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Symmetry analysis of electronic states for crystals with spiral magnetic order: II. Connection with limiting cases

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Abstract. Compatibility relations between the electronic states of crystals with spiral magnetic order and the states of non-magnetic, ferromagnetic and antiferromagnetic crystals are discussed. The results thus obtained permit one to predict the character of the electronic spectrum change on transition from a limiting case to a spiral structure. An anomaly in the optical characteristics of heavy rare-earth metals, which is observed on transition from the ferromagnetic structure to a spiral structure, is interpreted.

1. Introduction

In the previous paper [1], a general approach was developed for studying the symmetry of the electron spectrum exhibited by spiral magnetic configurations.

Ascertaining the changes that the spectrum undergoes with respect to one of the limiting cases of a non-magnetic, ferromagnetic, or antiferromagnetic crystal (see e.g. [2, 3]), well studied in terms of conventional band calculations, is vital to the qualitative interpretation of the electron spectrum of a spiral magnetic configuration. To perform a group-theoretical analysis of these changes, one needs to establish a relationship between the states of the limiting case as obtained in a conventional calculation and the states of the spiral that arise when the parameters of the spiral tend to values corresponding to a given limiting case. Knowledge of the compatibility relations for the states of the spiral and limiting magnetic structures permits one, in particular, to predict a change in the degeneracy of levels as the spiral parameters deviate from their limiting values. As a rule, a change in the degeneracy of states has important physical implications [2, 4].

The search for compatibility relations can be effected only on the basis of spin-space groups (SSG) and should contain the following stages: (i) describing the limiting-case symmetry in the language of SSG and constructing SSG irreducible representations (IR) whose basis is made up of electronic states that are calculated in a conventional approach and correspond to a given vector k_0; (ii) defining, in the approach based on the consideration of a spiral, the vectors k that correspond to the states belonging, in a conventional approach, to the vector k_0; and (iii) studying the interrelation between the constitutions of the groups of wavevectors k and k_0 in the two approaches under consideration.

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Next, knowing the constitutions of the wavevector groups and the characters of the IR of these groups, one can readily find representations at point k that correspond to a given IR at point k_0.

We shall consider peculiarities of the application of this scheme to different limiting cases.

A general approach to solving the problems of the first step is developed in [5]. The task of the second step has been discussed in [6]. We focus on aspects of the problem that were not discussed in those papers. The last section is devoted to the application of the results obtained to the experimental anomaly in the optical spectrum for heavy rare-earth metals (REM).

The present paper is closely connected with the previous paper [1]. Therefore, we use some notations of [1]. In the text there are also references to formulae of [1]. These formulae are labelled by two numbers.

All band-structure calculations represented in this paper have been carried out with the Korringa–Kohn–Rostoker (KKR) method [7] using the spin-polarized potential of Tb [8] as the local potential (2.3) in [1].

2. Non-magnetic crystal

The SSG of a non-magnetic crystal (NMC) involves operations $\{\alpha_S|\alpha_R|t\}$, where α_S is any spin rotation and $\{\alpha_R|t\}$ is an element of the space group (SG) of the crystal. The traditional classification of the NMC states is based on the use of IRS, $D^0_{p0k_0}$, of the group $G^0_{k_0}$ of the wavevector k_0. The group contains lattice symmetry transformations for which

$$\alpha_R k_0 = k_0 + K_\mu. \tag{1}$$

Here k_0 numbers the states satisfying the traditional Bloch condition

$$\{\varepsilon|\varepsilon|t_n\}\Psi_{k_0}(r) = \exp(-k_0 t_n)\Psi_{k_0}(r). \tag{2}$$

The corresponding IR of the group $\hat{G}_{k_0}$, which includes the SSG operators $\{\alpha_S|\alpha_R|t\}$ satisfying (1), can be represented in the form of a direct product:

$$\hat{D}_{p0k_0}(\{\alpha_S|\alpha_R|t\}) = U(\alpha_S) \times D^0_{p0k_0}(\{\alpha_R|t\}). \tag{3}$$

The doubling of the dimension of (3) relative to $D^0_{p0k_0}$ reflects the degeneracy of NMC states with opposite spin projections.

