^\mu_m(\mathbf{k})$. We use the generating relations $r_8^8 = m^2 = e$ and $r_8 m r_8 = m$, which impose equation (50) for the eightfold generator, equation (46) for the twofold generator and equation (49) for the additional generating relation $r_8 m r_8 = m$. We begin by noting that, if m is the mirror that leaves $\mathbf{b}^{(1)}$ invariant, then application of equation (46) to $\mathbf{b}^{(3)}$, which is perpendicular to m ($m\mathbf{b}^{(3)} = -\mathbf{b}^{(3)}$), yields

$$\Phi^{\mu^2}_e(\mathbf{b}^{(3)}) \equiv \Phi^\mu_m(m\mathbf{b}^{(3)} + \mathbf{b}^{(3)}) \equiv 0, \tag{57}$$

implying that $\Phi^{\mu^2}_e(\mathbf{b}^{(i)}) \equiv 0000$. Application of equation (46) to $\mathbf{b}^{(1)}$ then yields

$$0 \equiv 2\Phi^\mu_m(\mathbf{b}^{(1)}) \Longrightarrow \Phi^\mu_m(\mathbf{b}^{(1)}) \equiv 0 \text{ or } \tfrac{1}{2}, \tag{58}$$

and application of equation (46) to $\mathbf{b}^{(2)}$ and $\mathbf{b}^{(4)}$ shows that $\Phi^\mu_m(\mathbf{b}^{(2)}) \equiv \Phi^\mu_m(\mathbf{b}^{(4)})$ but provides no further information regarding the actual values of these phases. Next, we apply equation (49) to the horizontal generating vectors to obtain

$$\Phi^\mu_m(\mathbf{b}^{(i+1)}) \equiv \Phi^\mu_m(\mathbf{b}^{(i)}) + \Phi^{\mu^{-1}\delta\mu\delta}_e(\mathbf{b}^{(i)}). \tag{59}$$

Thus, the value of Φ^μ_m on $\mathbf{b}^{(1)}$ determines the values of Φ^μ_m on the remaining horizontal generating vectors through the phase function $\Phi^{\mu^{-1}\delta\mu\delta}_e$:

$$\Phi^\mu_m(\mathbf{b}^{(i)}) \equiv \begin{cases} 0000 \text{ or } \frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2} & \text{if } \Phi^{\mu^{-1}\delta\mu\delta}_e(\mathbf{b}^{(i)}) \equiv 0000, \\ 0\frac{1}{2}0\frac{1}{2} \text{ or } \frac{1}{2}0\frac{1}{2}0 & \text{if } \Phi^{\mu^{-1}\delta\mu\delta}_e(\mathbf{b}^{(i)}) \equiv \frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}. \end{cases} \tag{60}$$

For the vertical stacking vector in V lattices, for which $m\mathbf{z} = r_8\mathbf{z} = \mathbf{z}$, equation (51) remains unchanged, and equations (49) and (46) become

$$\Phi^{\mu^{-1}\delta\mu\delta}_e(\mathbf{z}) \equiv 2\Phi^\delta_{r_8}(\mathbf{z}) \tag{61a}$$

$$\Phi^{\mu^2}_e(\mathbf{z}) \equiv 2\Phi^\mu_m(\mathbf{z}). \tag{61b}$$

The solutions to these equations are

Table 6
Explicit list of octagonal spin-space-group types with $G = 8mm$ on V lattices.

The last column refers to line numbers in Table 4, where the possible phase functions are listed and rules are given to generate the spin-space-group symbol.

G_ε	G/G_ε	Γ	Generators	Line
$\Gamma_e = 1$				
$8mm$	1	1	$(r_8, \varepsilon)(m, \varepsilon)$	1
8	m	2	$(r_8, \varepsilon)(m, 2_{\bar{z}})$	1
		$2'$	$(r_8, \varepsilon)(m, 2'_{\bar{z}})$	1
		$1'$	$(r_8, \varepsilon)(m, \varepsilon')$	1
$4mm$	2	2^*	$(r_8, 2^*_{\bar{z}})(m, \varepsilon)$	1
		$1'$	$(r_8, \varepsilon')(m, \varepsilon)$	1
$4m'm'$	2	2^*	$(r_8, 2^*_{\bar{z}})(m, 2^*_{\bar{z}})$	1
		$1'$	$(r_8, \varepsilon')(m, \varepsilon')$	1
4	$2mm$	$2^*2^\dagger2^{*\dagger}$	$(r_8, 2^*_{\bar{z}})(m, 2^\dagger_{\bar{x}})$	1
		$21'$	$(r_8, 2^*_{\bar{z}})(m, \varepsilon')$	1
			$(r_8, \varepsilon')(m, 2^*_{\bar{z}})$	1
			$(r_8, 2^*_{\bar{z}})(m, 2'^*_{\bar{z}})$	1
2	$4mm$	$4^*2^\dagger2^{*\dagger}$	$(r_8, 4^*_{\bar{z}})(m, 2^\dagger_{\bar{x}})$	1
1	$8mm$	$8^*2^\dagger2^{*\dagger}$	$(r_8, 8^*_{\bar{z}})(m, 2^\dagger_{\bar{x}})$	1
			$(r_8, 8^{3*}_{\bar{z}})(m, 2^\dagger_{\bar{x}})$	1
$\Gamma_e = 2$				
$8mm$	1	2	$(r_8, \varepsilon)(m, \varepsilon)$	1
8	m	2^*2^*2	$(r_8, \varepsilon)(m, 2^*_{\bar{x}})$	1
		$21'$	$(r_8, \varepsilon)(m, \varepsilon')$	1
		4^*	$(r_8, \varepsilon)(m, 4^*_{\bar{z}})$	2
$4mm$	2	2^*2^*2	$(r_8, 2^*_{\bar{x}})(m, \varepsilon)$	1
		$21'$	$(r_8, \varepsilon')(m, \varepsilon)$	1
		4^*	$(r_8, 4^*_{\bar{z}})(m, \varepsilon)$	3
$4m'm'$	2	2^*2^*2	$(r_8, 2^*_{\bar{x}})(m, 2^*_{\bar{x}})$	1
		$21'$	$(r_8, \varepsilon')(m, \varepsilon')$	1
		4^*	$(r_8, 4^*_{\bar{z}})(m, 4^*_{\bar{z}})$	4
4	$2mm$	$4^*2^\dagger2^{*\dagger}$	$(r_8, 4^*_{\bar{z}})(m, 2^\dagger_{\bar{x}})$	1
			$(r_8, 2^\dagger_{\bar{x}})(m, 4^*_{\bar{z}})$	4
			$(r_8, 2^\dagger_{\bar{x}})(m, 2^{*\dagger}_{\bar{x}\bar{y}})$	3
		$41'$	$(r_8, 4^*_{\bar{z}})(m, \varepsilon')$	3
			$(r_8, \varepsilon')(m, 4^*_{\bar{z}})$	2
			$(r_8, 4^*_{\bar{z}})(m, 4'^*_{\bar{z}})$	4
		$2'2'2'$	$(r_8, 2^*_{\bar{x}})(m, \varepsilon')$	1
			$(r_8, \varepsilon')(m, 2^*_{\bar{x}})$	1
			$(r_8, 2^*_{\bar{x}})(m, 2'^*_{\bar{x}})$	1
2	$4mm$	$8^*2^\dagger2^{*\dagger}$	$(r_8, 8^*_{\bar{z}})(m, 2^\dagger_{\bar{x}})$	1
$\Gamma_e = 2'$				
$8mm$	1	$2'$	$(r_8, \varepsilon)(m, \varepsilon)$	1
8	m	$2'2^*2'^*$	$(r_8, \varepsilon)(m, 2^*_{\bar{x}})$	1
		$21'$	$(r_8, \varepsilon)(m, \varepsilon')$	1
$4mm$	2	$2'2^*2'^*$	$(r_8, 2^*_{\bar{x}})(m, \varepsilon)$	1
		$21'$	$(r_8, \varepsilon')(m, \varepsilon)$	1
$4m'm'$	2	$2'2^*2'^*$	$(r_8, 2^*_{\bar{x}})(m, 2^*_{\bar{x}})$	1
		$21'$	$(r_8, \varepsilon')(m, \varepsilon')$	1
4	$2mm$	$2'2'2'$	$(r_8, 2^*_{\bar{x}})(m, \varepsilon')$	1
			$(r_8, \varepsilon')(m, 2^*_{\bar{x}})$	1
			$(r_8, 2^*_{\bar{x}})(m, 2'^*_{\bar{x}})$	1
2	$4mm$	$4221'$	$(r_8, 4^*_{\bar{z}})(m, 2^\dagger_{\bar{x}})$	1
1	$8mm$	$8221'$	$(r_8, 8^*_{\bar{z}})(m, 2^\dagger_{\bar{x}})$	1
$\Gamma_e = 1'$				
$8mm$	1	$1'$	$(r_8, \varepsilon)(m, \varepsilon)$	1
8	m	$21'$	$(r_8, \varepsilon)(m, 2_{\bar{z}})$	1
$4mm$	2	$21'$	$(r_8, 2_{\bar{z}})(m, \varepsilon)$	1
$4m'm'$	2	$21'$	$(r_8, 2_{\bar{z}})(m, 2_{\bar{z}})$	1
4	$2mm$	$2'2'2'$	$(r_8, 2_{\bar{z}})(m, 2_{\bar{x}})$	1

