# QUASIPERIODIC SPIN SPACE GROUPS

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## ABSTRACT

An outline is given of the spin space-group classification of quasiperiodic arrangements of spins. It is based on an extension to multicomponent quasiperiodic fields of the Fourier-space approach to crystal symmetry. The classification of decagonal spin space groups in two dimensions is given as an example. A group theoretic argument is given which is used to determine extinctions in a neutron diffraction experiment, associated with a given spin space group.

## 1. Quasiperiodic Spin Density Fields

We consider quasiperiodic arrangements of spins, like the ones shown in Figure 1, described by a spin density field $\mathbf{S}(\mathbf{r})$ which transforms as an axial vector field under rotations and changes sign under time inversion. The symmetry groups of periodic spin density fields, called *spin groups*, were treated by Litvin and Opechowski.[1] Janner and Janssen[2] have suggested the possibility of extending the superspace procedure to treat quasiperiodic spin arrangements. Here I outline the symmetry classification of quasiperiodic as well as periodic spin density fields using the Fourier-space approach to crystal symmetry[3] which has been extended to deal with multicomponent fields.[4,5]

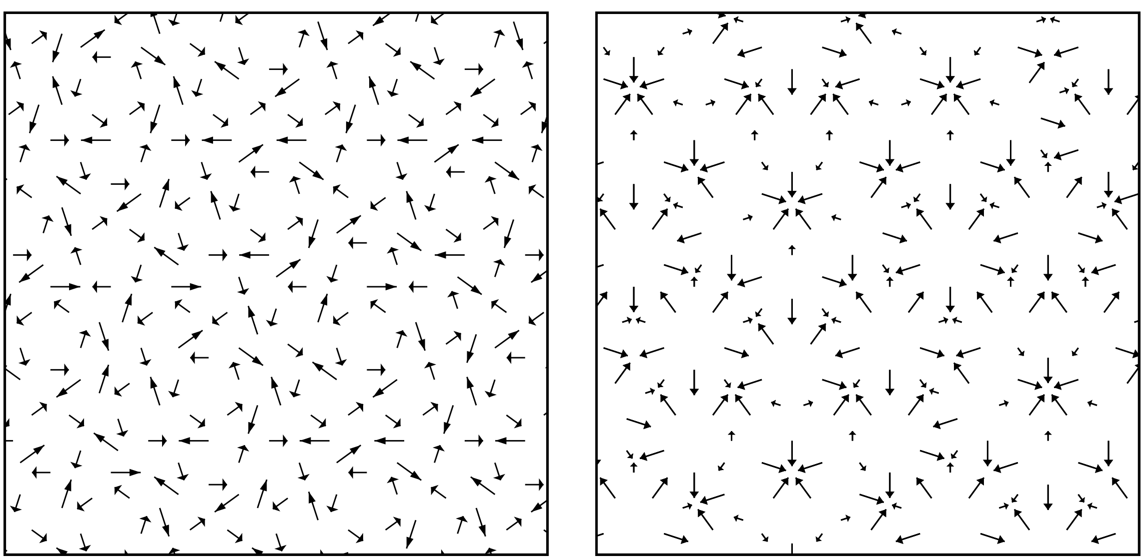

**Figure 1. Examples of Decagonal Spin Arrangements.** The left one has a spin point group with $G = 10mm$, $G_\epsilon = 1$, $\Gamma = (10)2'2'$, and $\Gamma_e = 1$, generated by $(10, 10_{\bar{z}}), (m, 2'_{\bar{x}})$. The right one has a spin point group with $G = 10mm$, $G_\epsilon = 2$, $\Gamma = 52'$, and $\Gamma_e = 1$, generated by $(10, 5^3_{\bar{z}}), (m, 2'_{\bar{x}})$. Both are decorations of the Penrose tiling. Spins are located at the tails of the arrows.