Let us find the compatibility relations between the states of an NMC and those of a spiral with vector q in the limit $V^+ \to V^-$ (see formula (2.3) in [1]). For the generalized translations, equality (3) takes the form

$$\hat{D}_{p0k_0}(\{\alpha(q\cdot t_n)|\alpha_R|t_n\}) = \begin{pmatrix} \exp[-i(\frac{1}{2}q + k_0)\cdot t_n] & 0 \\ 0 & \exp[-i(-\frac{1}{2}q + k_0)\cdot t_n] \end{pmatrix} \times E \tag{4}$$

where E is a unit matrix. Thus we obtain the well known result [6] that the NMC states with wavevector k_0 and spin projection σ are transformed into spiral states with wavevector $k_\sigma = k_0 + \frac{1}{2}\sigma q$. Therefore, in analysing the spectrum, it is useful at the outset to shift the non-magnetic bands with spin projection σ by the vector $\frac{1}{2}\sigma q$.

The subsequent analysis calls for a consideration of the constitution of the NMC group of wavevector k_0 and the constitution of wavevector k_σ group of the spiral structure. In view of (4.6*b*), the condition (5.5) imposed on the operations α_R of the wavevector k_σ group is equivalent, for operations of type I, to condition (1) for vector k_0. For operations of type II, the use of (4.7*b*) permits one to show that equality (5.5) is equivalent to the condition

$$\alpha_R k_0 = k_0 - \sigma q + K_\mu. \tag{5}$$

From (1) and (5) we can draw the following conclusions: (i) an operation of type I enters into the group of the wavevector k_0 if and only if this operation enters into the vector k_σ group; (ii) if q is not a reciprocal-lattice vector, then any operation of type II from the vector k_σ group will not enter into the group of the vector k_0; and (iii) if q is a reciprocal-lattice vector, then the groups of the vectors k_0 and k_σ contain the same set of type II operations.

Therefore, one needs to distinguish between the following three cases:

(*a*) q is not a reciprocal-lattice vector, G_{k_σ} does not contain operations of type II;
(*b*) q is a reciprocal-lattice vector; (6)
(*c*) q is not a reciprocal-lattice vector, G_{k_σ} contains operations of type II.

In the cases (*a*) and (*b*), G_{k_σ} is a subgroup of $\hat{G}_{k_0}$. Hence, to find an interconnection between the representation indices p_0 numbering the states in the traditional treatment of an NMC and the indices p numbering the states in the case of a spiral, it is sufficient to find the restriction of representation (3) on group G_{k_σ}. The representation thus obtained is, in general, reducible. The multiplicity factor of the pth IR in this reducible representation is defined by

$$n_p = \frac{1}{n(G_{k_\sigma})} \sum_{g \in G_{k_\sigma}} \chi_{p_0 k_0}(g)^* \chi_{pk_\sigma}(g) \tag{7}$$

where $\chi_{p_0 k_0}$ is the character of representation (3), χ_{pk_σ} the character of group G_{k_σ} IR, and $n(G_{k_\sigma})$ the number of group G_{k_σ} elements.

In case (*c*), G_{k_σ} is not a subgroup of $\hat{G}_{k_0}$. As is seen from formula (7.8), in this case the basis of a group G_{k_σ} IR may contain functions that belong to different IR in the traditional approach. Thus, the states corresponding to the same IR of the wavevector group of the spiral may belong to different representations (3). To study the interconnection of the states in case (*c*), one needs to find the restrictions of the group $\hat{G}_{k_0}$ representations (3) and also the G_{k_σ} IR on the greatest common subgroup of these groups, $G^{\mathrm{I}}_{k_\sigma}$. This subgroup consists of elements of G_{k_σ}, which belong to type I. Interconnected G_{k_σ} and $\hat{G}_{k_0}$ representations will be representations whose restrictions on subgroup $G^{\mathrm{I}}_{k_\sigma}$ contain the same IR of $G^{\mathrm{I}}_{k_\sigma}$.