Table 6 (continued)

G_ε	G/G_ε	Γ	Generators	Line
2	$4mm$	$4221'$	$(r_8, 4_{\bar{z}})(m, 2_{\bar{x}})$	1
1	$8mm$	$8221'$	$(r_8, 8_{\bar{z}})(m, 2_{\bar{x}})$	1
			$(r_8, 8^{3*}_{\bar{z}})(m, 2^\dagger_{\bar{x}})$	1
$\Gamma_e = 21'$				
$8mm$	1	$21'$	$(r_8, \varepsilon)(m, \varepsilon)$	1
8	m	$41'$	$(r_8, \varepsilon)(m, 4_{\bar{z}})$	2
		$2'2'2'$	$(r_8, \varepsilon)(m, 2_{\bar{x}})$	1
$4mm$	2	$41'$	$(r_8, 4_{\bar{z}})(m, \varepsilon)$	3
		$2'2'2'$	$(r_8, 2_{\bar{x}})(m, \varepsilon)$	1
$4m'm'$	2	$41'$	$(r_8, 4_{\bar{z}})(m, 4_{\bar{z}})$	4
		$2'2'2'$	$(r_8, 2_{\bar{x}})(m, 2_{\bar{x}})$	1
4	$2mm$	$4221'$	$(r_8, 4_{\bar{z}})(m, 2_{\bar{x}})$	1
			$(r_8, 2_{\bar{x}})(m, 4_{\bar{z}})$	4
			$(r_8, 2_{\bar{x}})(m, 2_{\bar{x}\bar{y}})$	3
2	$4mm$	$8221'$	$(r_8, 8_{\bar{z}})(m, 2_{\bar{x}})$	1
$\Gamma_e = n$				
$8mm$	1	n	$(r_8, \varepsilon)(m, \varepsilon)$	7
8	2	$(2n)^*$	$(r_8, \varepsilon)(m, (2n)^*_{\bar{z}})$	8
		$n1'$	$(r_8, \varepsilon)(m, \varepsilon')$	7
$4mm$	2	$(2n)^*$	$(r_8, (2n)^*_{\bar{z}})(m, \varepsilon)$	9
		$n1'$	$(r_8, \varepsilon')(m, \varepsilon)$	7
$4m'm'$	2	$(2n)^*$	$(r_8, (2n)^*_{\bar{z}})(m, (2n)^*_{\bar{z}})$	10
		$n1'$	$(r_8, \varepsilon')(m, \varepsilon')$	7
4	$2mm$	$(2n)1'$	$(r_8, (2n)^*_{\bar{z}})(m, \varepsilon')$	9
			$(r_8, \varepsilon')(m, (2n)^*_{\bar{z}})$	8
			$(r_8, (2n)^*_{\bar{z}})(m, (2n)'^*_{\bar{z}})$	10
$\Gamma_e = n'$				
$8mm$	1	n'	$(r_8, \varepsilon)(m, \varepsilon)$	7
8	m	$n1'$	$(r_8, \varepsilon)(m, \varepsilon')$	7
$4mm$	2	$n1'$	$(r_8, \varepsilon')(m, \varepsilon)$	7
$4m'm'$	2	$n1'$	$(r_8, \varepsilon')(m, \varepsilon')$	7
$\Gamma_e = n1'$ or n'				
$8mm$	1	$n1'$	$(r_8, \varepsilon)(m, \varepsilon)$	7
8	m	$(2n)1'$	$(r_8, \varepsilon)(m, (2n)_{\bar{z}})$	8
$4mm$	2	$(2n)1'$	$(r_8, (2n)_{\bar{z}})(m, \varepsilon)$	9
$4m'm'$	2	$(2n)1'$	$(r_8, (2n)^*_{\bar{z}})(m, (2n)^*_{\bar{z}})$	10
$\Gamma_e = 222$				
$8mm$	1	222	$(r_8, \varepsilon)(m, \varepsilon)$	5a
8	m	$2'2'2'$	$(r_8, \varepsilon)(m, \varepsilon')$	5a
$4mm$	2	$2'2'2'$	$(r_8, \varepsilon')(m, \varepsilon)$	5a
		4^*22^*	$(r_8, 4^*_{\bar{z}})(m, \varepsilon)$	6
$4m'm'$	2	$2'2'2'$	$(r_8, \varepsilon')(m, \varepsilon')$	5a
4	$2mm$	$4221'$	$(r_8, 4^*_{\bar{z}})(m, \varepsilon')$	6
$\Gamma_e = 2'2'2$				
$8mm$	1	$2'2'2$	$(r_8, \varepsilon)(m, \varepsilon)$	5
8	m	$2'2'2'$	$(r_8, \varepsilon)(m, \varepsilon')$	5
$4mm$	2	$2'2'2'$	$(r_8, \varepsilon')(m, \varepsilon)$	5
		4^*22^*	$(r_8, 4^*_{\bar{z}})(m, \varepsilon)$	6
$4m'm'$	2	$2'2'2'$	$(r_8, \varepsilon')(m, \varepsilon')$	5
4	$2mm$	$4221'$	$(r_8, 4^*_{\bar{z}})(m, \varepsilon')$	6
$\Gamma_e = 2'2'2'$				
$4mm$	2	$4221'$	$(r_8, 4_{\bar{z}})(m, \varepsilon)$	6

$$\Phi^{\delta}_{r_8}(\mathbf{z}) \equiv \tfrac{1}{2}\,\Phi^{\mu^{-1}\delta\mu\delta}_{e}(\mathbf{z}) + a, \tag{62a}$$

$$\Phi^{\mu}_{m}(\mathbf{z}) \equiv \tfrac{1}{2}\,\Phi^{\mu^2}_{e}(\mathbf{z}) + b, \tag{62b}$$

where a and b are independently 0 or 1/2.

Table 7
Explicit list of octagonal spin-space-group types with $G = 8mm$ on S lattices.

The last column refers to line numbers in Table 5, where the possible phase functions are listed, and rules are given to generate the spin-space-group symbol.

