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Symmetry analysis of electronic states for crystals with spiral magnetic order: I. General properties

L M Sandratskii
Institute of Metal Physics, Ural Division of the USSR Academy of Sciences, Sverdlovsk 620219, USSR

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Abstract. This paper is devoted to the systematic study of questions concerning the use of spin-space groups (SSG) in calculation and qualitative analysis of the electronic states for crystals with spiral magnetic order. The types of operators that may enter into the symmetry group of a spiral are investigated. Introduction of the wavevector of an electronic state on the basis of the generalized Bloch theorem is discussed, and it is shown that the possibility of the choice of the wavevector is not unique. The condition imposed on the symmetry operations belonging to the group of a given Bloch vector and the formula describing the symmetry of eigenvalues in reciprocal space are obtained and appear to be substantially different from counterparts used in traditional cases of collinear and non-magnetic crystals. It is shown that, contrary to the traditional cases, there are spiral structures whose spectral symmetry is described by non-symmorphic space groups. The irreducible domain of reciprocal space is found for a number of concrete spiral structures. Methods of construction of the SSG double-valued irreducible representations and also of their basis functions are suggested. Special attention is devoted to the possibility of using the corresponding tables of ordinary space groups. In particular, it is shown that for spirals with hexagonal close-packed crystal structure the traditional tables may be used after minor corrections. The peculiarities of allowance for the operation of time inversion are discussed.

1. Introduction

The success of electron band theory in describing the ground-state properties of collinear magnets is well known. In recent years, methods have been suggested [1–7] that permit calculation of electron states for non-collinear magnetic configurations. Special interest attaches to calculations of the electron spectrum of spiral magnetic configurations. This is because, first, this arrangement of magnetic moments is observed experimentally for a lot of substances (see e.g. [8]) and, secondly, calculating the electron structure for these simplest non-collinear magnetic configurations allows one to draw important qualitative conclusions concerning the electronic properties of collinear magnets at finite temperatures [1, 9–11].

In [3], it has been shown that allowance for the generalized symmetry of the problem on the basis of the theory of spin-space groups enables one to simplify fundamentally the calculation of the electron spectrum of spiral magnetic configurations. The generalized symmetry permits each electronic state to be specified by a definite wavevector $\boldsymbol{k}$ that belongs to the Brillouin zone (BZ) of the chemical lattice. The main feature distinguishing spin-space groups (SSG) from ordinary space groups (SG) is the possibility of independent

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transformations of spin and space sublattices. (According to terminology adopted by specialists in the theory of space groups, the SSG are a particular case of so-called 'colour' groups.) These transformations were introduced for the first time by Herring [12, 13]. A systematic study of the SSG has been made by Naish [14], in connection with the problem of describing the symmetry of magnetic structures, and by Brinkman and Elliott [15], who used SSG primarily to describe the Heisenberg spin Hamiltonian [16]. The present paper is devoted to a systematic investigation of questions connected with the use of SSG in the calculation and symmetry analysis of the electronic structure of spiral magnetic configurations.

The next section discusses the Hamiltonian of the problem and the principles of the construction of the SSG describing the symmetry of the Hamiltonian. In section 3, the generalized Bloch theorem is considered; it is shown that there is more than one way to choose the wavevector characterizing a given electron state. In section 4, classes of operators that may enter into the symmetry groups of spirals are investigated. In section 5, the condition imposed on the SSG operators involved in the group of a given wavevector is derived. The symmetry of the spectrum in reciprocal space is studied. It is shown that both the condition imposed on the operators belonging to the group of the wavevector and the formula describing the symmetry of the spectrum differ greatly from the corresponding traditional results for collinear magnets, which may be described on the basis of SG. It is pointed out that, contrary to the traditional problems, the spectral symmetry for some spiral structures is described by a non-symmorphic space group. Section 6 is closely connected with section 5 and includes a discussion of the irreducible domains of reciprocal space where the spectrum is to be calculated. Sections 7 and 8 are devoted to the construction of irreducible representations (IR) and symmetrized functions. Special attention is paid to the possibility of using the corresponding tables for point groups. In section 9, peculiarities in taking into account the time inversion operation are discussed for the case of spiral structures.

2. One-electron Hamiltonian and its symmetry

In the present paper, we shall restrict ourselves to a consideration of spiral structures of the form

$$e_{jn\perp} = \sin\theta \exp[i\boldsymbol{q}\cdot(\boldsymbol{a}_j + \boldsymbol{t}_n)] \tag{2.1a}$$

$$e_{jnz} = \cos\theta \tag{2.1b}$$

where the vectors $\boldsymbol{e}$ define the directions of atomic magnetic moments, the $\boldsymbol{t}_n$ are the lattice translations, the $\boldsymbol{a}_j$ are the radius vectors of unit-cell atoms, and $\boldsymbol{q}$ is the vector of the spiral. We shall suppose that $\boldsymbol{a}_1 = 0$. Formulae (2.1) give the projections of vector $\boldsymbol{e}$ on the xy plane and the z axis; θ is the angle between the magnetic moments and the z axis. In (2.1a) the representation of the vector in the form of a complex number is used.

The one-electron Hamiltonian of a non-collinear structure (2.1) may be written as [3]

$$H = -\Delta + \sum_{j,n} U_{jn} V(|\boldsymbol{r} - \boldsymbol{t}_n - \boldsymbol{a}_j|)(U_{jn})^{-1} \tag{2.2}$$

where

$$V(r) = \begin{pmatrix} V_+(r) & 0 \\ 0 & V_-(r) \end{pmatrix}$$

is a potential in the local atomic systems of coordinates, the z axes of which are parallel to the directions of atomic moments. The spin rotation matrices

$$U = \begin{pmatrix} \cos(\tfrac{1}{2}\beta)\exp[-i(\alpha+\gamma)/2] & -\sin(\tfrac{1}{2}\beta)\exp[-i(\alpha-\gamma)/2] \\ \sin(\tfrac{1}{2}\beta)\exp[i(\alpha-\gamma)/2] & \cos(\tfrac{1}{2}\beta)\exp[i(\alpha+\gamma)/2] \end{pmatrix} \tag{2.4}$$

determine the transition between the laboratory coordinate system and the atomic systems; α, β, γ are Euler angles; Δ is the kinetic energy operator.

In [15], it has been shown that the traditional machinery of space groups does not give a complete description of the symmetry of Hamiltonian (2.2), so the use of SSG is needed. The action of a SSG operator on a two-component spinor may be defined by

$$\{\alpha_S|\alpha_R|t\}\Psi(r) = U(\alpha_S)\Psi(\{\alpha_R|t\}^{-1}r) = U(\alpha_S)\Psi(\alpha_R^{-1}r - \alpha_R^{-1}t) \tag{2.5}$$

where α_S is the spin rotation, $\{\alpha_R|t\}$ is a space transformation that contains a rotation α_R and a translation t. From the commutation relations of the operators (2.5) and the Hamiltonian (2.2), it follows [17] that the symmetry group of the problem includes operators that leave the magnetic structure (2.1) invariant. The action of SSG operator on the vector function (2.1), determined at the crystal lattice sites, is defined by

$$e'_{jn} = \{\alpha_S|\alpha_R|t\}e_{jn} = \alpha_S e_{j'n'} \tag{2.6}$$

where the indices j', n' may be found from the equality

$$\{\alpha_R|t\}^{-1}(a_j + t_n) = a_{j'} + t_{n'}. \tag{2.7}$$

At the same time there is an important difference between the group of operators (2.5) commuting with the Hamiltonian (2.2) and the group of transformations (2.6) leaving the magnetic structure (2.1) invariant: two operators (2.5) of opposite sign correspond to each transformation (2.6). This sign uncertainty is typical of operators acting on spinors and is a consequence of the homomorphism of the group of rotations α_S and the group of matrices $U(\alpha_S)$ [18]. (Using the same notation for the transformations defined by (2.5) and (2.6) should not lead to difficulties. In this paper, we use mainly the operators (2.5).)