Figure 1 shows the transformation of the electron spectrum on the transition from an NMC to a spiral. Indices of the IR labelling the states of the NMC in the traditional approach (figure 1(*a*)) and in the consideration of the NMC as a limiting case of the spiral (figure 1(*b*)) are given in the figure. We note only the most substantial points. Two states corresponding, in the traditional treatment, to the two-dimensional IR A_1 are shifted in the case of the spiral by a distance $\frac{1}{2}q$ and belong to two different representations, Δ_1 and Δ_2. As a result, the appearance of a non-zero exchange field leads to lifting of the

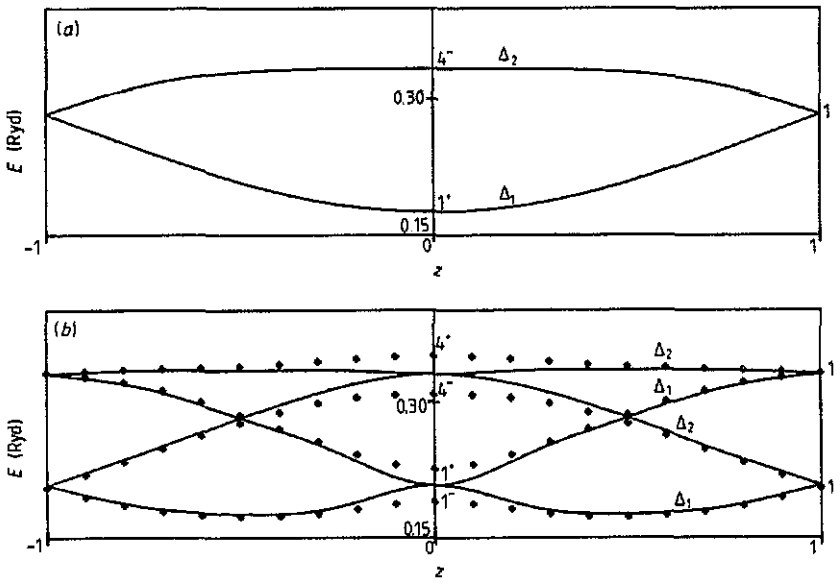

Figure 1. Transformation of the electronic spectrum on transition from NMC to spiral. (*a*) The spectrum of the NMC for the z axis points in the traditional approach. (*b*) The spectrum of the NMC considered as a limit of the spiral with $q = (0, 0, \pi/c)$ (full curves) and the spectrum of the SS with the same q (points). The scale of the abscissa is given in π/c units. To calculate the non-magnetic state, the spin components of the spin-polarized potential of Tb [8] were averaged.

degeneracy of the Δ_1 and Δ_2 states at points $\pm\frac{1}{2}q$. (As the intersecting bands belong to different representations, their intersections near the points $\pm\frac{1}{2}q$ persist (figure 1(*b*)); but the points of intersection are accidental.) In the case of the spiral, the point with $z = 1$ corresponds to type (*c*). In the non-magnetic limit, A_1 unites the states that in the traditional classification (figure 1(*a*)) are described by the IR Δ_1 at point $\frac{1}{2}q + \pi/c$ and by the IR Δ_2 at point $-\frac{1}{2}q + \pi/c$, and also by the opposite spin indices $\sigma = 1$ and $\sigma = -1$, respectively. (The state Δ_2 at point $\frac{1}{2}q + \pi/c$ is equivalent to the state Δ_1 at point $-\pi/c + \frac{1}{2}q$ shown in figure 1.) This degeneracy of states is a result of the symmetry of the problem and remains for a non-zero exchange field. The degeneracy of the NMC states at point Γ (figure 1(*b*)) is accidental from the viewpoint of the symmetry of the spiral and is lifted for a non-zero exchange field. As both intersecting bands correspond to the same IR at the points of the direction Δ, the degeneracy of states does not shift to another point but disappears.

Figure 1(*b*) shows that, for the given spiral parameters, the main changes of the electron spectrum as the NMC transforms to a crystal with a spiral magnetic structure may be treated as a mutual 'repulsion' of non-magnetic bands near point Γ. In this connection, it is useful to devote some attention to the term 'super-zone boundary', which is often used in the analysis of the electron spectrum of spiral magnetic configurations [2, 4].

Let α_R be a transformation entering into the symmetry group of an NMC and leading to the invariance of the spectrum under a reflection in a plane, and let the spiral vector q be perpendicular to that plane. Then, on displacing the spin sub-bands of the NMC by

the vectors $\pm\frac{1}{2}q$, we again obtain the degeneracy of states with opposite spin projections at the points of the plane. For the spiral considered in figure 1, the degeneracy takes place at the points of the $z = 0$ and $z = \pi/c$ planes, in particular at the points Γ and A shown in figure 1(*b*). The degeneracy lifting (because of the non-zero spiral exchange field) at all points of the plane may be interpreted as the appearance of 'super-zone boundaries'. But here it is worth pointing out that, first, for the spirals described by the Hamiltonian (2.2), the change of the Brillouin zone (BZ) does not actually take place and, as was mentioned in [1], the bands of the spiral magnet are continuous in the BZ of the NMC. In fact, we deal with the lifting of the degeneracy for definite states that have equal energies in the non-magnetic limit. Secondly, the application of the term 'super-zone boundary' calls for an exhaustive symmetry analysis, as degeneracy can take place in the case of a non-zero spiral field, too (see the point with $z = 1$ in figure 1(*b*)).