Two quasiperiodic fields $\mathbf{S}(\mathbf{r})$ and $\mathbf{S}'(\mathbf{r})$ are *indistinguishable* if the positionally averaged autocorrelation functions of $\mathbf{S}(\mathbf{r})$ of any order, and for any choice of components, are identical to the corresponding autocorrelation functions of $\mathbf{S}'(\mathbf{r})$. As such, $\mathbf{S}(\mathbf{r})$ and $\mathbf{S}'(\mathbf{r})$ have the same distribution of substructures on any scale. Lifshitz and Mermin[5] prove that an equivalent statement of indistinguishability is that the Fourier coefficients of the two fields are related by

$$\mathbf{S}'(\mathbf{k}) = e^{2\pi i\chi(\mathbf{k})}\mathbf{S}(\mathbf{k}) \ , \tag{1}$$

where $\chi$, called a *gauge function*, is the same for all components and is linear modulo an integer over the lattice $L$ of wave vectors. The *lattice* is the set of all integral linear combinations of wave vectors at which at least one component of the field has a non-vanishing Fourier coefficient.

## 2. The Classification Scheme

The *point group* $G$ of $\mathbf{S}(\mathbf{r})$ is the set of all operations $g$ from $O(3)$ that leave it indistinguishable to within a transformation $\gamma$ of its components. For every pair $(g,\gamma)$ there exists a gauge function, $\Phi_g^\gamma(\mathbf{k})$, called a *phase function*, which satisfies

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

The transformations $\gamma$ in spin space are proper rotations possibly combined with time inversion. It is enough to consider only proper rotations because the spins are axial vectors. The identity in spin space is denoted by $\epsilon$, the time inversion operator by $\epsilon'$, and any spin rotation $\gamma$ followed by the time inversion is denoted by $\gamma'$. The rotations in spin space are decoupled from those in physical space so there can be many different $\gamma$'s associated with each element of $G$.

The possible relations between elements of the point group $G$ and the spin transformations $\gamma$ are severely constrained by Eq. (2). If $(g,\gamma)$ and $(h,\delta)$ both satisfy (2) then so does $(gh,\gamma\delta)$. The set $\Gamma$ of all the transformations $\gamma$ is a group, and the set of pairs $(g,\gamma)$ satisfying (2) is a subgroup of $G\times\Gamma$, called the *spin point group* $G_{\mathbf{S}}$. The corresponding phase functions must satisfy the *group compatibility condition*:

$$\Phi_{gh}^{\gamma\delta}(\mathbf{k}) \equiv \Phi_g^\gamma(h\mathbf{k}) + \Phi_h^\delta(\mathbf{k}) \ , \tag{3}$$

where '$\equiv$' denotes equality modulo an integer.

When enumerating the possible symmetry classes of a field $\mathbf{S}$, for a given lattice $L$ and point group $G$, one first needs to consider all distinct spin point groups, associating a set $\Gamma_g$ of spin transformations with every point group operation $g$. These must satisfy the following requirements imposed by Eq. (2):

*(1)* The set of transformations $\Gamma_e$ associated with the identity of $G$ forms an abelian normal subgroup of $\Gamma$, where each $\Gamma_g$ is a coset of $\Gamma_e$ in $\Gamma$. It follows from (3) that if $\gamma$ is in $\Gamma_g$ and $\delta$ is in $\Gamma_e$ then

$$\Phi_e^{\gamma^{-1}\delta\gamma}(\mathbf{k}) \equiv \Phi_e^\delta(g\mathbf{k}) \ . \tag{4}$$

*(2)* The set of point group operations $G_\epsilon$ associated with the identity of $\Gamma$ is a normal subgroup of $G$.

*(3)* The two quotient groups $G/G_\epsilon$ and $\Gamma/\Gamma_e$ are isomorphic, with $\Gamma_g = \Gamma_h$ if and only if $g$ and $h$ are in the same coset of $G_\epsilon$.