The multiplication law for the operators (2.5) reads

$$\{\alpha_S|\alpha_R|t\}\{\alpha'_S|\alpha'_R|t'\} = c_s\{\alpha_S\alpha'_S|\alpha_R\alpha'_R|\alpha_R t' + t\} \tag{2.8}$$

where c_s is $+1$ or -1, according to the signs that we choose for matrices U in the definition (2.5) of the operators involved in (2.8). In the general case, this uncertainty cannot be removed by any choice of the signs of operators. The group multiplication law may be fulfilled only for double groups [19] containing two operators with opposite signs for each transformation (2.6).

The wavefunctions corresponding to an energy level form the basis of some IR of the Hamiltonian symmetry group [18]. In the case of spinor wavefunctions, this statement holds good for the IR of double groups or, in other terminology, for the double-valued representations of the group of the transformations (2.6).

Thus in constructing the symmetry group of the Hamiltonian (2.2), it is sufficient to

find the symmetry group for the vector function (2.1) on the basis of transformations (2.6). But to describe the electronic structure, we need to take into account the sign uncertainty of the operators (2.5).

Note that the potentials $V_o(r)$ in (2.3) may be defined in both the atomic sphere and the whole space. Therefore the consideration is not restricted to the muffin-tin potential only. We believe that the important conclusion drawn in the previous paragraph and, as a consequence, all further considerations should be valid within any consistent theory of electron states of non-collinear magnets neglecting spin–orbit interaction (see also [16]) and do not depend on the representation of one-electron potential.

3. Generalized Bloch theorem

As in traditional cases whose symmetry may be described by ordinary SG, the most important role is played by the translational symmetry of the problem, because this symmetry permits a wavevector of a state to be introduced [3, 13, 15].

Let us consider SSG elements of the form

$$T_n = \{\alpha(\boldsymbol{q}\cdot\boldsymbol{t}_n)\,|\,\varepsilon\,|\,\boldsymbol{t}_n\} \tag{3.1}$$

where ε is the unit element of the group of rotations, and $\alpha(\varphi)$ is a rotation by an angle φ about the z axis. We call these elements 'generalized translations'. For the group of generalized translations, T, the use of the double-valued representations may be avoided if, in the definition (2.5) of operators (3.1), we use matrices (2.4) corresponding to angles $\alpha = \beta = 0$, $\gamma = \boldsymbol{q}\cdot\boldsymbol{t}_n$. For these matrices we introduce the notation $U(\boldsymbol{q}\cdot\boldsymbol{t}_n)$. For this choice of the signs of the matrices we can write

$$U(\boldsymbol{q}\cdot\boldsymbol{t}_n)U(\boldsymbol{q}\cdot\boldsymbol{t}_m) = U(\boldsymbol{q}\cdot(\boldsymbol{t}_n+\boldsymbol{t}_m)) \tag{3.2}$$

and the set of generalized translations forms an Abelian group that is isomorphic to the group of space translations $\boldsymbol{t}_n$. Therefore the IR of these groups are identical and we can write the IR of T in the form

$$D_k(T_n) = \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}_n). \tag{3.3}$$

Thus we arrive at the generalized Bloch theorem

$$T_n\Psi(\boldsymbol{r}) = \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}_n)\Psi(\boldsymbol{r}) \tag{3.4}$$

where Ψ is the eigenfunction of the Hamiltonian (2.2).

Hence in labelling the states, it is sufficient to use wavevectors from the BZ that corresponds to the lattice of vectors $\boldsymbol{t}_n$. The electron spectrum $\varepsilon(\boldsymbol{k})$ may also be considered as defined at all points of reciprocal space and as having the periodicity of the reciprocal lattice.

Note that, although we may avoid the use of double-valued representations of the generalized translation group, the sign uncertainty in the definition of operators (2.5) leads to the following important property: the possibility to connect the electronic state with the vector $\boldsymbol{k}$ of the BZ on the basis of the generalized Bloch theorem (3.4) is not unique.

Indeed, let us show that there are other possibilities to choose the signs of the operators T_n, which also lead to the isomorphism of the group T and the group of space translations $\boldsymbol{t}_n$.

Rewrite formula (3.3) in the form

$$D_k(T_n) = \sum_{i=1}^{3} [\exp(-i\boldsymbol{k}\cdot\boldsymbol{f}_i)]^{n_i} \tag{3.5}$$

where we have used the equality

$$\boldsymbol{t}_n = \sum_{i=1}^{3} n_i \boldsymbol{f}_i \tag{3.6}$$

and the $\boldsymbol{f}_i$ are the unit translations. The sign uncertainty in the formula (2.5) allows one to change the definitions of the generalized translations corresponding to the vectors $\boldsymbol{f}_i$ in such a way that the value of the representation corresponding to the translation $\boldsymbol{t}_n$ takes the form

$$\sum_i [c_i \exp(-i\boldsymbol{k}\cdot\boldsymbol{f}_i)]^{n_i} \tag{3.7}$$

where c_i may be equal to $+1$ or -1 depending on the choice of sign in the definition of unit translations. Expression (3.7) may be rewritten in the form $\exp(-i\boldsymbol{k}'\cdot\boldsymbol{t}'_n)$; that is we obtain, as before, the traditional form of representation (3.3) but for a different vector

$$\boldsymbol{k}' = \boldsymbol{k} + \sum_i \nu_i \boldsymbol{b}_i \tag{3.8}$$

where the $\boldsymbol{b}_i$ are the unit translations of the reciprocal lattice, ν_i is equal to 0 if $c_i = 1$ and to $1/2$ if $c_i = -1$. Therefore depending on choice of signs in the definition of operators T_n, the same electronic state will satisfy the Bloch condition (3.4) for different values of wavevector, which differ by half the reciprocal-lattice vector.

The change of sign of the operators that leads to equality (3.8) may be defined, in calculating the spin rotation angle in (3.1), by the replacement of spiral vector $\boldsymbol{q}$ by

$$\boldsymbol{q}' = \boldsymbol{q} + 2\sum_i \nu_i \boldsymbol{b}_i. \tag{3.9}$$

In this case, the spin rotation accompanying lattice translation changes by a value that is multiple of 2π. The translation thus obtained is again a symmetry operation that leaves the magnetic structure (2.1) unchanged but leads to some operators T_n changing sign due to the properties of the matrix U.

In the following consideration it is supposed that the choice of the spiral vector $\boldsymbol{q}$ has been made and, therefore, the wavevector of each state is uniquely fixed.

4. Properties of the symmetry operations of spiral structures

The symmetry of the Hamiltonian (2.2) relative to the elements of the group of generalized translations has allowed us to characterize each electron state by a wavevector. For the investigation of the properties of the electron spectrum, which follow from the presence of other symmetry operations, it is useful to find classes of operators that may enter the symmetry group of spiral structures.

In this section we restrict our attention to strictly non-collinear structures (although a ferromagnet and an antiferromagnet may be considered as the limiting case of a

spiral). Then, in the SSG of a spiral, the only spin rotation α_S corresponds to each space transformation $\{\alpha_R|t\}$ because in the opposite case the group has to contain a transformation that is a purely spin rotation.

Let $g = \{\alpha_S|\alpha_R|t\}$ be a transformation from the SSG of the spiral. For the space part of this transformation, the following relation is true:

$$\{\alpha_R|t\}^{-1}\{\varepsilon|t_n\}\{\alpha_R|t\} = \{\varepsilon|\alpha_R^{-1}t_n\}. \tag{4.1}$$

Then, for the operations (2.6) we can write

$$g^{-1}T(t_n)g = T(\alpha_R^{-1}t_n) \tag{4.2}$$

where the space translations corresponding to the generalized translations are shown in brackets. For the spin parts of the operations we shall obtain

$$\alpha_S^{-1}\alpha(t_n)\alpha_S = \alpha(\alpha_R^{-1}t_n). \tag{4.3}$$

Supposing that the spin rotation α_S is defined by the angles α, β, γ and using formula (2.4), we can write

$$\begin{pmatrix} d^*\cos^2(\frac{1}{2}\beta) + d\sin^2(\frac{1}{2}\beta) & \frac{1}{2}\sin\beta\, e^{i\gamma}(d-d^*) \\ \frac{1}{2}\sin\beta\, e^{-i\gamma}(d-d^*) & d^*\sin^2(\frac{1}{2}\beta) + d\cos^2(\frac{1}{2}\beta) \end{pmatrix} = c_s \begin{pmatrix} f^* & 0 \\ 0 & f \end{pmatrix} \tag{4.4}$$

which follows from (4.3). In (4.4) $d = \exp(\frac{1}{2}i\boldsymbol{q}\cdot\boldsymbol{t}_n)$, $f = \exp[\frac{1}{2}i\boldsymbol{q}\cdot(\alpha_R^{-1}\boldsymbol{t}_n)]$, the constant c_s arises from the homomorphism of the rotation group and the group of the matrices U and is equal to $+1$ or -1.