3. Ferromagnetic crystal

The SSG of a ferromagnetic crystal (FMC) contains operations $\{\alpha_S|\alpha_R|t\}$, where α_S is any spin rotation about the magnetization axis and $\{\alpha_R|t\}$ is an element of the lattice SG. The IR of the SSG of the wavevector k_0 may be represented in the form

$$D_{\sigma p 0 k_0}(\{C_\varphi|\alpha_R|t\}) = \exp(-\tfrac{1}{2}i\sigma\varphi)D^0_{p0k_0}(\{\alpha_R|t\}) \tag{8}$$

where C_φ is a spin rotation by an angle φ. States with opposite spin projections σ on the magnetization direction belong to different representations of the SSG.

The transition from a spiral structure to a ferromagnetic structure may be obtained by letting the angle θ or the vector q tend to zero (see formula (2.1) in [1]).

If we let θ tend to zero, we obtain, analogously to the case of an NMC, the result that if a ferromagnetic state with spin index σ corresponds to a vector k_0 in the traditional classification, that state will correspond, from the viewpoint of the spiral, to point $k_\sigma = k_0 + \frac{1}{2}\sigma q$. Hence, to compare the spectra of the ferromagnet and spiral, it is useful to shift ferromagnetic bands by the vector $\frac{1}{2}\sigma q$. For $\theta \neq \pi/2$ a spiral structure has no symmetry operations of type II. Therefore, the case (*c*) in (6) is never realized and the group of the wavevector k_σ for the spiral is always a subgroup of the vector k_0 group for the FMC. Hence, with the bands shifted, the main changes of the FMC spectrum reside in the splitting of multidimensional representations and in the 'repulsion' of the bands near the points of their intersection if, from the 'spiral' viewpoint, the bands belong to the same IR. (A figure illustrating this process can be found in [9].)

With the vector q tending to zero, the spiral states turn into ferromagnet states with the same value of the wavevector. Therefore, the changes in the spectrum are connected with a decrease in the number of operations in the wavevector group and include the 'repulsion' of bands belonging to the same IR of the spiral SSG and the splitting of multivalued IR.

Figure 2 allows one to compare the electron spectra of an FMC and an SS for three directions in the BZ of an HCP crystal. Although the value of the spiral vector is not very small, the spectra are close. As was supposed, substantial changes are obtained only in the regions where the 'repulsion' of opposite-spin bands arises. The splitting of multidimensional representations does not take place because all operations α_R of the HCP-lattice crystal class enter into the symmetry group of the SS (see table 1 of [1]). We do not show the indices of the IR in figure 2 because the corresponding tables of IR were not given in [1]. Note that, in accord with the analysis of section 7 of [1], the SSG of the