For each spin point group $G_{\mathbf{S}}$ one needs to find all the inequivalent sets of phase functions satisfying the associated group compatibility conditions (3). The *spin space-group* classification is merely an organization of these sets of phase functions into equivalence classes according to two criteria:

**Table 1. Decagonal Spin Space Groups in 2 Dimensions.** Spin point groups are specified in the right-hand column by their generators $(g,\gamma)$ and separated by semicolons. The 5-fold symmetry of the lattice restricts $\Gamma_e$ to be either the identity or the point group 5. In the first case I consider for each point group $G$ and each of its normal subgroups $G_\epsilon$ all groups $\Gamma$ which are isomorphic to $G/G_\epsilon$, and all inequivalent isomorphisms between $\Gamma$ and $G/G_\epsilon$. When $\Gamma_e = 5$, further constraints are imposed by Eq. (4) which restrict the possible choices for the normal subgroup $G_\epsilon$. There is only a single spin space group for each spin point group which is a result of having only symmorphic space groups in the scalar case. In a suitable gauge (5), all phase functions for the generators given in the table are zero everywhere except for $\Phi_e^{5_{\bar z}}$ which, using scale equivalence (6), can be shown to have the value 1/5 at a 5-fold star of wave vectors which generate the lattice. Spin groups with $\Gamma = 1$ are the trivial ferromagnetic groups. Spin groups where $\Gamma$ is the time-inversion group $T = \{\epsilon, \epsilon'\}$ are equivalent to black-and-white groups, often called magnetic groups. $\bar x$, $\bar y$, and $\bar z$ denote the coordinate system in spin space which is decoupled from that in physical space.