If the vector $\boldsymbol{q}$ coincides with a vector of the lattice reciprocal to the lattice of vectors $\boldsymbol{t}_n$, that is,

$$\boldsymbol{q}\cdot\boldsymbol{t}_n = 2\pi k \qquad k \text{ is an integer} \tag{4.5}$$

then equality (4.4) is true for any α_S.

For other $\boldsymbol{q}$ the condition (4.4) is fulfilled if

$$\beta = 0 \tag{4.6a}$$

$$\alpha_R\boldsymbol{q} = \boldsymbol{q} + \boldsymbol{K}_\alpha \tag{4.6b}$$

or

$$\beta = \pi \tag{4.7a}$$

$$\alpha_R\boldsymbol{q} = -\boldsymbol{q} + \boldsymbol{K}_\alpha \tag{4.7b}$$

where $\boldsymbol{K}_\alpha$ is a reciprocal-lattice vector. In the case (4.6), the spin rotation is carried out about the z axis; in the case (4.7), the rotation is carried out by an angle π about an axis perpendicular to the z axis. We shall call the operations fulfilling the conditions (4.6) and (4.7) operations of type I and II, respectively.

As the operations of type II change the sign of the projection of the magnetic moments on the z axis, they can enter into the symmetry group only for spiral structures (2.1) with $\theta = \pi/2$, when all spins are parallel to the $z = 0$ plane.

To solve the question whether conditions (4.6) and (4.7) suffice for the corresponding transformations to be involved in the SSG of the spiral, we transform the crystal by the

symmetry operations of the space subsystem $\{\alpha_R|t\}$ without changing the directions of atomic spins. Then, instead of $e_{jn\perp}$ in (2.1), we shall obtain

$$e'_{jn\perp} = \sin\theta \exp[i\alpha_R q \cdot (a_j + t_n) - iq \cdot (\alpha_R^{-1} t)]. \tag{4.8}$$

For operations of type I, using (4.6*b*), we can write

$$e'_{jn\perp} = \sin\theta \exp[iq \cdot (a_j + t_n) + iK_\alpha \cdot a_j - iq \cdot (\alpha_R^{-1} t)]. \tag{4.9}$$

The function (4.9) will coincide with (2.1*a*) as a result of a spin rotation about the z axis if and only if the expression $-K_\alpha \cdot a_j + q \cdot (\alpha_R^{-1} t)$ gives a j-independent value of the angle of rotation. As $a_1 = 0$, we can write this condition in the form

$$K_\alpha \cdot a_j = 2\pi k \qquad k \text{ is an integer} \tag{4.10}$$

for any j. Therefore, K_α has to fulfil the condition imposed on the reciprocal-lattice vectors not only for lattice translations t_n, but also for atomic basis a_j.

For operations of type II, using (4.7*b*) yields

$$e^{-1}_{jn\perp} = \sin\theta \exp[-iq \cdot (a_j + t_n) + iK_\alpha \cdot a_j - iq \cdot (\alpha_R^{-1} t)] \tag{4.11}$$

instead of (4.9).

Taking into account that a rotation by an angle π about any axis perpendicular to the z axis may be considered as a rotation by an angle π about the x axis followed by a rotation through an angle about the z axis, and allowing for the fact that a rotation by an angle π about the x axis corresponds to a complex conjugation of the function (4.11), we again obtain the equality (4.10) as a necessary and sufficient condition for the operations of type II to enter the symmetry group of the spiral.

Note that for lattices with one atom per unit cell and also for q and α_R for which $K_\alpha = 0$, the condition (4.10) is always fulfilled.

5. Groups of the wavevectors and the symmetry of the spectrum in reciprocal space

With respect to the electron state Ψ_k corresponding to a given k, all symmetry operators g may be separated into two sets. The first set contains operators that transform the function Ψ_k to a function $g\Psi_k$ corresponding to the same vector k. These operators form the wavevector group, G_k, whose irreducible representations determine the character of the degeneracy of states at the point k. The second set contains operators for which the function $g\Psi_k$ fulfils the condition (3.4) for a vector k' that is not equal to k. This part of the operators determines the symmetry of the spectrum in reciprocal space. We shall show that both the condition imposed on the operators belonging to the wavevector group and the formula describing the symmetry of the spectrum differ substantially from the corresponding traditional results for collinear magnets, the symmetry of which may be described on the basis of ordinary space groups.

Let the generalized translation $T(t_n)$ act on the function $g\Psi_k$:

$$T_n(g\Psi_k) = g\{\alpha_S^{-1}\alpha(q \cdot t_n)\alpha_S|\varepsilon|\alpha_R^{-1} t_n\}\Psi_k. \tag{5.1}$$

For operations of type I, rotations α_S are performed about the z axis. Therefore these

operations commute with $\alpha(\boldsymbol{q}\cdot\boldsymbol{t}_n)$, and we can rewrite the operator on the right-hand side of (5.1):

$$\{\alpha(\boldsymbol{q}\cdot\boldsymbol{t}_n)|\varepsilon|\alpha_R^{-1}\boldsymbol{t}_n\}=\{\alpha(\boldsymbol{q}\cdot\boldsymbol{t}_n-\boldsymbol{q}\cdot(\alpha_R^{-1}\boldsymbol{t}_n))|\varepsilon|0\}T(\alpha_R^{-1}\boldsymbol{t}_n). \tag{5.2}$$

As

$$\boldsymbol{q}\cdot\boldsymbol{t}_n-\boldsymbol{q}\cdot(\alpha_R^{-1}\boldsymbol{t}_n)=-\boldsymbol{K}_\alpha\cdot\boldsymbol{t}_n \tag{5.3}$$

this value of the angle of spin rotation is a multiple of 2π and the corresponding matrix $U(-\boldsymbol{K}_\alpha\cdot\boldsymbol{t}_n)$ is a scalar and equal to $+1$ or -1. Allowing for (5.2), (5.3) and (3.4), we have from (5.1)

$$T_n(g\Psi_k)=\exp[-\mathrm{i}(\alpha_R\boldsymbol{k}-\tfrac{1}{2}\boldsymbol{K}_\alpha)\cdot\boldsymbol{t}_n](g\Psi_k). \tag{5.4}$$

Thus the function $g\Psi_k$ corresponds to the wavevector $\alpha_R\boldsymbol{k}-\frac{1}{2}\boldsymbol{K}_\alpha$. If

$$\alpha_R\boldsymbol{k}-\tfrac{1}{2}\boldsymbol{K}_\alpha=\boldsymbol{k}+\boldsymbol{K}_\mu \tag{5.5}$$

where $\boldsymbol{K}_\mu$ is a reciprocal-lattice vector, then the type I operation g is involved in the group of the wavevector $\boldsymbol{k}$. In the opposite case we obtain the symmetry property of the spectrum

$$\varepsilon(\boldsymbol{k})=\varepsilon(\alpha_R\boldsymbol{k}-\tfrac{1}{2}\boldsymbol{K}_\alpha). \tag{5.6}$$

For operations of type II the product of three spin rotations may be written in the form

$$\alpha_S^{-1}\alpha(\boldsymbol{q}\cdot\boldsymbol{t}_n)\alpha_S=\alpha(-\boldsymbol{q}\cdot\boldsymbol{t}_n)=\alpha(-\boldsymbol{K}_\alpha\cdot\boldsymbol{t}_n)\alpha(\boldsymbol{q}\cdot(\alpha_R^{-1}\boldsymbol{t}_n)) \tag{5.7}$$

where formula (4.7*b*) was used. Further, in complete analogy with the consideration for operators of type I, we obtain the result that formulae (5.4)–(5.6) are true in the case of operators of type II, too.