G_ε	G/G_ε	Γ	Generators	Line
$\Gamma_e = 1$				
$8mm$	1	1	$(r_8, \varepsilon)(m, \varepsilon)$	1
8	m	2	$(r_8, \varepsilon)(m, 2_{\bar z})$	1
		$2'$	$(r_8, \varepsilon)(m, 2'_{\bar z})$	1
		$1'$	$(r_8, \varepsilon)(m, \varepsilon')$	1
$4mm$	2	2^*	$(r_8, 2^*_{\bar z})(m, \varepsilon)$	1
		$1'$	$(r_8, \varepsilon')(m, \varepsilon)$	1
$4m'm'$	2	2^*	$(r_8, 2^*_{\bar z})(m, 2^*_{\bar z})$	1
		$1'$	$(r_8, \varepsilon')(m, \varepsilon')$	1
4	$2mm$	$2^*2^\dagger 2^{*\dagger}$	$(r_8, 2^*_{\bar z})(m, 2^\dagger_{\bar x})$	1
		$21'$	$(r_8, 2^*_{\bar z})(m, \varepsilon')$	1
			$(r_8, \varepsilon')(m, 2^*_{\bar z})$	1
			$(r_8, 2^*_{\bar z})(m, 2'^*_{\bar z})$	1
2	$4mm$	$4^*2^\dagger 2^{*\dagger}$	$(r_8, 4^*_{\bar z})(m, 2^\dagger_{\bar x})$	1
1	$8mm$	$8^*2^\dagger 2^{*\dagger}$	$(r_8, 8^*_{\bar z})(m, 2^\dagger_{\bar x})$	1
			$(r_8, 8^{3*}_{\bar z})(m, 2^\dagger_{\bar x})$	1
$\Gamma_e = 2$				
$8mm$	1	2	$(r_8, \varepsilon)(m, \varepsilon)$	1
8	m	2^*2^*2	$(r_8, \varepsilon)(m, 2^*_{\bar x})$	1
		$21'$	$(r_8, \varepsilon)(m, \varepsilon')$	1
		4^*	$(r_8, \varepsilon)(m, 4^*_{\bar z})$	2
$4mm$	2	2^*2^*2	$(r_8, 2^*_{\bar x})(m, \varepsilon)$	1
		$21'$	$(r_8, \varepsilon')(m, \varepsilon)$	1
		4^*	$(r_8, 4^*_{\bar z})(m, \varepsilon)$	3
$4m'm'$	2	2^*2^*2	$(r_8, 2^*_{\bar x})(m, 2^*_{\bar x})$	1
		$21'$	$(r_8, \varepsilon')(m, \varepsilon')$	1
		4^*	$(r_8, 4^*_{\bar z})(m, 4^*_{\bar z})$	4
4	$2mm$	$4^*2^\dagger 2^{*\dagger}$	$(r_8, 4^*_{\bar z})(m, 2^\dagger_{\bar x})$	1
			$(r_8, 2^\dagger_{\bar x})(m, 4^*_{\bar z})$	2
			$(r_8, 2^\dagger_{\bar x})(m, 2^{*\dagger}_{\bar x y})$	3
		$41'$	$(r_8, 4^*_{\bar z})(m, \varepsilon')$	3
			$(r_8, \varepsilon')(m, 4^*_{\bar z})$	2
			$(r_8, 4^*_{\bar z})(m, 4'^*_{\bar z})$	4
		$2'2'2'$	$(r_8, 2^*_{\bar x})(m, \varepsilon')$	1
			$(r_8, \varepsilon')(m, 2^*_{\bar x})$	1
			$(r_8, 2^*_{\bar x})(m, 2'^*_{\bar x})$	1
2	$4mm$	$8^*2^\dagger 2^{*\dagger}$	$(r_8, 8^*_{\bar z})(m, 2^\dagger_{\bar x})$	1
$\Gamma_e = 2'$				
$8mm$	1	$2'$	$(r_8, \varepsilon)(m, \varepsilon)$	1
8	m	$2'2^*2'^*$	$(r_8, \varepsilon)(m, 2^*_{\bar x})$	1
		$21'$	$(r_8, \varepsilon)(m, \varepsilon')$	1
$4mm$	2	$2'2^*2'^*$	$(r_8, 2^*_{\bar x})(m, \varepsilon)$	1
		$21'$	$(r_8, \varepsilon')(m, \varepsilon)$	1
$4m'm'$	2	$2'2^*2'^*$	$(r_8, 2^*_{\bar x})(m, 2^*_{\bar x})$	1
		$21'$	$(r_8, \varepsilon')(m, \varepsilon')$	1
4	$2mm$	$2'2'2'$	$(r_8, 2^*_{\bar x})(m, \varepsilon')$	1
			$(r_8, \varepsilon')(m, 2^*_{\bar x})$	1
			$(r_8, 2^*_{\bar x})(m, 2'^*_{\bar x})$	1
2	$4mm$	$4221'$	$(r_8, 4^*_{\bar z})(m, 2^\dagger_{\bar x})$	1
1	$8mm$	$8221'$	$(r_8, 8^*_{\bar z})(m, 2^\dagger_{\bar x})$	1
$\Gamma_e = 1'$				
$8mm$	1	$1'$	$(r_8, \varepsilon)(m, \varepsilon)$	1
8	m	$21'$	$(r_8, \varepsilon)(m, 2_{\bar z})$	1
$4mm$	2	$21'$	$(r_8, 2_{\bar z})(m, \varepsilon)$	1
$4m'm'$	2	$21'$	$(r_8, 2_{\bar z})(m, 2_{\bar z})$	1
4	$2mm$	$2'2'2'$	$(r_8, 2_{\bar z})(m, 2_{\bar x})$	1

Table 7 (continued)

G_ε	G/G_ε	Γ	Generators	Line
2	$4mm$	$4221'$	$(r_8, 4_{\bar z})(m, 2_{\bar x})$	1
1	$8mm$	$8221'$	$(r_8, 8_{\bar z})(m, 2_{\bar x})$	1
			$(r_8, 8^{3*}_{\bar z})(m, 2^\dagger_{\bar x})$	1
$\Gamma_e = n$				
$8mm$	1	n	$(r_8, \varepsilon)(m, \varepsilon)$	6
8	2	$(2n)^*$	$(r_8, \varepsilon)(m, (2n)^*_{\bar z})$	7
		$n1'$	$(r_8, \varepsilon)(m, \varepsilon')$	6
$4mm$	2	$(2n)^*$	$(r_8, (2n)^*_{\bar z})(m, \varepsilon)$	8
		$n1'$	$(r_8, \varepsilon')(m, \varepsilon)$	6
$4m'm'$	2	$(2n)^*$	$(r_8, (2n)^*_{\bar z})(m, (2n)^*_{\bar z})$	9
		$n2^*2^*$	$(r_8, 2^*_{\bar x})(m2^*_{\bar x})$	10
		$n1'$	$(r_8, \varepsilon')(m, \varepsilon')$	6
4	222	$(2n)^*2^\dagger 2^{*\dagger}$	$(r_8, (2n)_{\bar z}2^{*\dagger}_{\bar x})(m, 2^\dagger_{\bar x})$	11
		$n221'$	$(r_8, 2^*_{\bar x})(m, 2'^*_{\bar x})$	10
		$(2n)1'$	$(r_8, (2n)^*_{\bar z})(m, \varepsilon')$	8
			$(r_8, \varepsilon')(m, (2n)^*_{\bar z})$	7
			$(r_8, (2n)^*_{\bar z})(m, (2n)'^*_{\bar z})$	9
$\Gamma_e = n'$				
$8mm$	1	n'	$(r_8, \varepsilon)(m, \varepsilon)$	6
8	m	$n1'$	$(r_8, \varepsilon)(m, \varepsilon')$	6
$4mm$	2	$n1'$	$(r_8, \varepsilon')(m, \varepsilon)$	6
$4m'm'$	2	$n'2^*2'^*$	$(r_8, 2^*_{\bar x})(m, 2^*_{\bar x})$	10
		$n1'$	$(r_8, \varepsilon')(m, \varepsilon')$	6
4	222	$n221'$	$(r_8, 2^*_{\bar x})(m, 2'^*_{\bar x})$	10
$\Gamma_e = 2^*2^*2$				
$4m'm'$	2	$4^\dagger 2^*2^{*\dagger}$	$(r_8, 4^\dagger_{\bar z})(m, 4^\dagger_{\bar z})$	5
4	$2mm$	$4221'$	$(r_8, 4^\dagger_{\bar z})(m, 4'^\dagger_{\bar z})$	5