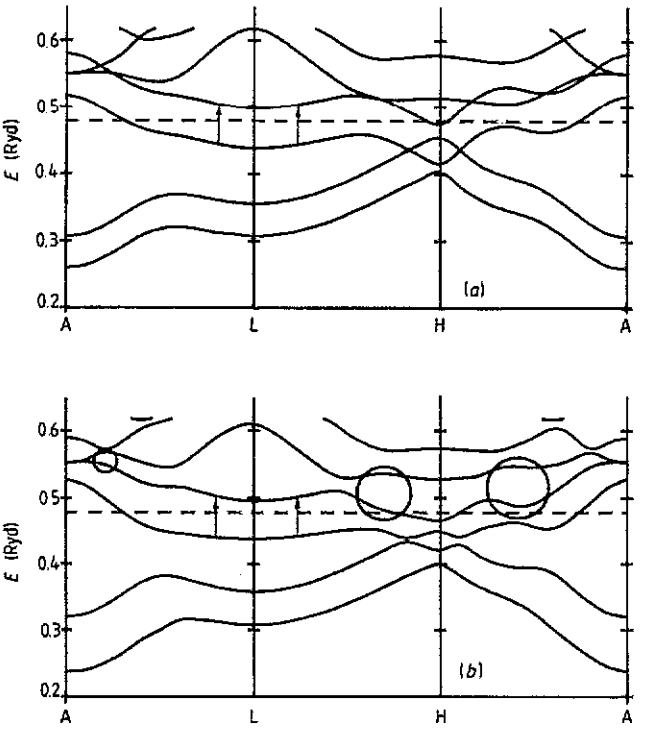

Figure 2. The energy spectrum of HCP crystal with ferromagnetic (*a*) and spiral magnetic (*b*) structures. The spiral parameters are $q = (0, 0, \pi/2c)$ and $\theta = 90°$. The regions of the main changes on transition from the FMC to the spiral are marked by circles. The arrows show the electronic transitions between stable parts of the bands. These transitions determine a weak dependence of the position of the optical peak with respect to the variation of magnetic structure [10, 11].

spiral for the directions AH and LH have, just as in the traditional case of the SG D_{6h}^4, only one IR. That is why all the intersections of the bands have disappeared for these directions.

4. Antiferromagnetic crystal

The conventional treatment of the electron structure of a two-sublattice antiferromagnetic crystal (AFC) rests on the use of a space group that contains operations leaving the magnetic sublattices invariant. For the sake of brevity we shall discuss only the crystals with one atom per unit cell.

Each sublattice can be considered as a ferromagnetic crystal. Hence, the operations of the sublattice SSG may be written in the form $\{C_\varphi \,|\, \alpha_R \,|\, t_n^s\}$, where C_φ is a spin rotation through an arbitrary angle φ about the axis parallel to magnetic moments; the t_n^s are translations that connect the sublattice atoms. Let $G_{k_0}^0$ be the SG of the vector k_0 and

$G^s_{k_0}$ be the corresponding SSG of the sublattice. Then, for the IR of these groups, we can write, by analogy with (8),

$$D_{\sigma k_0 p_0}(\{C_\varphi \,|\, \alpha_R \,|\, t^s_n\}) = \exp(-\tfrac{1}{2}\mathrm{i}\sigma\varphi) D^0_{k_0 p_0}(\{\alpha_R \,|\, t^s_n\}). \tag{9}$$

In addition to the symmetry operations of the sublattice, the SSG of an AFC also contains operations transforming one sublattice into other. As a representative of this class of transformations, we can take the operation $g_2 = \{\alpha(\pi)\,|\,\varepsilon\,|\,t_0\}$, where $\alpha(\pi)$ is a spin rotation through an angle π about the z axis (without restricting the generality of the consideration, we may suppose that the magnetic moments are parallel to the x axis) and t_0 is a translation connecting the sublattices. To construct the IR of the group

$$\hat{G}_{k_0} = G^s_{k_0} + G^s_{k_0} g_2 \tag{10}$$

we can use the method used in section 7 of [1] for the construction of the IR of a group on the basis of the IR of its half-subgroup. The formula for the characters of the subgroup representations (9) takes the form

$$\chi_{\sigma k_0 p_0}(g_2 h g_2^{-1}) = \chi_{(-\sigma)k_0 p_0}(h) \exp[-\mathrm{i}k_0 \cdot (-\alpha_R t_0 + t_0)] = \chi_{(-\sigma)k_0 p'_0}(h) \tag{11}$$

where $p_0 = p'_0$ if the exponent is always equal to 1 and $p_0 \neq p'_0$ in the opposite case; $h \in G^s_{k_0}$. The representations $D_{\sigma k_0 p_0}$ and $D_{(-\sigma)k_0 p_0}$ are inequivalent because they correspond to opposite σ values. Therefore, to construct the IR of $\hat{G}_{k_0}$, one needs to use formulae (7.8). The representation takes the form

$$\hat{D}_{k_0 p_0 p'_0}(h) = \begin{pmatrix} D_{k_0 p_0}(h) & 0 \\ 0 & D_{(-\sigma)k_0 p'_0}(h) \end{pmatrix} \tag{12a}$$

$$\hat{D}_{k_0 p_0 p'_0}(h g_2) = \begin{pmatrix} 0 & D_{\sigma k_0 p_0}(h) \\ -D_{(-\sigma)k_0 p_0}(h) \exp[-\mathrm{i}k_0 \cdot (\alpha_R t_0 + t_0)] & 0 \end{pmatrix}. \tag{12b}$$

The dimension doubling for the representation (12) relative to the representation (9) reflects the degeneracy of AFC states with opposite spin projections on magnetic moment direction. This degeneracy takes place at any point of reciprocal space. As is apparent from (12), the degenerate states may belong to different representations, p and p', coupled by condition (11).