So we see that formulae (5.5) and (5.6) differ from the corresponding formulae in the traditional case:

$$\alpha_R\boldsymbol{k}=\boldsymbol{k}+\boldsymbol{K}_\mu \tag{5.8}$$

$$\varepsilon(\alpha_R\boldsymbol{k})=\varepsilon(\boldsymbol{k}) \tag{5.9}$$

and coincide with them only for $\boldsymbol{K}_\alpha=0$.

To understand more deeply the sense of the relation (5.6), we replace the variable

$$\boldsymbol{k}=\boldsymbol{k}'+\tfrac{1}{2}\boldsymbol{q} \tag{5.10}$$

and introduce the notation $\varepsilon'(\boldsymbol{k}')=\varepsilon(\boldsymbol{k}'+\frac{1}{2}\boldsymbol{q})$. Formula (5.6) takes the form

$$\varepsilon'(\boldsymbol{k}')=\varepsilon'(\alpha_R\boldsymbol{k}') \tag{5.11}$$

that is we have obtained the traditional formula (5.9). Hence the type I operations determine the symmetry of the spectrum relative to a point transformation with the centre at the point $\frac{1}{2}\boldsymbol{q}$. For operations of type II the use of (5.10) allows us to represent (5.6) in the form

$$\varepsilon\big(I((I\alpha_R)\boldsymbol{k}'+\tfrac{1}{2}\boldsymbol{q})\big)=\varepsilon(\boldsymbol{k}'+\tfrac{1}{2}\boldsymbol{q}) \tag{5.12}$$

where I is the operation of inversion. Therefore, an operation of type II leads to the

coincidence of the spectrum at a point $\boldsymbol{k}$ with the spectrum at the point obtained from $\boldsymbol{k}$ by a transformation $I\alpha_R$ relative to the point $\frac{1}{2}\boldsymbol{q}$ and by a subsequent inversion relative to the coordinate origin.

If the group contains operations that are a superposition of point transformations with different centres, an unusual result can arise: the symmetry of the spectrum in reciprocal space will be described by a non-symmorphic space group, a situation that is impossible in the traditional case (5.9). (A corresponding example will be considered below.)

The spiral structure spectrum symmetry can be visualized better if we rewrite equalities (5.6), (4.6) and (4.7) in the form

$$\varepsilon(\boldsymbol{k}) = \varepsilon(\{\alpha_R \mid -\tfrac{1}{2}\boldsymbol{K}_\alpha + \boldsymbol{K}_\mu\}\boldsymbol{k}) \tag{5.13}$$

$$\{\alpha_R \mid -\tfrac{1}{2}\boldsymbol{K}_\alpha\}\tfrac{1}{2}\boldsymbol{q} = \tfrac{1}{2}\boldsymbol{q} \tag{5.14}$$

$$\{\alpha_R \mid -\tfrac{1}{2}\boldsymbol{K}_\alpha\}\tfrac{1}{2}\boldsymbol{q} = -\tfrac{1}{2}\boldsymbol{q}. \tag{5.15}$$

From this it follows that the symmetry group of the spiral spectrum includes only operations that leave unchanged the crystal lattice made up of the vectors $\boldsymbol{K}_\mu$ and having two atoms (at the points $\frac{1}{2}\boldsymbol{q}$ and $-\frac{1}{2}\boldsymbol{q}$) per unit cell. Moreover, operations of the first type (5.14) leave the atoms of the basis unchanged, and operations of the second type (5.15) transfer one atom of the basis into the other atom.

Finally, in the case (4.5) where the spiral vector is equal to a reciprocal-lattice vector, a consideration analogous to the foregoing treatment shows again that formula (5.6) is true for any symmetry operation.

6. Irreducible domain of reciprocal space

One of the main tasks of the investigation of spectral symmetry is to determine a minimum domain of reciprocal space such that knowledge of the spectrum in this domain allows one to find the spectrum at any point of space. The volume of the irreducible domain (ID) is equal to the $(1/n)$th part of the BZ volume, where n is the number of different point transformations α_R entering into the symmetry operations.

Let us consider the ID for a number of concrete spiral structures.

6.1. BCC lattice, $\boldsymbol{q} = (0, 0, \alpha)$, $0 < \alpha \leq 2\pi/a$

For magnetic structures (2.1) with $\alpha \neq 2\pi/a$ and $\theta \neq \pi/2$ the symmetry group contains eight of 48 operations of the crystal class of cubic lattices [20]. These are operations that satisfy the condition

$$\alpha_R\boldsymbol{q} = \boldsymbol{q} \tag{6.1}$$

and are rotations about the z axis and reflections in the planes going through the z axis. For the same α and $\theta = \pi/2$ the volume of the ID decreases by the factor of 2 because of the type II operations, for which

$$\alpha_R\boldsymbol{q} = -\boldsymbol{q}. \tag{6.2}$$

These operations may be obtained from the previous eight operations by multiplying by the inversion. For all of the 16 operations the vector $\boldsymbol{K}_\alpha$ in formulae (4.6) and (4.7) is

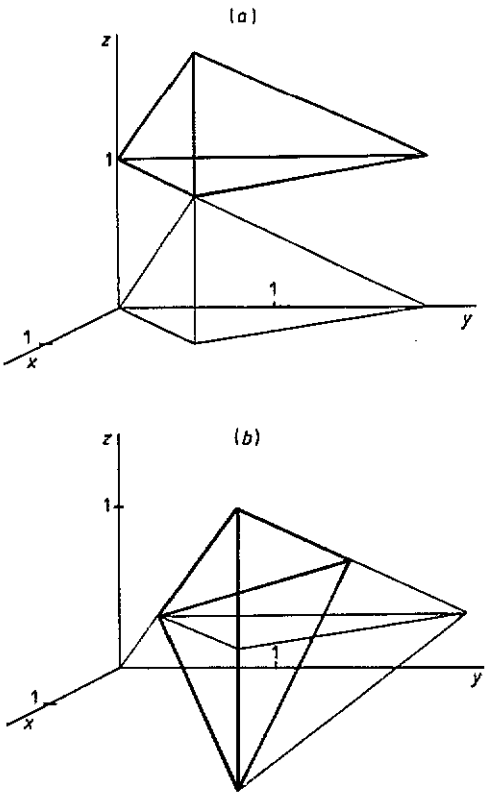

Figure 1. Irreducible domains in reciprocal space for spiral structures with BCC lattice. (*a*) The traditional ID of BCC lattice (thin line) and the ID for spiral structure with $q = (0, 0, 2\pi/a)$ and $\theta \neq 90°$ (heavy line). (*b*) The ID for spiral structure with $q = (\pi,\pi,\pi)/a$ and $\theta = 90°$ (heavy line). The tetrahedron of doubled volume is the ID for spiral structure with $q = (\pi,\pi,\pi)/a$ and $\theta \neq 90°$. The coordinate scales are given in $2\pi/a$ units.

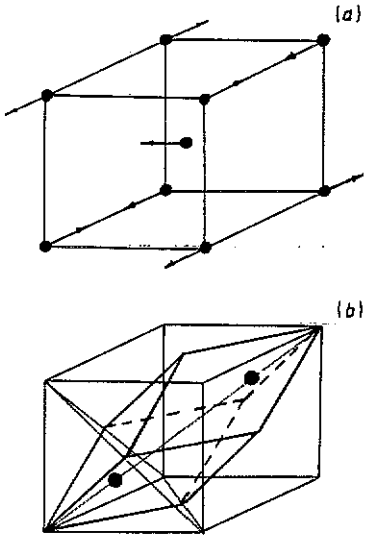

Figure 2. (*a*) Magnetic structure with $q = (\pi,\pi,\pi)/a$ and $\theta = 90°$. (*b*) The crystal structure whose symmetry is described by the same symmetry group as the symmetry of the spectrum of the magnetic crystal shown in (*a*).

zero and the symmetry of the spectrum has the traditional form (5.9). Therefore, the construction of the ID has no peculiarities connected with the non-collinearity of magnetic structure. It suffices to separate the $(1/n)$th part of the traditional BZ of the lattice being considered, by allowing for the point transformations α_R.