| $\Gamma_e$ | $G$ | $G_\epsilon$ | $G/G_\epsilon$ | $\Gamma$ | Generators of the Spin Point Group |
|---|---|---|---|---|---|
| 1 | $10mm$ | $10mm$ | 1 | 1 | $(10,\epsilon),(m,\epsilon)$; |
| | | 10 | $m$ | 2; $2'$; $T$; | $(10,\epsilon),(m,2_{\bar z})$; $(10,\epsilon),(m,2'_{\bar z})$; $(10,\epsilon),(m,\epsilon')$; |
| | | $5m1$ | 2 | 2; $2'$; $T$; | $(10,2_{\bar z}),(m,\epsilon)$; $(10,2'_{\bar z}),(m,\epsilon)$; $(10,\epsilon'),(m,\epsilon)$; |
| | | $51m$ | 2 | 2; $2'$; $T$; | $(10,2_{\bar z}),(m,2_{\bar z})$; $(10,2'_{\bar z}),(m,2'_{\bar z})$; $(10,\epsilon'),(m,\epsilon')$; |
| | | 5 | $2mm$ | 222; | $(10,2_{\bar z}),(m,2_{\bar x})$; |
| | | | | $2'2'2$; | $(10,2'_{\bar z}),(m,2_{\bar x})$; $(10,2_{\bar z}),(m,2'_{\bar x})$; $(10,2'_{\bar z}),(m,2'_{\bar x})$; |
| | | | | $2\times T$; | $(10,2_{\bar z}),(m,\epsilon')$; $(10,2'_{\bar z}),(m,\epsilon')$; $(10,2_{\bar z}),(m,2'_{\bar z})$; |
| | | | | | $(10,\epsilon'),(m,2_{\bar z})$; $(10,\epsilon'),(m,2'_{\bar z})$; $(10,2'_{\bar z}),(m,2_{\bar z})$; |
| | | 2 | $5m$ | 52; | $(10,5_{\bar z}^{\pm1}),(m,2_{\bar x})$; $(10,5_{\bar z}^{\pm2}),(m,2_{\bar x})$; |
| | | | | $52'$; | $(10,5_{\bar z}^{\pm1}),(m,2'_{\bar x})$; $(10,5_{\bar z}^{\pm2}),(m,2'_{\bar x})$; |
| | | 1 | $10mm$ | (10)22; | $(10,10_{\bar z}^{\pm1}),(m,2_{\bar x})$; $(10,10_{\bar z}^{\pm3}),(m,2_{\bar x})$; |
| | | | | $(10)2'2'$; | $(10,10_{\bar z}^{\pm1}),(m,2'_{\bar x})$; $(10,10_{\bar z}^{\pm3}),(m,2'_{\bar x})$; |
| | | | | $(10')22'$; | $(10,10_{\bar z}^{\pm1\prime}),(m,2_{\bar x})$; $(10,10_{\bar z}^{\pm3\prime}),(m,2_{\bar x})$; |
| | | | | $(10')2'2$; | $(10,10_{\bar z}^{\pm1\prime}),(m,2'_{\bar x})$; $(10,10_{\bar z}^{\pm3\prime}),(m,2'_{\bar x})$; |
| | 10 | 10 | 1 | 1 | $(10,\epsilon)$; |
| | | 5 | 2 | 2; $2'$; $T$; | $(10,2_{\bar z})$; $(10,2'_{\bar z})$; $(10,\epsilon')$; |
| | | 2 | 5 | 5 | $(10,5_{\bar z}^{\pm1})$; $(10,5_{\bar z}^{\pm2})$; |
| | | 1 | 10 | 10; | $(10,10_{\bar z}^{\pm1})$; $(10,10_{\bar z}^{\pm3})$; |
| | | | | $10'$; | $(10,10_{\bar z}^{\pm1\prime})$; $(10,10_{\bar z}^{\pm3\prime})$; |
| 5 | $10mm$ | $5m1$ | 2 | 52; $52'$; | $(e,5_{\bar z}),(10,2_{\bar x}),(m,\epsilon)$; $(e,5_{\bar z}),(10,2'_{\bar x}),(m,\epsilon)$; |
| | | 5 | $2mm$ | $52\times T$; | $(e,5_{\bar z}),(10,2_{\bar x}),(m,\epsilon')$; $(e,5_{\bar z}),(10,2'_{\bar x}),(m,\epsilon')$; |
| | | | | (10)22 | $(e,5_{\bar z}),(10,2_{\bar x}),(m,2_{\bar z})$; |
| | | | | $(10)2'2'$ | $(e,5_{\bar z}),(10,2'_{\bar x}),(m,2_{\bar z})$; |
| | | | | $(10')22'$ | $(e,5_{\bar z}),(10,2_{\bar x}),(m,2'_{\bar z})$; |
| | | | | $(10')2'2$ | $(e,5_{\bar z}),(10,2'_{\bar x}),(m,2'_{\bar z})$; |
| | 10 | 5 | 2 | 52; $52'$; | $(e,5_{\bar z}),(10,2_{\bar x})$; $(e,5_{\bar z}),(10,2'_{\bar x})$; |

1. Two sets of phase functions $\Phi$ and $\Phi'$ that describe indistinguishable fields $\mathbf{S}$ and $\mathbf{S}'$, related by a gauge function $\chi$, should clearly be associated with the same spin space group. Two such sets are related by a *gauge transformation*

$$\Phi'^{\gamma}_{g}(\mathbf{k}) \equiv \Phi^{\gamma}_{g}(\mathbf{k}) + \chi([g-1]\mathbf{k}) \ , \tag{5}$$

and belong to the same *gauge-equivalence class.*

2. Two sets of phase functions $\Phi$ and $\Phi'$ may also be counted as *scale-equivalent* if there is a symmetry $s$ of the lattice $L$, for which $G \to sGs^{-1}$ is an automorphism of $G$, and there is an automorphism $\sigma$ of $\Gamma$, which together take one set into the other

$$\Phi'^{\gamma}_{g}(\mathbf{k}) = \Phi^{\sigma\gamma\sigma^{-1}}_{sgs^{-1}}(s\mathbf{k}) \ . \tag{6}$$

The classes of phase functions under gauge and scale equivalence for a given spin point group correspond to the spin space groups in the periodic case, and constitute the extension of the spin space group classification scheme to the general case of aperiodic spin density fields. In Table 1 I illustrate, as an example, the classification of all decagonal spin space groups in two dimensions.