To clarify the interconnection of the AFC states obtained in the traditional approach, and the same states obtained as a limit of the spiral states, we find the restriction of (12) on the group of generalized translations $\{\alpha(\boldsymbol{q}\cdot t_n)\,|\,\varepsilon\,|\,t_n\}$, where t_n runs over all sites of the lattice $t^s_n + t_0$. The representation thus obtained may be reduced with the help of the unitary matrix

$$U = 2^{-1/2} \begin{pmatrix} 1 & 1 \\ \mathrm{i}\exp(-\mathrm{i}k_0 \cdot t_0) & -\mathrm{i}\exp(-\mathrm{i}k_0 \cdot t_0) \end{pmatrix} \tag{13}$$

and takes the form

$$U D_{k_0 p_0}(T_n) U^{-1} = \begin{pmatrix} \exp[-\mathrm{i}(\boldsymbol{k}_0 + \frac{1}{2})\boldsymbol{q}) \cdot t_n] & 0 \\ 0 & \exp[-\mathrm{i}(\boldsymbol{k}_0 - \frac{1}{2}\boldsymbol{q}) \cdot t_n] \end{pmatrix} E. \tag{14}$$

Hence, just as with an NMC and an FMC, the states corresponding to $\boldsymbol{k}_0$ in the traditional consideration of an AFC correspond to the wavevectors $\boldsymbol{k}_\zeta = \boldsymbol{k}_0 - \frac{1}{2}\zeta\boldsymbol{q}$, $\zeta = \pm 1$, in the

treatment of the AFC as the limit of the spiral. But the AFC case has the following important difference.

For all three limiting cases, the Hamiltonian (2.2) commutes with the operator of the spin projection on a 'global' z axis. Hence, one can find the electronic states in a form where they have a definite projection on the 'global' axis. This possibility is used in traditional approaches.

In the case of an FMC and an NMC, the operator of the spin projection on the 'global' axis commutes also with all ordinary and generalized translations. The ordinary and generalized translations commute with each other. Thus, in the NMC and FMC the states having a definite spin projection on the 'global' axis satisfy both the traditional (2) and generalized (3.4) Bloch theorems. Contrary to the NMC and FMC, generalized translations of the AFC that connect different sublattices fail to commute with the operator of the spin projection on the 'global' axis. Hence, the AFC states used traditionally, which have a definite spin projection and satisfy Bloch's theorem (2), cannot satisfy the generalized Bloch condition (3.4) for all generalized translations.

Therefore, restricting the representations (3) and (7), obtained in the traditional approach to the NMC and FMC, on the group of generalized translations immediately gives diagonal matrices with the values $\exp(-ik_\sigma \cdot t_n)$ on the diagonal. In the AFC case this result is obtained only after a unitary transformation with the matrix (13). This transformation mixes pairs of states that have opposite spin projections on the 'global' axis and that satisfy Bloch's theorem (2) for the space translations from the sublattice symmetry group. As a result, we obtain states that satisfy the generalized Bloch theorem but have no definite spin projection of the 'global' axis.

Thus, two different approaches are possible in the AFC case. The first is based on the sublattice symmetry group and reflects the inequivalence of atoms of different sublattices with respect to the 'global' axis parallel to the magnetic moments. The second approach allows for the equivalence of all atoms, which is reflected in the invariance of the crystal relative to generalized translations.

Note that for strictly non-collinear structures the electron states cannot be characterized by a definite spin projection on any axis and one can use only the second approach, which rests on the generalized Bloch theorem.