In the case $\alpha = 2\pi/a$ and $\theta \neq \pi/2$ the symmetry group of the spiral contains all the 48 operations α_R of the cubic lattice crystal class as the condition (4.6*b*) is fulfilled for any α_R. In this case all operations belong to type I, and formula (5.11) works well for any operation. Hence the spectrum is invariant under 48 point transformations with the centre at point $q/2$. Therefore, the ID may be taken in the form of the polyhedron shown in figure 1(*a*) and obtained from the traditional ID of the BCC structure via displacement by the vector $q/2$.

Finally, for $\alpha = 2\pi/a$ and $\theta = \pi/2$ we obtain a collinear antiferromagnetic structure, which has been well studied by the traditional methods.

6.2. BCC lattice, $q = (\pi, \pi, \pi)/a$

For $\theta \neq \pi/2$ the group contains 24 operations, for which the equality (4.6*b*) is true. The corresponding ID (figure 1(*b*)) is shifted by $\frac{1}{2}q$ relative to the ID obtained for the same set of α_R in the traditional case. For $\theta = \pi/2$ the volume of the ID is equal to 1/48th the BZ volume (figure 1(*b*)), although the location and orientation of the ID differ from the traditional case (figure 1(*a*)).

The magnetic structure with $\theta = \pi/2$ (figure 2(*a*)) is of special interest because at this parameter the symmetry of the spectrum is described by a non-symmorphic space group. Figure 2(*b*) shows a crystal structure whose symmetry is described by the same space group as the spectrum of the spiral. As was noted in the previous section, that is a crystal with an FCC lattice and two atoms per unit cell at the points $\frac{1}{2}q$ and $-\frac{1}{2}q$. In particular, the symmetry group of the structure shown in figure 2(*b*) contains a transformation that consists of a reflection in the $z = 0$ plane and a subsequent translation by the vector $(\pi, \pi, 0)/a$ parallel to that plane. This indicates the presence of a slip plane in the symmetry group of the spectrum.

6.3. HCP structure, $q = (0, 0, \alpha)$, $0 < \alpha \leqslant 2\pi/c$

For $\alpha \neq 2\pi/c$ and $\theta \neq \pi/2$ the spiral structure symmetry group contains, of the 24 operations of the HCP structure crystal class [20], 12 operations that fulfil condition (6.1). For $\theta = \pi/2$ the volume of the ID becomes equal to 1/24th the BZ volume, owing to the operations satisfying (6.2). In the latter case the ID coincides with that used in traditional calculations for HCP crystals [20].

For $\alpha = 2\pi/c$ and $\theta \neq \pi/2$ equalities (4.6*b*) and (4.10) are fulfilled for all the 24 operations α_R and we obtain again the traditional polyhedron of the HCP crystal.

7. Irreducible representations of the wavevector group

A principal role in the consideration of the symmetry of quantum-mechanical problems is played by the irreducible representations (IR) of the symmetry group of the Hamiltonian. In the investigation of crystals, the task reduces to finding permissible IR of the wavevector groups [21] for various points of reciprocal space.

Comparing the multiplication law for the SSG operators (2.8) with the corresponding formula for the space parts of the operators

$$\{\alpha_R \,|\, t\}\{\alpha'_R \,|\, t'\} = \{\alpha_R \alpha'_R \,|\, \alpha_R t' + t\} \tag{7.1}$$

and taking into consideration the one-to-one correspondence of the spin and space parts of the SSG operators for non-collinear structures, we may conclude that double-valued IR of the ordinary space group of the operators $\{\alpha_R | t\}$, but with sign distribution defined by spin rotations, are needed in this case. On constructing the multiplication table, the IR can be found by the traditional group-theory methods; that is, in principle, the problem has been solved.

In this section we shall formulate a simple statement that allows us to base the construction of the SSG IR on the existing tables of IR of ordinary space groups. As an example we shall consider the application of the method to a crystal with HCP structure (SG of the D^4_{6h} type).

Table 1. Elements of the crystal class[a].

	α_R								
No.	Angle (deg)	Axis	τ_α	α_S	Type	No.	τ_α	α_S	Type
1	0	0,0,1	0	ε	I	13	τ	$C_{\varphi v}$	II
2 3	60	0,0,1 0,0,−1	τ	C_φ	I	14 15	0	C_{2v}	II
4 5	120	0,0,1 0,0,−1	0	ε	I	16 17	τ	$C_{\varphi v}$	II
6	180	0,0,1	τ	C_φ	I	18	0	C_{2v}	II
7 8 9	180	1,0,0 $\frac{1}{2},\sqrt{3}/2,0$ $-\frac{1}{2},\sqrt{3}/2,0$	τ	$C_{\varphi v}$	II	19 20 21	0	ε	I
10 11 12	180	$\sqrt{3}/2,\frac{1}{2},0$ 0,1,0 $-\sqrt{3}/2,\frac{1}{2},0$	0	C_{2v}	II	22 23 24	τ	C_φ	I

[a] Transformations α_R with numbers from 13 to 24 differ from the corresponding operations with numbers from 1 to 12 in the addition of inversion. The following notations are used: $\tau = a_2$; C_φ is the rotation by an angle $\varphi = \boldsymbol{q}\cdot\boldsymbol{\tau}$ about the z axis; C_{2v} is the rotation by an angle π about $\boldsymbol{e}_1$; $C_{\varphi v} = C_\varphi C_{2v}$. The symmetry group of the FS contains the operations of type I only.

It may be shown that for the subgroup containing symmetry transformations $\{\alpha_S|\alpha_R|t\}$ belonging to type I and fulfilling condition (6.1) the signs of the operators acting on the spinors may be chosen such that the isomorphism of this subgroup and of the corresponding subgroup of pure space transformations $\{\alpha_R|t\}$ takes place. The proof of this statement is based on the property following from the results of section 4 that for operators $\{\alpha_S|\alpha_R|t\}$, which satisfy (6.1), spin rotations are carried out by an angle $\boldsymbol{q}\cdot\boldsymbol{t}$ about the z axis. The isomorphism will be established if we fix the sign of the matrix (2.4) in definition (2.5) by using the angles $\gamma = \boldsymbol{q}\cdot\boldsymbol{t}$, $\beta = \alpha = 0$. This isomorphism allows one to use the IR of the ordinary SG of the operators $\{\alpha_R|t\}$ as the IR of the SSG of the operators $\{\alpha(\boldsymbol{q}\cdot\boldsymbol{t})|\alpha_R|t\}$.

Let us consider the construction of the IR of the SSG of a spiral with an HCP structure. In accord with experiment [8], we take a vector $\boldsymbol{q}$ parallel to the z axis. We shall restrict our consideration to vectors $\boldsymbol{q}$ that are not equal to a reciprocal-lattice vector. We shall use the form of the unit cell of the HCP structure defined by unit translations

$$\boldsymbol{f}_1 = a(1/2, \sqrt{3}/2, 0) \qquad \boldsymbol{f}_2 = a(-1/2, \sqrt{3}/2, 0) \qquad \boldsymbol{f}_3 = c(0,0,1)$$

and by atomic basis

$$\boldsymbol{a}_1 = (0,0,0) \qquad \boldsymbol{a}_2 = (0, \sqrt{3}a/3, c/2)$$

where a and c are the lattice parameters of the HCP structure. In table 1 the elements of the crystal class of the SSG are given for a ferromagnetic spiral (FS) with θ in (2.1) not equal to $\pi/2$, and for a simple spiral (SS) with $\theta = \pi/2$. These structures were experimentally observed for Tb, Dy, Ho and Er [8]. The symmetry elements entering into the group of the wavevector for various BZ points are given in table 2.

Table 2. Symmetry of the reciprocal space points[a].