## 3. Extinctions

For every wave vector $\mathbf{k}$ in the lattice we define $(G_\mathbf{S})_\mathbf{k}$ to be the subgroup of the spin point group containing all pairs with physical-space rotations leaving $\mathbf{k}$ invariant. The associated phases satisfy

$$\Phi_{gh}^{\gamma\delta}(\mathbf{k}) \equiv \Phi_g^\gamma(\mathbf{k}) + \Phi_h^\delta(\mathbf{k}) \tag{7}$$

as a special case of (3), and so the complex numbers $e^{2\pi i \Phi_g^\gamma(\mathbf{k})}$ constitute a 1-dimensional representation of the subgroup $(G_\mathbf{S})_\mathbf{k}$. In addition we find from (2) that

$$\gamma\mathbf{S}(\mathbf{k}) = e^{-2\pi i \Phi_g^\gamma(\mathbf{k})}\mathbf{S}(\mathbf{k}) \ . \tag{8}$$

Equation (8) implies that the action of the elements of the subgroup $(G_\mathbf{S})_\mathbf{k}$ on $\mathbf{S}(\mathbf{k})$ is to transform it under (the inverse of) this 1-dimensional representation, and requires $\mathbf{S}(\mathbf{k})$ to have a specific form.

Since $\mathbf{S}(\mathbf{k})$ is an axial vector, it transforms under the 3-dimensional representation of the $(g, \gamma)$ which is defined by the action of the $3\times 3$ matrices $\gamma$ on its components (with the $g$'s leaving it invariant). It is then easy to determine whether $\mathbf{S}(\mathbf{k})$ can have the form required by (8), by checking whether the decomposition of this 3-dimensional representation of $(G_\mathbf{S})_\mathbf{k}$ contains the 1-dimensional representation (8). If it does than $\mathbf{S}(\mathbf{k})$ will have the required from; if it does not then $\mathbf{S}(\mathbf{k})$ will necessarily vanish.

It follows from Eq. (5) that the phases $\Phi_g^\gamma(\mathbf{k})$ for all $(g, \gamma)$ in $(G_\mathbf{S})_\mathbf{k}$ are gauge-invariant. The restrictions on the form of $\mathbf{S}(\mathbf{k})$ are therefore independent of the choice of gauge. Using these we can determine the extinctions in neutron diffraction experiments via standard formulae which give the neutron diffraction intensity at $\mathbf{k}$ in terms of $\mathbf{S}(\mathbf{k})$ and its orientation relative to $\mathbf{k}$.

As an example, note that in the case of spin point groups with a non-trivial $\Gamma_e$, $(G_\mathbf{S})_\mathbf{k}$ contains $\{e\}\times\Gamma_e$ for any $\mathbf{k}$, restricting the form of $\mathbf{S}(\mathbf{k})$ everywhere according to (8). In the example of decagonal spin space groups with $\Gamma_e = 5$, given in Table 1, it can easily be shown that the only non-vanishing $\mathbf{S}(\mathbf{k})$ are at $\mathbf{k}$'s with $\Phi_e^\gamma(\mathbf{k}) \equiv 0$, requiring $\mathbf{S}(\mathbf{k}) = (0, 0, S)$, or with $\Phi_e^\gamma(\mathbf{k}) \equiv \pm\frac{1}{5}$, requiring $\mathbf{S}(\mathbf{k}) = (S, \pm iS, 0)$. The form of $\mathbf{S}(\mathbf{k})$ at vectors $\mathbf{k}$ with $(G_\mathbf{S})_\mathbf{k}$ larger than $\{e\}\times\Gamma_e$ may be further constrained.

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## 4. References

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