For the staggered stacking vector in S lattices, for which $r_8(\mathbf{z}+\mathbf{h}) = \mathbf{z}+\mathbf{h}+\mathbf{b}^{(4)}$ and $m(\mathbf{z}+\mathbf{h}) = \mathbf{z}+\mathbf{h}-\mathbf{b}^{(3)}$, we obtain equation (53) together with

$$\Phi_e^{\mu^{-1}\delta\mu\delta}(\mathbf{z}+\mathbf{h}) \equiv 2\Phi_{r_8}^{\delta}(\mathbf{z}+\mathbf{h}) + \Phi_m^{\mu}(\mathbf{b}^{(4)}) \qquad (63a)$$

$$\Phi_e^{\mu^2}(\mathbf{z}+\mathbf{h}) \equiv 2\Phi_m^{\mu}(\mathbf{z}+\mathbf{h}) - \Phi_m^{\mu}(\mathbf{b}^{(3)}) \qquad (63b)$$

Noting that the signs of the phases $\Phi_m^{\mu}(\mathbf{b}^{(i)})$ are unimportant, the solutions to these equations are

$$\Phi_{r_8}^{\delta}(\mathbf{z}+\mathbf{h}) \equiv \tfrac{1}{2}\Phi_m^{\mu}(\mathbf{b}^{(4)}) + \tfrac{1}{2}\Phi_e^{\mu^{-1}\delta\mu\delta}(\mathbf{z}+\mathbf{h}) + a, \qquad (64a)$$

$$\Phi_m^{\mu}(\mathbf{z}+\mathbf{h}) \equiv \tfrac{1}{2}\Phi_m^{\mu}(\mathbf{b}^{(3)}) + \tfrac{1}{2}\Phi_e^{\mu^2}(\mathbf{z}+\mathbf{h}) + b, \qquad (64b)$$

where a and b are independently 0 or 1/2, but we still need to check for gauge equivalence using the remaining gauge freedom given by the gauge functions (45). A gauge transformation with $\chi_3(\mathbf{b}^{(i)}) \equiv 1/2$ changes both of the phases in equations (64) by 1/2, implying that the two solutions with $ab \equiv 00$ and $\frac{1}{2}\frac{1}{2}$ are gauge equivalent and the two solutions $ab \equiv 0\frac{1}{2}$ and $\frac{1}{2}0$ are also gauge equivalent. As representatives of the gauge-equivalence classes, we take the solutions with $a \equiv 0$.

We finally note that equations (51) and (53) further imply that for both lattice types

$$\Phi_e^{\delta^8}(\mathbf{c}) \equiv 4\Phi_e^{\mu^{-1}\delta\mu\delta}(\mathbf{c}), \qquad (65)$$

which is true for the horizontal generating vectors as well and therefore $\delta^8 = (\mu^{-1}\delta\mu\delta)^4$.

Table 8
Restrictions on the form of $\mathbf{S}(\mathbf{k})$ for any wavevector $\mathbf{k}$ in the magnetic lattice L when $\Gamma_e = 2, 2'$ or $1'$.

In each case, the form of $\mathbf{S}(\mathbf{k})$ depends on the particular values of the phases $\Phi_e^\gamma(\mathbf{b}^{(i)}\mathbf{c})$, where γ is the generator of Γ_e, and on the parities of $\sum n_i$ and l, where $\mathbf{k} = \sum_{i=1}^4 n_i \mathbf{b}^{(i)} + l\mathbf{c}$. Each entry in the table contains three values for the form of $\mathbf{S}(\mathbf{k})$: the one on the left is for $\Gamma_e = 2$; the one in the center is for $\Gamma_e = 2'$; and the one on the right is for $\Gamma_e = 1'$.

Lattice spin group		$\sum n_i$ even		$\sum n_i$ odd	
Symbols	$\Phi_e^\gamma(\mathbf{b}^{(i)}\mathbf{c})$	l even	l odd	l even	l odd
$P_{2c}^\gamma, S_P^\gamma$	$0\frac{1}{2}$	$\mathbf{S}_z/\mathbf{S}_{xy}/0$	$\mathbf{S}_{xy}/\mathbf{S}_z/\mathbf{S}$	$\mathbf{S}_z/\mathbf{S}_{xy}/0$	$\mathbf{S}_{xy}/\mathbf{S}_z/\mathbf{S}$
P_P^γ	$\frac{1}{2}0$	$\mathbf{S}_z/\mathbf{S}_{xy}/0$	$\mathbf{S}_z/\mathbf{S}_{xy}/0$	$\mathbf{S}_{xy}/\mathbf{S}_z/\mathbf{S}$	$\mathbf{S}_{xy}/\mathbf{S}_z/\mathbf{S}$
P_S^γ	$\frac{1}{2}\frac{1}{2}$	$\mathbf{S}_z/\mathbf{S}_{xy}/0$	$\mathbf{S}_{xy}/\mathbf{S}_z/\mathbf{S}$	$\mathbf{S}_{xy}/\mathbf{S}_z/\mathbf{S}$	$\mathbf{S}_z/\mathbf{S}_{xy}/0$

Table 9
Restrictions on the form of $\mathbf{S}(\mathbf{k})$ for any wavevector $\mathbf{k} \in L$ when $\Gamma_e = 21'$.

In each case, the form of $\mathbf{S}(\mathbf{k})$ depends on the particular values of the phase functions for the generators of Γ_e, and on the parities of $\sum n_i$ and l, where $\mathbf{k} = \sum_{i=1}^4 n_i \mathbf{b}^{(i)} + l\mathbf{c}$.

Lattice spin group			$\sum n_i$ even		$\sum n_i$ odd	
Symbols	$\Phi_e^{2_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c})$	$\Phi_e^{\varepsilon'}(\mathbf{b}^{(i)}\mathbf{c})$	l even	l odd	l even	l odd
$P_{2c,P}^{21'}$	$0\frac{1}{2}$	$\frac{1}{2}0$	0	0	$\mathbf{S}_z$	$\mathbf{S}_{xy}$
$P_{2c,S}^{21'}$	$0\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}$	0	$\mathbf{S}_{xy}$	$\mathbf{S}_z$	0
$P_{P,2c}^{21'}$	$\frac{1}{2}0$	$0\frac{1}{2}$	0	$\mathbf{S}_z$	0	$\mathbf{S}_{xy}$
$P_{P,S}^{21'}$	$\frac{1}{2}0$	$\frac{1}{2}\frac{1}{2}$	0	$\mathbf{S}_z$	$\mathbf{S}_{xy}$	0
$P_{S,2c}^{21'}$	$\frac{1}{2}\frac{1}{2}$	$0\frac{1}{2}$	0	$\mathbf{S}_{xy}$	0	$\mathbf{S}_z$
$P_{S,P}^{21'}$	$\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}0$	0	0	$\mathbf{S}_{xy}$	$\mathbf{S}_z$

The phase functions for point group $G = 8mm$ are summarized in Table 4 for V lattices and Table 5 for S lattices.