Symbol	k			Symmetry elements	
	k_x	k_y	k_z	Type I	Type II
Δ	0	0	μ	1–6, 19–24	–
Γ	0	0	0	1–6, 19–24	7–18
A	0	0	1	1–6, 19–24	7–18
U	0	$\sqrt{3}/3$	μ	1, 6, 19, 23	–
M	0	$\sqrt{3}/3$	0	1, 6, 19, 23	7, 11, 13, 18
L	0	$\sqrt{3}/3$	1	1, 6, 19, 23	7, 11, 13, 18
P	1/3	$\sqrt{3}/3$	μ	1, 4, 5, 22–24	–
K	1/3	$\sqrt{3}/3$	0	1, 4, 5, 22–24	7–9, 14, 15, 18
H	1/3	$\sqrt{3}/3$	1	1, 4, 5, 22–24	7–9, 14, 15, 18
α	$\omega/3$	$\sqrt{3}/3\nu$	0	1	18
β	$\omega/3$	$\sqrt{3}/3\nu$	1	1	18
γ	$\nu/3$	$\sqrt{3}/3\nu$	μ	1, 24	–
T	$\nu/3$	$\sqrt{3}/3\nu$	0	1, 24	8, 18
S	$\nu/3$	$\sqrt{3}/3\nu$	1	1, 24	8, 18
δ	0	$\sqrt{3}/3\nu$	μ	1, 19	–
Σ	0	$\sqrt{3}/3\nu$	0	1, 19	11, 18
R	0	$\sqrt{3}/3\nu$	1	1, 19	11, 18
ξ	$\nu/3$	$\sqrt{3}/3$	μ	1, 23	–
T'	$\nu/3$	$\sqrt{3}/3$	0	1, 23	7, 18
S'	$\nu/3$	$\sqrt{3}/3$	1	1, 23	7, 18

[a] The symmetry group of the FS contains the operations of type I only. Coordinates k_x, k_y are given in $2\pi/a$ units, k_z in $2\pi/c$ units. $0 < \nu, \omega < 1$, $-1 < \mu \leq 1$ in the case of the FS and $0 < \mu < 1$ in the case of SS.

In the case of an FS all points of any straight line parallel to the z axis have the same symmetry. That is why the isolated points of high symmetry are absent for the FS. In the ID there are only three vertical directions Δ, P, U and three vertical planes γ, δ, ξ the groups of which contain non-unit elements of the crystal class. As the symmetry group of the FS contains only type I operations that satisfy (6.1), the IR of all the wavevector groups may be found from the isomorphism with the corresponding space group. Moreover, for all the six symmetry objects the wavevector groups contain the same elements α_R as those in the traditional consideration of these points on the basis of SG D_{6h}^4 [20]. Therefore we can immediately use tables of IR of ordinary SG for these symmetry directions and planes. In table 3 the IR for the direction Δ are given.

In the case of SS for points of the planes $z = 0$ and $z = \pi/c$, the number of symmetry elements is doubled owing to the operations of type II, which satisfy condition (6.2). For the points k of these planes the theory of the SG IR (see e.g. [21]) permits one to find the IR of the SSG of the wavevector k for the SS, based on the corresponding representations at this point for the FS. For the points of these planes the wavevector group in the case of an FS, H, is a half-subgroup of the group of the same wavevector in the case of an SS, G. Then

$$G = Hg_1 + Hg_2 \tag{7.2}$$

where g_1 is the unit element and the element numbered 18 in table 1 may be used as g_2.

Table 3. Irreducible representations of the wavevector group for the z axis points in the case of FS[a].

	α											
p	1	2	3	4	5	6	19	20	21	22	23	24
1, 2	1	± 1		1		± 1		1			± 1	
3, 4	1	± 1		1		± 1		-1			∓ 1	
	2	∓ 1		-1		± 2		0			0	
5, 6	$\begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$	$\begin{pmatrix} \pm\omega^2 & \\ & \pm\omega \end{pmatrix}$	$\begin{pmatrix} \pm\omega & \\ & \pm\omega^2 \end{pmatrix}$	$\begin{pmatrix} \omega & \\ & \omega^2 \end{pmatrix}$	$\begin{pmatrix} \omega^2 & \\ & \omega \end{pmatrix}$	$\begin{pmatrix} \pm 1 & \\ & \pm 1 \end{pmatrix}$	$\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$	$\begin{pmatrix} & \omega \\ \omega^2 & \end{pmatrix}$	$\begin{pmatrix} & \omega^2 \\ \omega & \end{pmatrix}$	$\begin{pmatrix} & \pm\omega^2 \\ \pm\omega & \end{pmatrix}$	$\begin{pmatrix} & \pm 1 \\ \pm 1 & \end{pmatrix}$	$\begin{pmatrix} & \pm\omega \\ \pm\omega^2 & \end{pmatrix}$

[a] In the table the matrices are given to be multiplied by $\exp(i\boldsymbol{k}\cdot\boldsymbol{\tau}_\alpha)$, $\omega = \exp(i2\pi/3)$. For two-dimensional representations the characters are shown above matrices. The upper sign corresponds to the first value of p, the lower sign to the second value. In the writing of the matrices of representations 5 and 6 zero elements are omitted.

H is an invariant subgroup [21] of G. We can write the following formula for the characters $\chi_p(h)$ of representations $d_p(h)$ of H, $h \in H$,

$$\chi_p(g_2 h g_2^{-1}) = \chi_{p'}(h). \tag{7.3}$$

Further steps depend on whether p is equal to p' or not.

With $p = p'$, G is the little group [21] of the representation d_p and its IR may be found by the direct product

$$D_{p\zeta}(hg_m) = (d_p(h)U(g_m)) \times \delta_\zeta(g_m) \tag{7.4}$$

where the unitary matrices U are defined by the formula

$$d_p(g_m h g_m^{-1}) = U(g_m) d_p(h) U(g_m)^{-1} \tag{7.5}$$

and δ_ζ are the projection representations [21] of the factor group G/H defined by formulae

$$\delta(g_m)\delta(g_{m'}) = \omega_{mm'}\delta(g_m g_{m'}) \tag{7.6}$$

$$U(g_m g_{m'}) = \omega_{mm'} U(g_m) U(g_{m'}). \tag{7.7}$$

In the case of $p \neq p'$, two representations (d_p and $d_{p'}$) form an orbit and give one IR of group G:

$$D(h) = \begin{pmatrix} d_p(h) & 0 \\ 0 & d_{p'}(h) \end{pmatrix} \tag{7.8a}$$

and for $g \in G$, but $g \notin H$,

$$D(g) = \begin{pmatrix} 0 & d_p(gg_2^{-1}) \\ d_p(g_2 g) & 0 \end{pmatrix}. \tag{7.8b}$$

Thus the main question is whether p' in (7.4) will be equal to p or not. In the case of HCP structure we can write

$$\chi_p(g_2 h g_2^{-1}) = \exp[-i\boldsymbol{t}\cdot(\alpha_{18}\boldsymbol{k} - \boldsymbol{k})]\chi_p(h) \tag{7.9}$$

where α_{18} is the space rotation of the 18th operation from table 1. For all points of the $z = 0$ plane $\alpha_{18}\boldsymbol{k} - \boldsymbol{k} = 0$ and, consequently, p' is always equal to p. For the points of the $z = \pi/c$ plane the equality $p = p'$ holds either for operations with $\tau_\alpha = 0$ (see table 1) or for the case $\chi_p(h) = 0$. Let us consider some details of the construction of the IR for the $z = 0$ and $z = \pi/c$ planes.

The $z = 0$ plane. For all points of the plane

$$U(g_1) = U(g_2) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \omega_{11} = \omega_{12} = \omega_{22} = 1 \qquad \omega_{22} = -1.$$

In this case the isomorphism with an ordinary space group cannot be established,

because $g_2^2 = -g_1$ for any choice of sign of g_2. Two projection representations of the factor group have the form

$$\delta_\zeta(g_1) = 1 \qquad \delta_\zeta(g_2) = \zeta i \qquad \text{where } \zeta = \pm 1. \tag{7.10}$$

These permit us to write the representations (7.4) at any point of the $z = 0$ plane. In particular, to obtain the IR at the point Γ, it suffices to use the relation

$$\Gamma_{p\zeta}(hg_m) = d_p(h)\delta_\zeta(g_m) \tag{7.11}$$

where the d_p are the IR from table 3, which correspond to the point $k = 0$.

Note that for the space group D_{6h}^4 a quite analogous consideration may be carried out to construct the IR at the points of the $z = 0$ plane. The only difference lies in the replacement of the imaginary unity in (7.10) by unity. Thus all IR $D_{p\zeta}$ of the SSG of the spiral for the points of the $z = 0$ plane may be obtained from the representations $D^\circ_{p\zeta}$ of the ordinary space group by multiplying the matrices of symmetry elements numbered 7 through to 18 by an imaginary unity; that is

$$D_{p\zeta}(h) = D^\circ_{p\zeta}(h) \tag{7.12a}$$

$$D_{p\zeta}(hg_2) = iD^\circ_{p\zeta}(hg_2). \tag{7.12b}$$

Point A. All representations of the subgroup H belong to the case where equality (7.3) is valid for $p \neq p'$. The representations of the subgroup (table 3) are separated into three orbits: $(p = 1, p' = 2)$; $(p = 3, p' = 4)$; $(p = 5, p' = 6)$. Using (7.8) we obtain three irreducible representations of the wavevector group at the point A.

The length of the present paper does not allow us to consider all points of reciprocal space in detail and to furnish tables of IR. A complete consideration of the problem enables us to draw the following conclusions about the connection between the SSG IR in the case of the SS and the group D_{6h}^4 IR. (i) For all points of reciprocal space, the number and dimensions of the IR of the SS coincide with the counterparts for space group D_{6h}^4. (ii) For points that do not belong to the $z = 0$ and $z = \pi/c$ planes, the IR coincide completely. (iii) At the points of the $z = 0$ and $z = \pi/c$ planes SSG IR of the type (7.4) (for the $z = 0$ plane all IR belong to this type) differ from the corresponding group D_{6h}^4 IR by multiplier i for matrices of type II elements. (iv) For IR of type (7.8), this difference resides in the change of sign of the lower left-hand block of the matrices of type II elements. (v) For the SG D_{6h}^4 the IR of the wavevector lying in the $z = \pi/c$ plane belongs to the type (7.4) if its restriction on the subgroup of elements fulfilling condition (6.1) is irreducible. In the opposite case this IR belongs to the type (7.8). This information allows one to construct easily the IR for a SS on the basis of tables of SG D_{6h}^4 IR.

8. The construction of symmetrized functions

Complete allowance for the symmetry of the problem in band-structure calculations is based on representing the electron wavefunction as a linear combination of functions forming the basis of the IR of the Hamiltonian symmetry group. Detailed symmetry analysis of electronic states may be useful, for instance, in the description of spectral properties connected with the electron transitions between different states because the symmetry of states influences substantially the probability of transition. Another application of this analysis is the prediction of the character of the change in electron bands as a response to the change of the one-electron potential symmetry. (As an

example, see the following paper for a discussion of the influence of magnetic structure change on optical properties of crystals.)

We shall restrict ourselves to the construction of symmetrized bases of the functions

$$\gamma_{lm}^{jn\sigma} = f(|\boldsymbol{r} - \boldsymbol{a}_j - \boldsymbol{t}_n|)Y_{lm}(\boldsymbol{r} - \boldsymbol{a}_j - \boldsymbol{t}_n)\chi_\sigma^{jn}. \tag{8.1}$$

These will allow one to carry out symmetry considerations for the Korringa–Kohn–Rostoker (KKR) [3], tight-binding [3], augmented spherical-wave (ASW) [6] and linear muffin-tin orbitals (LMTO) [7] methods. In (8.1), f is an arbitrary function, Y_{lm} are spherical harmonics and χ_σ^{jn} is a spinor, which in the local coordinate systems takes the form

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{or} \qquad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

that is

$$\chi_\sigma^{jn} = U_{jn}\chi_\sigma. \tag{8.2}$$

It is convenient to choose directions of the x and y axes of the local coordinate systems such that the following equality holds:

$$U_{jn} = U(\boldsymbol{q} \cdot (\boldsymbol{t}_n + \boldsymbol{a}_j))U_{10}. \tag{8.3}$$

Any element of the wavevector group G_k can be represented as $T_n\hat{\alpha}$ where $\hat{\alpha}$ is an operator $\{\alpha_S|\alpha_R|\boldsymbol{\tau}_\alpha\}$ for which the vector $\boldsymbol{\tau}_\alpha$ lies inside the unit cell. To obtain the symmetrized functions, we act on the functions (8.1) by a projection operator

$$O_{\beta\gamma}^p = [l_p/n(T)n(g_k)] \sum_{n,\hat{\alpha}} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{t}_n)D_{\beta\gamma}^p(\hat{\alpha})^*(T_n\hat{\alpha}) \tag{8.4}$$

where the value of γ is fixed; $\beta = 1, 2, \ldots, l_p$; l_p is the dimension of the representation D_p; $n(T)$ and $n(g_k)$ are the numbers of elements T_n and $\hat{\alpha}$ in G_k.

On performing transformations we have

$$O_{\beta\gamma}^p Y_{lm}^{j\sigma} = [1/n(T)] \sum_n \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{t}_n) \sum_{j',m'} a_{lm'j'\sigma}^{p\beta} Y_{lm'}^{j'n\sigma} \tag{8.5}$$

$$a_{lm'j'\sigma}^{p\beta} = [1/n(g_k)] \sum_{\hat{\alpha}} \delta_{j'j_\alpha} \exp(-\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{t}_{\alpha j})D_{\beta\gamma}^p(\hat{\alpha})^* D_{m'm}^l(\alpha_R) \exp(-\tfrac{1}{2}\varphi_{\alpha j}\sigma). \tag{8.6}$$

Here $D^l(\alpha_R)$ are the matrices of the representation of the space rotation group. Lattice vectors $\boldsymbol{t}_{\alpha j}$ are defined by equality

$$\{\alpha_R|\boldsymbol{\tau}_\alpha\}\boldsymbol{a}_j = \boldsymbol{a}_{j_\alpha} + \boldsymbol{t}_{\alpha j}. \tag{8.7}$$

The important difference between (8.5), (8.6) and the corresponding formulae for the ordinary space groups is the presence of the factor $\exp(-\frac{1}{2}\varphi_{\alpha j}\sigma)$ in (8.6). The value of $\varphi_{\alpha j}$ is defined by equality

$$U_{j0}^{-1}U(-\boldsymbol{q} \cdot \boldsymbol{t}_{\alpha j})U(\alpha_S)U_{j\alpha} = \begin{pmatrix} \exp(-\mathrm{i}\varphi_{\alpha j}/2) & 0 \\ 0 & \exp(\mathrm{i}\varphi_{\alpha j}/2) \end{pmatrix}. \tag{8.8}$$

(The product of four matrices on the left side of (8.8) always corresponds to a spin rotation about the z axis.) The coefficients (8.6) enter into the formula for the symmetrized secular matrix [3]. The action of the projection operator on the function (8.1) with $n \neq 0$ gives symmetrized functions that differ from (8.5) and (8.6) only in an unimportant multiplier.

Table 4. Indices of the representation the basis of which may be constructed from the functions with $l = 2^a$.

Type of point	SSG of SS		
	$\sigma = 1$	$\sigma = -1$	D_{6h}^4
Γ	$2^+, 5^+, 6^+, 1^-, 5^-, 6^-$	$1^+, 5^+, 6^+, 2^-, 5^-, 6^-$	$1^+, 5^+, 6^+, 2^-, 5^-, 6^-$
Δ	1, 2, 5(2), 6(2)	1, 2, 5(2), 6(2)	1, 2, 5(2), 6(2)
A	1, 3(2)	1, 3(2)	1, 3(2)

[a] In parentheses, the value of $n_{l\sigma}^p$ is given if it differs from 1.

The analysis of formula (8.8) with the use of (4.6*b*), (4.7*b*), (8.7) and (4.10) shows that

$$\varphi_{\alpha j} = -\boldsymbol{K}_\alpha(\alpha_R \boldsymbol{a}_j) \tag{8.9}$$

for operations of type I and

$$\varphi_{\alpha j} = -\boldsymbol{K}_\alpha(\alpha_R \boldsymbol{a}_j) + \pi \tag{8.10}$$

for operations of type II.