7. Spin-group tables

Tables B-1 to B-16 in Appendix *B* contain in compact form all the information needed to generate the complete list of octagonal spin space-group types (shown here are only Tables 4 and 5 for the case of point group $G = 8mm$ as examples). All that is still required is to explicitly identify the spin-space operations δ, and whenever necessary μ, α and η, recalling that these operations must also satisfy the constraints, summarized in Table 3, that are due to the isomorphism between G/G_ε and Γ/Γ_e. Once these operations are identified, their different combinations—δ^8, $\delta\gamma\delta^{-1}$, $\mu^{-1}\delta\mu\delta$ *etc.*—that determine the phase functions can be calculated to give the different spin-space-group types. The explicit identification of spin-space operations for point group $G = 8mm$ are listed in Table 6 for V lattices and in Table 7 for S lattices. The complete set of tables for all octagonal point groups are listed in Appendix *C*. For each spin-space-group table (Tables B-1 to B-16), there is a corresponding table in Appendix *C* that lists all the possible identifications of spin-space operations and, for each one, indicates the line in the spin-space-group table to which it corresponds.

To each spin space-group type, we give a unique symbol 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, which for the case of octagonal quasicrystals is explained in detail by Rabson *et al.* (1991), in the following ways: (i) the symbol for the lattice spin group Γ_e is added as a superscript over the lattice symbol, unless $\Gamma_e = 1$ or $1'$; (ii) the values of the phase functions, associated with the elements of Γ_e, are encoded by subscripts under the lattice symbol, describing the sublattices defined by the zeros of the phase functions for the operations in the symbol for Γ_e (as explained in §4); (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 can be ε, we omit it, if it can be ε', we simply add a prime, and we omit the axis about which rotations are performed if it is the $\bar{z}$ axis); (iv) the values of phase functions for the spin-point-group generators $\Phi_{r_8}^\delta$, $\Phi_{\bar{r}_8}^\delta$, Φ_m^μ, Φ_d^α and Φ_h^η are encoded by making changes and adding subscripts to the point-group symbol (similar to the way it is done for the regular space groups), as described in the captions of Tables B-1 to B-16, where we use the same notation, simply without explicitly listing Γ_e and its associated phase functions, and without explicitly identifying the spin-space operations paired with the point-group generators. Specific examples of spin-space-group symbols can be found in the captions of Table 4 as well as Tables B-1, B-2, B-5 and B-16.

8. Magnetic selection rules

We calculate the symmetry-imposed constraints on $\mathbf{S}(\mathbf{k})$ for any wavevector $\mathbf{k} = \sum_{i=1}^4 n_i \mathbf{b}^{(i)} + l\mathbf{c}$ in the magnetic lattice L, as described in the companion paper (Lifshitz & Even-Dar Mandel, 2004), by considering all spin-point-group operations (g, γ) for which $g\mathbf{k} = \mathbf{k}$. The point-group condition for each of these operations provides an eigenvalue equation

$$\gamma\mathbf{S}(\mathbf{k}) = e^{-2\pi i \Phi_g^\gamma(\mathbf{k})}\mathbf{S}(\mathbf{k}), \tag{66}$$

from which we obtain the constraints on $\mathbf{S}$. These constraints may require $\mathbf{S}(\mathbf{k})$ to vanish or to take a particular form that transforms under the operations γ in (66) according to the one-dimensional representation dictated by the phases $\Phi_g^\gamma(\mathbf{k})$. When there are no constraints then $\mathbf{S} = (S_{\bar{x}}, S_{\bar{y}}, S_{\bar{z}})$ is an arbitrary three-component axial vector. When there are constraints, $\mathbf{S}(\mathbf{k})$ takes one of the following forms:

$$\begin{aligned} &\mathbf{S}_x = (S_{\bar{x}}, 0, 0), && \mathbf{S}_y = (0, S_{\bar{y}}, 0), && \mathbf{S}_z = (0, 0, S_{\bar{z}}), \\ &\mathbf{S}_{yz} = (0, S_{\bar{y}}, S_{\bar{z}}), && \mathbf{S}_{zx} = (S_{\bar{x}}, 0, S_{\bar{z}}), && \mathbf{S}_{xy} = (S_{\bar{x}}, S_{\bar{y}}, 0), \\ &\mathbf{S}_+ = (S_{\bar{x}}, +iS_{\bar{x}}, 0), && \mathbf{S}_- = (S_{\bar{x}}, -iS_{\bar{x}}, 0), \end{aligned} \tag{67}$$

as explained below.

In §8.1, we determine the selection rules due to elements in Γ_e. These affect all wavevectors $\mathbf{k} \in L$, and are summarized in Tables 8–12. In §8.2, we determine the remaining selection rules for wavevectors that lie in the invariant subspaces of the different point-group elements. These selection rules are expressed in a general manner in terms of the spin-space

Table 10
Restrictions on the form of $\mathbf{S}(\mathbf{k})$ for any wavevector $\mathbf{k}$ in the magnetic lattice L when $\Gamma_e = 222$ and $2'2'2$.

In each case, the form of $\mathbf{S}(\mathbf{k})$ depends on the particular values of the phase functions for the generators $2^*_{\bar{x}}$ and $2^*_{\bar{y}}$ of Γ_e, where the asterisk denotes an optional prime, and on the parities of n_1+n_3, n_2+n_4 and l, where $\mathbf{k} = \sum_{i=1}^4 n_i \mathbf{b}^{(i)} + l\mathbf{c}$. Each entry in the table contains two values for the form of $\mathbf{S}(\mathbf{k})$: the one on the left is for $\Gamma_e = 222$; and the one on the right is for $\Gamma_e = 2'2'2$.

Lattice spin group			n_1+n_3 even				n_1+n_3 odd			
			n_2+n_4 even		n_2+n_4 odd		n_2+n_4 even		n_2+n_4 odd	
Symbols	$\Phi_e^{2^*_{\bar{x}}}(\mathbf{b}^{(i)}\mathbf{c})$	$\Phi_e^{2^*_{\bar{y}}}(\mathbf{b}^{(i)}\mathbf{c})$	l even	l odd	l even	l odd	l even	l odd	l even	l odd
$P^{222}_{2c,P,S}$, $P^{2'2'2}_{2c,P,S}$	$0\,\frac{1}{2}$	$\frac{1}{2}\,0$	$0/\mathbf{S}_z$	$\mathbf{S}_y/\mathbf{S}_x$	$\mathbf{S}_x/\mathbf{S}_y$	$\mathbf{S}_z/0$	$\mathbf{S}_x/\mathbf{S}_y$	$\mathbf{S}_z/0$	$0/\mathbf{S}_z$	$\mathbf{S}_y/\mathbf{S}_x$
$P^{2'2'2}_{2c,S,P}$	$0\,\frac{1}{2}$	$\frac{1}{2}\,\frac{1}{2}$	$0/\mathbf{S}_z$	$\mathbf{S}_z/0$	$\mathbf{S}_x/\mathbf{S}_y$	$\mathbf{S}_y/\mathbf{S}_x$	$\mathbf{S}_x/\mathbf{S}_y$	$\mathbf{S}_y/\mathbf{S}_x$	$0/\mathbf{S}_z$	$\mathbf{S}_z/0$
$P^{2'2'2}_{P,S,2c}$, $S^{222}_{I\times p,P}$, $S^{2'2'2}_{I\times p,P}$	$\frac{1}{2}\,0$	$\frac{1}{2}\,\frac{1}{2}$	$0/\mathbf{S}_z$	$\mathbf{S}_x/\mathbf{S}_y$	$\mathbf{S}_z/0$	$\mathbf{S}_y/\mathbf{S}_x$	$\mathbf{S}_z/0$	$\mathbf{S}_y/\mathbf{S}_x$	$0/\mathbf{S}_z$	$\mathbf{S}_x/\mathbf{S}_y$
$P^{222}_{P+p,P}$, $P^{2'2'2}_{P+p,P}$	$A_0 0$	$A_1 0$	$0/\mathbf{S}_z$	$0/\mathbf{S}_z$	$\mathbf{S}_y/\mathbf{S}_x$	$\mathbf{S}_y/\mathbf{S}_x$	$\mathbf{S}_x/\mathbf{S}_y$	$\mathbf{S}_x/\mathbf{S}_y$	$\mathbf{S}_z/0$	$\mathbf{S}_z/0$
$P^{222}_{I+p,P}$, $P^{2'2'2}_{I+p,P}$	$A_0\,\frac{1}{2}$	$A_1\,\frac{1}{2}$	$0/\mathbf{S}_z$	$\mathbf{S}_z/0$	$\mathbf{S}_y/\mathbf{S}_x$	$\mathbf{S}_x/\mathbf{S}_y$	$\mathbf{S}_x/\mathbf{S}_y$	$\mathbf{S}_y/\mathbf{S}_x$	$\mathbf{S}_z/0$	$0/\mathbf{S}_z$

Table 11
Restrictions on the form of $\mathbf{S}(\mathbf{k})$ for any wavevector $\mathbf{k} \in L$ when $\Gamma_e = 2'2'2'$.

In each case, the form of $\mathbf{S}(\mathbf{k})$ depends on the particular values of the phase functions for the generators $2'_{\bar{x}}$, $2'_{\bar{y}}$ and $2'_{\bar{z}}$ of Γ_e, and on the parities of n_1+n_3, n_2+n_4 and l, where $\mathbf{k} = \sum_{i=1}^4 n_i \mathbf{b}^{(i)} + l\mathbf{c}$.

Lattice spin group				n_1+n_3 even				n_1+n_3 odd			
				n_2+n_4 even		n_2+n_4 odd		n_2+n_4 even		n_2+n_4 odd	
Symbols	$\Phi_e^{2'_{\bar{x}}}(\mathbf{b}^{(i)}\mathbf{c})$	$\Phi_e^{2'_{\bar{y}}}(\mathbf{b}^{(i)}\mathbf{c})$	$\Phi_e^{2'_{\bar{z}}}(\mathbf{b}^{(i)}\mathbf{c})$	l even	l odd	l even	l odd	l even	l odd	l even	l odd
$P^{2'2'2'}_{P+p,2c}$	$A_0 0$	$A_1 0$	$0\,\frac{1}{2}$	0	$\mathbf{S}_z$	$\mathbf{S}_x$	0	$\mathbf{S}_y$	0	0	0
$P^{2'2'2'}_{P+p,S}$	$A_0 0$	$A_1 0$	$\frac{1}{2}\,\frac{1}{2}$	0	$\mathbf{S}_z$	0	$\mathbf{S}_x$	0	$\mathbf{S}_y$	0	0
$P^{2'2'2'}_{I+p,2c}$	$A_0\,\frac{1}{2}$	$A_1\,\frac{1}{2}$	$0\,\frac{1}{2}$	0	0	$\mathbf{S}_x$	0	$\mathbf{S}_y$	0	0	$\mathbf{S}_z$
$P^{2'2'2'}_{I+p,S}$	$A_0\,\frac{1}{2}$	$A_1\,\frac{1}{2}$	$\frac{1}{2}\,\frac{1}{2}$	0	0	0	$\mathbf{S}_y$	0	$\mathbf{S}_x$	0	$\mathbf{S}_z$

operations paired with these point-group elements, without identifying them explicitly.

8.1. Calculation of selection rules due to Γ_e

If γ is an operation of order 2 then its phases $\Phi_e^\gamma(\mathbf{k})$ are either 0 or 1/2. In this case, equation (66) reduces to

$$\gamma\mathbf{S}(\mathbf{k}) = \begin{cases} \mathbf{S}(\mathbf{k}) & \text{if } \Phi_e^\gamma(\mathbf{k}) \equiv 0, \\ -\mathbf{S}(\mathbf{k}) & \text{if } \Phi_e^\gamma(\mathbf{k}) \equiv \frac{1}{2}, \end{cases} \tag{68}$$

so, if $\Phi_e^\gamma(\mathbf{k}) \equiv 0$, $\mathbf{S}(\mathbf{k})$ must be invariant under γ and, if $\Phi_e^\gamma(\mathbf{k}) \equiv 1/2$, it must change its sign under γ. This implies different constraints on the form of $\mathbf{S}(\mathbf{k})$ depending on the particular type of operation of order 2:

1. If γ is the time inversion ε', then $\mathbf{S}(\mathbf{k}) = 0$ if $\Phi_e^\gamma(\mathbf{k}) \equiv 0$ and there are no constraints on $\mathbf{S}(\mathbf{k})$ if $\Phi_e^\gamma(\mathbf{k}) \equiv 1/2$.
2. If γ is a twofold rotation $2_{\bar{z}}$, then $\mathbf{S}(\mathbf{k}) = \mathbf{S}_z$ if $\Phi_e^\gamma(\mathbf{k}) \equiv 0$ and $\mathbf{S}(\mathbf{k}) = \mathbf{S}_{xy}$ if $\Phi_e^\gamma(\mathbf{k}) \equiv 1/2$. Similar constraints are obtained for rotations about the other two axes.
3. If γ is a twofold rotation followed by time inversion $2'_{\bar{z}}$, then $\mathbf{S}(\mathbf{k}) = \mathbf{S}_{xy}$ if $\Phi_e^\gamma(\mathbf{k}) \equiv 0$ and $\mathbf{S}(\mathbf{k}) = \mathbf{S}_z$ if $\Phi_e^\gamma(\mathbf{k}) \equiv 1/2$. Similar constraints are obtained for primed rotations about the other two axes.

Thus, for lattice spin groups Γ_e containing only operations of order 2, the form of $\mathbf{S}(\mathbf{k})$ depends on whether the phases at $\mathbf{k} = \sum_{i=1}^4 n_i \mathbf{b}^{(i)} + l\mathbf{c}$, associated with all the operations, are 0 or 1/2. This can easily be calculated for each Γ_e from the values of its phase functions on the lattice-generating vectors. The outcome depends, at most, on the parities of n_1+n_3, n_2+n_4 and l. Tables 8–11 summarize the results for all such Γ_e.

For operations of order greater than 2, we find that

4. If γ is an n-fold rotation $n_{\bar{z}}$ ($n > 2$), then equation (66) requires $\mathbf{S}(\mathbf{k})$ to acquire the phase $2\pi\Phi_e^{n_{\bar{z}}}(\mathbf{k})$ upon application of the n-fold rotation. One can directly verify that the only possible forms that $\mathbf{S}$ can have that satisfy this requirement are

$$\mathbf{S}(\mathbf{k}) = \begin{cases} \mathbf{S}_z & \text{if } \Phi_e^{n_{\bar{z}}}(\mathbf{k}) \equiv 0, \\ \mathbf{S}_\pm & \text{if } \Phi_e^{n_{\bar{z}}}(\mathbf{k}) \equiv \pm\frac{1}{n}, \\ 0 & \text{otherwise.} \end{cases} \tag{69}$$

5. If γ is an n-fold rotation followed by time inversion $n'_{\bar{z}}$, then one can obtain the constraints on the form of $\mathbf{S}$ from the constraints (69) by adding 1/2 to the phases, thus

$$\mathbf{S}(\mathbf{k}) = \begin{cases} \mathbf{S}_z & \text{if } \Phi_e^{n'_{\bar{z}}}(\mathbf{k}) \equiv \frac{1}{2}, \\ \mathbf{S}_\pm & \text{if } \Phi_e^{n'_{\bar{z}}}(\mathbf{k}) \equiv \frac{1}{2} \pm \frac{1}{n}, \\ 0 & \text{otherwise.} \end{cases} \tag{70}$$

Table 12 summarizes the results for lattice spin groups $\Gamma_e = n$, n' and $n1'$, containing operations of order greater than 2.

Table 12
Restrictions on the form of $\mathbf{S}(\mathbf{k})$ for any wavevector $\mathbf{k} \in L$ when $\Gamma_e = n, n'$ and $n1'$.