Formula (8.5) shows that symmetrized functions may be constructed from 'atomic-like' functions (8.1) with fixed l and σ. It is useful to obtain a formula giving the number, $n_{l\sigma}^p$, of different pth representation basis sets that may be constructed from functions with given l and σ. Acting by the group G_k operators on functions

$$\sum_n \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}_n) Y_{lm}^{in\sigma}$$

with fixed l and σ shows that these functions form the basis of a group G_k representation that is, generally speaking, reducible. The character of this representation has the form

$$\chi_{l\sigma}(T_n\hat{\alpha}) = \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}_n)(-1)^{ln_\alpha}\frac{\sin(l+\frac{1}{2})\mu_\alpha}{\sin(\mu_\alpha/2)}$$
$$\times \sum_i \exp(-\mathrm{i}\sigma\varphi_{\alpha j}/2)\exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}_{\alpha j})\delta_{ij_\alpha} \tag{8.11}$$

where $n_\alpha = 0$ if α_R is a proper rotation, and $n_\alpha = 1$ in the opposite case; μ_α is the angle of rotation corresponding to α_R. Hence

$$n_{l\sigma}^p = [1/n(g_k)]\sum_\alpha \chi_{l\sigma}(\hat{\alpha})\chi_p(\hat{\alpha})^* \tag{8.12}$$

where χ_p is the character of the pth IR of G_k.

As an illustration, we consider the calculation of the numbers (8.12) and symmetrized functions (8.5) and (8.6) for the case of an SS with an HCP structure. Some results of the calculations are collected in tables 4 and 5. Table 4 furnishes, for the points k belonging to the z axis, the indices of the IR whose basis may be constructed from the functions with $l = 2$ (i.e. $n_{2\sigma}^p \neq 0$). In table 5 the bases constructed of the functions with $l = 2$ and $m = 0$ are represented.

As was mentioned in section 7, for an HCP structure $\boldsymbol{K}_\alpha = 0$ for all symmetry operations. Hence for operations of type I the angle (8.9) is equal to zero, and the contribution

Table 5. Basic functions of the IR.

SSG of SS			
$\Gamma_{1+}: Y_{20}^{1-} + Y_{20}^{2-}$	$\Gamma_{2+}: Y_{20}^{1+} - Y_{20}^{2+}$	$\Gamma_{1-}: Y_{20}^{1+} + Y_{20}^{2+}$	$\Gamma_{2-}: Y_{20}^{1-} - Y_{20}^{2-}$
$\Delta_1: Y_{20}^{1\sigma} + \exp(i\boldsymbol{k}\cdot\boldsymbol{a}_2)Y_{20}^{2\sigma}$	$\Delta_2: Y_{20}^{1\sigma} - \exp(i\boldsymbol{k}\cdot\boldsymbol{a}_2)Y_{20}^{2\sigma}$	$\sigma = \pm 1$	
$A_1: Y_{20}^{1\sigma} + iY_{20}^{2\sigma}$	$\sigma(iY_{20}^{1\sigma} + Y_{20}^{2\sigma})$	$\sigma = \pm 1$	
D_{6h}^4			
$\Gamma_{1+}: Y_{20}^{1} + Y_{20}^{2}$	$\Gamma_{2-}: Y_{20}^{1} - Y_{20}^{2}$		
$\Delta_1: Y_{20}^{1} + \exp(i\boldsymbol{k}\cdot\boldsymbol{a}_2)Y_{20}^{2}$	$\Delta_2: Y_{20}^{1} - \exp(i\boldsymbol{k}\cdot\boldsymbol{a}_2)Y_{20}^{2}$		
$A_1: Y_{20}^{1} + iY_{20}^{2}$	$Y_{20}^{1} - iY_{20}^{2}$		

of these operations to expressions (8.12) and (8.6) is independent of σ. Moreover, owing to the aforementioned coincidence of the matrices of this type of element with the matrices of the corresponding representations for the SG D_{6h}^4, we shall obtain the same contributions to the sums (8.6) and (8.12) as those in the traditional consideration of an HCP structure. Therefore, when the wavevector group contains only operations of type I, the numbers of symmetrized basis sets (8.12) and the coefficients of the symmetrized functions (8.6) are σ-independent and coincide with the corresponding values for SG D_{6h}^4. (See point Δ in tables 4 and 5.)

For operations of type II $\varphi_{\alpha j} = \pi$ and

$$\exp(-i\tfrac{1}{2}\varphi_{\alpha j}\sigma) = -i\sigma \tag{8.13}$$

that is the quantities (8.6) and (8.12) become σ-dependent. Further consideration depends on the type of representation.

For the representations of the type (7.4), the matrices corresponding to the elements of type II differ from the counterparts for the SG D_{6h}^4 in multiplier i. Accounting for (8.13), the parameters (8.12) and coefficients (8.6) for the representation $D_{p\xi}$ and spin index σ will coincide with the corresponding values for the IR $D_{p(-\xi)}^{\circ}$ of SG D_{6h}^4. That is for $\sigma = -1$ we shall have the same values as in the case of the SG D_{6h}^4 (see point Γ in tables 4 and 5). Another implication is that the number and form of symmetrized functions for the representation $D_{p\xi}$ and spin index σ coincide with the corresponding characteristics for the IR $D_{p(-\xi)}$ and spin index $-\sigma$.

For IR of the type (7.8), the characters of the matrices corresponding to type II operations are equal to zero. Therefore, the σ dependence of the parameters (8.12) is absent. If we use in (8.4) the first column of IR matrices (i.e. $\gamma = 1$), then the coefficients (8.6) for the functions corresponding to the upper half of rows will be independent of σ and coincide with the corresponding values for the SG D_{6h}^4 because only type I operations make a contribution to these functions. The rest of the functions are defined by the operations of type II and are of opposite signs for different values of σ. These functions differ from the corresponding functions for SG D_{6h}^4 in factor i. (See point A in tables 4 and 5.)

9. Time inversion operator

Some additional properties of the spectrum may be obtained by taking into consideration the time inversion operation θ [18]. To act on a two-component spinor, this operation

may be taken in the form

$$\theta = -i\sigma_y K = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} K \tag{9.1}$$

where K is the operator of complex conjugation.

For any magnetic crystal, that is in the case of $V^+ \neq V^-$ in (2.3), the operator (9.1) can enter the symmetry group only in combination with unitary operations. From the condition for the Hamiltonian (2.2) and the anti-unitary operators $g_a = \theta\{\alpha_S|\alpha_R|t\}$ to commute, it follows [17] that, just as in the case of unitary operators, the symmetry group includes operators that transform the magnetic structure (2.1) into itself. (When acting on the magnetic structure, the operation (9.1) reverses the directions of magnetic moments.)

Below we give, without proof, some important statements connected with taking into account the time inversion operator:

(i) The restriction (4.6) and (4.7) imposed on the unitary parts of the operators g_a are the same as those for the unitary operators. But in this case transformations of type I enter into the symmetry group only for the SS.

(ii) If Ψ_k is a generalized Bloch function corresponding to the vector k, then $g_a\Psi_k$ is also a generalized Bloch function, but one corresponding to the wavevector $-\alpha_R k + \frac{1}{2}K_\alpha$. Hence we obtain the following additional property of spectral symmetry:

$$\varepsilon(-\alpha_R k + \tfrac{1}{2}K_\alpha) = \varepsilon(k). \tag{9.2}$$

(iii) The operation (9.1) may lead to an additional degeneracy at a given point k. Information about this degeneracy can be obtained using the following generalization of the well known Herring criterion [22]:

$$\sum_{\alpha_R k = -k + \frac{1}{2}K_\alpha + K_\mu} \chi_k((\theta\{\alpha_S|\alpha_R|\tau_\alpha\})^2) = \begin{cases} n_k & \text{case } (a) \\ 0 & \text{case } (b) \\ -n_k & \text{case } (c) \end{cases} \tag{9.3}$$

where χ_k is the character of the wavevector group IR being considered. The summation in (9.3) is carried out over anti-unitary symmetry operations that fulfil the condition specified under the summation sign. In cases (b) and (c), an additional degeneracy of levels takes place, which is due to the presence of anti-unitary elements. In case (a) such degeneracy is absent.

The main difference of formulae (9.2) and (9.3) from analogous formulae for space and magnetic groups [22, 23] is in the presence of a vector K_α in these formulae. The length of this paper does not allow us to carry out more detailed discussions of questions connected with operation θ.

Note that for the SS in HCP crystals, in complete analogy with traditional results for HCP structures [20], all representations for points of the interval AL and for internal points of the triangle ALH belong to the case (b). Therefore, all states of the ALH plane turn out to be at least doubly degenerate. Thus, for an SS one can use the double BZ, which is often convenient in the traditional consideration of HCP crystals [24].

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