In each case, the form of $\mathbf{S}(\mathbf{k})$ depends on the particular value of the phase functions for the generators of Γ_e, on the parity of $\sum n_i$, and on the value of l, where $\mathbf{k} = \sum_{i=1}^{4} n_i \mathbf{b}^{(i)} + l\mathbf{c}$. The conditions for obtaining non-extinct $\mathbf{S}(\mathbf{k})$ are listed separately for $\Gamma_e = n$, $\Gamma_e = n'$ (even n) and $\Gamma_e = n'$ (odd n). The restrictions on the form of $\mathbf{S}(\mathbf{k})$ for $\Gamma_e = n1'$ are obtained from those of $\Gamma_e = n$ with the additional requirement that $\mathbf{S}(\mathbf{k}) = 0$ if: (i) $\Phi_e^{\varepsilon'}(\mathbf{b}^{(i)}\mathbf{c}) \equiv 0\frac{1}{2}$ and l is even; (ii) $\Phi_e^{\varepsilon'}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \frac{1}{2}0$ and $\sum n_i$ is even; or (iii) $\Phi_e^{\varepsilon'}(\mathbf{b}^{(i)}\mathbf{c}) \equiv \frac{1}{2}\frac{1}{2}$ and $\sum n_i + l$ is even.

$\Gamma_e = n$		$\Gamma_e = n'$ (even n)		$\Gamma_e = n'$ (odd n)			
$\Phi_e^{n_{\bar z}}(\mathbf{b}^{(i)}\mathbf{c})$	lj (mod n)	$\Phi_e^{n'_{\bar z}}(\mathbf{b}^{(i)}\mathbf{c})$	lj (mod n)	$\Phi_e^{n'_{\bar z}}(\mathbf{b}^{(i)}\mathbf{c})$	lj (mod $2n$)	$\sum n_i$ even	$\sum n_i$ odd
$P^n_{n_jc}, S^n_{n_jc}$		$P^{n'}_{n_jc}, S^{n'}_{n_jc}$		$P^{n'}_{(2n)_jc}, S^{n'}_{(2n)_jc}$			
$0\frac{j}{n}$	0	$0\frac{j}{n}$	$\frac{n}{2}$	$0\frac{j}{2n}$	n	$\mathbf{S}_z$	$\mathbf{S}_z$
	+1		$\frac{n}{2}+1$		$n+2$	$\mathbf{S}_+$	$\mathbf{S}_+$
	−1		$\frac{n}{2}-1$		$n-2$	$\mathbf{S}_-$	$\mathbf{S}_-$
	otherwise		otherwise		otherwise	0	0
$P^n_{n_jS}, S^4_{4_jS}$		$P^{n'}_{n_jS}, S^{4'}_{4_jS}$		$P^{n'}_{(2n)_jS}$			
$\frac{1}{2}\frac{j}{n}$	0	$\frac{1}{2}\frac{j}{n}$	$\frac{n}{2}$	$\frac{1}{2}\frac{j}{2n}$	n	$\mathbf{S}_z$	0
	+1		$\frac{n}{2}+1$		$n+2$	$\mathbf{S}_+$	0
	−1		$\frac{n}{2}-1$		$n-2$	$\mathbf{S}_-$	0
	$\frac{n}{2}$		0		0	0	$\mathbf{S}_z$
	$\frac{n}{2}+1$		+1		+1	0	$\mathbf{S}_+$
	$\frac{n}{2}-1$		−1		−1	0	$\mathbf{S}_-$
	otherwise		otherwise		otherwise	0	0
$P^n_{(n/2)_jP}$		$P^{n'}_{(n/2)_jP}$		$P^{n'}_{n_jP}$			
$\frac{1}{2}\frac{2j}{n}$	0 or $\frac{n}{2}$	$\frac{1}{2}\frac{2j}{n}$	0 or $\frac{n}{2}$	$\frac{1}{2}\frac{j}{n}$	0 or n	$\mathbf{S}_z$	0
	$\frac{n}{4}+\frac{1}{2}$ or $\frac{3n}{4}+\frac{1}{2}$		$\frac{n}{4}+\frac{1}{2}$ or $\frac{3n}{4}+\frac{1}{2}$		$\frac{n}{2}+1$ or $\frac{3n}{2}+1$	0	$\mathbf{S}_+$
	$\frac{n}{4}-\frac{1}{2}$ or $\frac{3n}{4}-\frac{1}{2}$		$\frac{n}{4}-\frac{1}{2}$ or $\frac{3n}{4}-\frac{1}{2}$		$\frac{n}{2}-1$ or $\frac{3n}{2}-1$	0	$\mathbf{S}_-$
	otherwise		otherwise		otherwise	0	0

8.2. Additional selection rules on invariant subspaces of nontrivial point-group operations

In addition to the selection rules arising from Γ_e, there are also selection rules that occur when $\mathbf{k}$ lies along one of the rotation axes or within one of the mirror planes and is therefore invariant under additional operations (g, γ) with non-trivial g. In this case, the eigenvalue equation (66) imposes further restrictions on the Fourier coefficients of the spin density field.

8.2.1. Selection rules along the *z* axis. When the eightfold rotation r_8 is in the point group G, it leaves all the wavevectors along the z axis invariant. These wavevectors are given by $\mathbf{k} = l\mathbf{z}$, where l is any integer if the lattice is vertical and l is even if the lattice is staggered. For both lattice types, equation (66), determining the selection rules for these wavevectors, becomes

$$\delta\mathbf{S}(l\mathbf{z}) \equiv e^{-2\pi i l \Phi^{\delta}_{r_8}(\mathbf{c})}\mathbf{S}(l\mathbf{z}), \tag{71}$$

where $\mathbf{c}$ is the appropriate stacking vector. When G is generated by $\bar r_8$ and does not contain r_8, the wavevectors along the z axis are left invariant by $\bar r_8^2$ and its powers. The phase $\Phi^{\bar\delta^2}_{\bar r_8^2}(l\mathbf{z}) \equiv \Phi^{\bar\delta}_{\bar r_8}(\bar r_8 l\mathbf{z}) + \Phi^{\bar\delta}_{\bar r_8}(l\mathbf{z})$ is necessarily zero because $\bar r_8 l\mathbf{z} = -l\mathbf{z}$. Equation (66) can therefore be written as

$$\bar\delta^2\mathbf{S}(l\mathbf{z}) = \mathbf{S}(l\mathbf{z}), \tag{72}$$

requiring $\mathbf{S}(l\mathbf{z})$ to be invariant under $\bar\delta^2$, where $\bar\delta$ is the spin-space operation paired with $\bar r_8$.

8.2.2. Selection rules within the horizontal mirror *h*. If the horizontal mirror h is present in the point group then all the Fourier coefficients of the spin density field associated with wavevectors $\mathbf{k}_h = \sum_i n_i\mathbf{b}^{(i)}$ in the horizontal sublattice are subject to selection rules, dictated by the values of the phase function Φ^{η}_h. Equation (66), for both lattice types, is simply

$$\eta\mathbf{S}(\mathbf{k}_h) \equiv e^{-2\pi i \sum_{i=1}^{4} n_i \Phi^{\eta}_h(\mathbf{b}^{(i)})}\mathbf{S}(\mathbf{k}_h). \tag{73}$$

Thus, if a horizontal mirror is present in the point group, then $\mathbf{S}(\mathbf{k}_h)$, for $\mathbf{k}_h = \sum_i n_i\mathbf{b}^{(i)}$ in the horizontal sublattice, must remain invariant under η unless (*a*) $\Phi^{\eta}_h(\mathbf{b}^{(i)}) \equiv \frac{1}{2}0\frac{1}{2}0$ and $n_1 + n_3$ is odd; or (*b*) $\Phi^{\eta}_h(\mathbf{b}^{(i)}) \equiv 0\frac{1}{2}0\frac{1}{2}$ and $n_2 + n_4$ is odd; or (*c*) $\Phi^{\eta}_h(\mathbf{b}^{(i)}) \equiv \frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$ and $\sum_i n_i$ is odd; in which case, $\mathbf{S}(\mathbf{k}_h)$ must change its sign under η.

8.2.3. Selection rules within vertical mirrors and along dihedral axes. There are two sets of conjugate vertical mirrors which we have labeled m and m' and two sets of conjugate dihedral axes d and d'. It is sufficient to determine the selection rules for a single member of each of these four sets because the selection rules for the remaining conjugate operations can be inferred from the eightfold rotational symmetry of the spin density field. To see this, take for example the operation (m, μ) and examine all the wavevectors $\mathbf{k}$, satisfying $m\mathbf{k} = \mathbf{k}$, to obtain the general selection rules for the invariant subspace of m,

$$\mu\mathbf{S}(\mathbf{k}) \equiv e^{-2\pi i \Phi^{\mu}_m(\mathbf{k})}\mathbf{S}(\mathbf{k}). \tag{74}$$

If g is the eightfold generator of the point group (r_8 or $\bar r_8$), paired with the spin-space operation δ, then the selection rules on the invariant subspaces of the remaining three conjugate operations are simply given by

$$\delta^n \mu \delta^{-n} \mathbf{S}(g^n \mathbf{k}) \equiv e^{-2\pi i \Phi_m^\mu(\mathbf{k})} \mathbf{S}(g^n \mathbf{k}), \quad n = 1, 2, 3, \tag{75}$$

where we have used the fact that, since $m\mathbf{k} = \mathbf{k}$, it follows from successive applications of the group compatibility condition (1) that

$$\Phi_{gmg^{-1}}^{\delta\mu\delta^{-1}}(g\mathbf{k}) \equiv \Phi_m^\mu(\mathbf{k}). \tag{76}$$

Similar expressions can be derived for the other operations and so we proceed below to obtain the general selection rules only for the vertical mirrors and dihedral axes that are oriented either along the generating vector $\mathbf{b}^{(1)}$ or between the two generating vectors $\mathbf{b}^{(1)}$ and $\mathbf{b}^{(2)}$ (as depicted in Fig. 1).

Wavevectors along the dihedral axis d, containing the generating vector $\mathbf{b}^{(1)}$, on either lattice type, can be expressed as $\mathbf{k}_d = n_1\mathbf{b}^{(1)} + n_2(\mathbf{b}^{(2)} - \mathbf{b}^{(4)})$ for any two integers n_1 and n_2. Since it is always the case that $\Phi_d^\alpha(\mathbf{b}^{(2)} - \mathbf{b}^{(4)}) \equiv 0$, the selection rules for such wavevectors are determined by

$$\alpha \mathbf{S}(\mathbf{k}_d) \equiv e^{-2\pi i n_1 \Phi_d^\alpha(\mathbf{b}^{(1)})} \mathbf{S}(\mathbf{k}_d). \tag{77}$$

Thus, if a dihedral operation (d, α) is present in the spin point group, then $\mathbf{S}(\mathbf{k}_d)$, for $\mathbf{k}_d$ along the axis of d, must remain invariant under α, unless $\Phi_d^\alpha(\mathbf{b}^{(1)}) \equiv \frac{1}{2}$ and n_1 is odd, in which case $\mathbf{S}(\mathbf{k}_d)$ must change its sign under α.

Wavevectors along the dihedral axis d', between the generating vectors $\mathbf{b}^{(1)}$ and $\mathbf{b}^{(2)}$, on either lattice type, can be expressed as $\mathbf{k}_{d'} = n_1(\mathbf{b}^{(1)} + \mathbf{b}^{(2)}) + n_3(\mathbf{b}^{(3)} - \mathbf{b}^{(4)})$ for any two integers n_1 and n_3. Since it is always the case that $\Phi_{d'}^{\alpha'}(\mathbf{b}^{(1)} - \mathbf{b}^{(3)}) \equiv \Phi_{d'}^{\alpha'}(\mathbf{b}^{(2)} + \mathbf{b}^{(4)}) \equiv 0$, the selection rules are determined by

$$\alpha' \mathbf{S}(\mathbf{k}_{d'}) \equiv e^{-2\pi i (n_1+n_3) \Phi_{d'}^{\alpha'}(\mathbf{b}^{(1)}+\mathbf{b}^{(2)})} \mathbf{S}(\mathbf{k}_{d'}). \tag{78}$$

Thus, if a dihedral operation (d', α') is present in the spin point group then $\mathbf{S}(\mathbf{k}_{d'})$, for $\mathbf{k}_{d'}$ along the axis of d', must remain invariant under α', unless $\Phi_{d'}^{\alpha'}(\mathbf{b}^{(i)}) \equiv 0\frac{1}{2}0\frac{1}{2}$ or $\frac{1}{2}0\frac{1}{2}0$ and $n_1 + n_3$ is odd, in which case, $\mathbf{S}(\mathbf{k}_{d'})$ must change its sign under α'. The operation α', as well as the values of the phase function $\Phi_{d'}^{\alpha'}$, are determined for each separate spin point group according to the generating relations for that group, namely, $(d', \alpha') = (r_8, \delta)(d, \alpha)$ for point group 822, $(d', \alpha') = (\bar{r}_8, \delta)(m, \mu)$ for point group $\bar{8}m2$ and $(d', \alpha') = (r_8, \delta)(m, \mu)(h, \eta)$ for point group $8/mmm$.

Wavevectors within the vertical mirror m, containing the generating vector $\mathbf{b}^{(1)}$, can be expressed as $\mathbf{k}_m = n_1\mathbf{b}^{(1)} + n_2(\mathbf{b}^{(2)} - \mathbf{b}^{(4)}) + l\mathbf{z}$, where l is any integer if the lattice is vertical and l is even if the lattice is staggered. This is because there are no wavevectors in odd layers of S lattices that are invariant under mirrors of type m (Rabson *et al.*, 1991, footnote 46). Since it is always the case that $\Phi_m^\mu(\mathbf{b}^{(2)} - \mathbf{b}^{(4)}) \equiv 0$, the selection rules for such wavevectors are determined by

$$\mu \mathbf{S}(\mathbf{k}_m) \equiv e^{-2\pi i [n_1 \Phi_m^\mu(\mathbf{b}^{(1)}) + l \Phi_m^\mu(\mathbf{c})]} \mathbf{S}(\mathbf{k}_m). \tag{79}$$

Finally, wavevectors within the vertical mirror m', between the generating vectors $\mathbf{b}^{(1)}$ and $\mathbf{b}^{(2)}$, on both lattice types, can be expressed as $\mathbf{k}_{m'} = n_1(\mathbf{b}^{(1)} + \mathbf{b}^{(2)}) + n_3(\mathbf{b}^{(3)} - \mathbf{b}^{(4)}) + l\mathbf{c}$ for any three integers n_1, n_3 and l, where $\mathbf{c}$ is the appropriate stacking vector. Since it is always the case that $\Phi_{m'}^{\mu'}(\mathbf{b}^{(1)} - \mathbf{b}^{(3)}) \equiv \Phi_{m'}^{\mu'}(\mathbf{b}^{(2)} + \mathbf{b}^{(4)}) \equiv 0$, the selection rules are determined by

$$\mu' \mathbf{S}(\mathbf{k}_{m'}) \equiv e^{-2\pi i [(n_1+n_3)\Phi_{m'}^{\mu'}(\mathbf{b}^{(1)}+\mathbf{b}^{(2)}) + l \Phi_{m'}^{\mu'}(\mathbf{c})]} \mathbf{S}(\mathbf{k}_{d'}). \tag{80}$$

This completes the general calculation of selection rules on invariant subspaces of point-group operations. One can apply these rules in a straightforward manner to each spin space group once the spin-space operations δ, η, μ and α are explicitly identified.

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