The mutual inequivalence of both approaches to AFC leads to the following peculiarity of the antiferromagnetic spectrum. For an AFC the spiral vector q is a vector of the lattice reciprocal to the lattice of vectors t_n^s, but it is equal to only half a vector of the lattice reciprocal to the set of all translations t_n. Therefore, the reciprocal-space volume containing all inequivalent states (that is, the volume of the BZ) in the traditional case is a factor of 2 smaller than that used in the approach to the AFC from the viewpoint of the spiral. However, the irreducible domains that contain the states not connected by symmetry are the same in both cases because in the 'spiral' approach the spectrum of the AFC satisfies the symmetry condition [6]

$$\varepsilon(k) = \varepsilon(k + q). \tag{15}$$

Thus, an energy level of the AFC is characterized in the traditional approach by a point k_0 and indices p_0 and p_0' of the IR of $G_{k_0}^s$. In the 'spiral' approach, to this level there correspond states at the points k_ζ. To find the corresponding indices of the IR of the group G_{k_ζ}, one can use the circumstance easily proved that G_{k_ζ} is always a subgroup of $\hat{G}_{k_0}$. Hence, to define the indices of the IR of G_{k_ζ}, one needs to find the restriction of the representation (12) on the group G_{k_ζ} and, using tables of characters and a formula analogous to (7), to decompose the reducible representation thus obtained.

5. Application to analysis of optical anomaly in rare-earth metals

Thus, the methods of group theory permit us to predict the character of the energy band change in going from one of the limiting magnetic structures to a spiral structure. The foregoing analysis has shown that the appearance of 'super-zone boundaries' in the NMC spectrum (figure 1) and the disappearance of some intersections of bands in the FMC spectrum (figure 2) are processes of similar physical nature. Both processes are associated with the 'repulsion' of the electron states that have opposite spin projections and belong, in the case of the spiral, to the same IR of the SSG. The difference between NMC and FMC lies in the fact that, in the NMC case, the points where the lifting of the degeneracy takes place form planes in reciprocal space and may be predicted from symmetry considerations. In the FMC case the positions of these points are accidental and depend on the physical parameters of the crystal.

To give a qualitative interpretation of a spiral electron spectrum, it is natural to use a limiting spectrum closest to the spectrum being studied. An analysis of changes in the FMC spectrum on transition to a spiral structure is of special interest for rare-earth metals (REM), where these transitions are actually observed in experiment.

In particular, a comparison of the spectra given in figure 2 allows us to give an interpretation of the following experimental anomaly of the optical characteristics of heavy REM. Numerous optical experiments (see reviews [10, 11]) have detected an absorption peak whose position on the energy scale is proportional to the spin moment of an isolated REM atom. This peak has been ascribed to the electron transitions between the valence states split by the exchange field of the 4f shell. A non-trivial feature of the experiments is that the peak position depends weakly on magnetic-structure changes caused by temperature and magnetic field. In [12], to explain the weak temperature dependence of the 'exchange' peak position in Gd, the concept of a spin polaron [13] was used. The authors assumed that the width of the valence bands in Gd was much less than the value of the exchange splitting. As a result, for a non-collinear configuration, just as for a ferromagnet, the valence-state spin direction near any atom is collinear to the direction of the atomic magnetic moment. Consequently, the energy distances between electron states are defined by the intra-atomic exchange field and have a weak dependence on the angles between the magnetic moments.

The spin-polaron concept, explaining easily the weak dependence of optical peak on magnetic configuration, disagrees with the results of many works (see e.g. [2]), pointing out that it is the substantial magnetic-configuration dependence of the electron spectrum that defines the behaviour of the resistivity and of other physical characteristics.

An analysis of figure 2 permits us to resolve this contradiction. In the FMC case (figure 2(*a*)) the optical peak is connected with the transitions between the states of the third and fourth bands, which are split by the 4f-shell exchange field and are characterized by opposite spin projections. (Obviously, the exchange splitting and the bandwidth are values of the same order.) In accord with the conclusions of the group-theoretical consideration, substantial changes of the third and fourth bands at a transition from a ferromagnet to a spiral arise only near the points where these bands intersect the opposite-spin bands. This permits us to separate out a considerable part of the bands that is situated near the points L and remains practically unchanged. A calculation shows that for this part of the spectrum the maximal admixture of states with an opposite local spin projection is close to 15%. The weak change of the third and fourth bands near the point L is connected evidently with their isolation from the other bands. Conversely, near the points of intersection of the ferromagnetic bands a strong spin hybridization is observed. The contribution by the opposite-spin states reaches 35%.

Thus, in spite of the inapplicability of the spin-polaron concept to the whole spectrum of REMs, the similarity between the general spectrum structure of a ferromagnet and that of a spiral allows one to indicate a spectral region that may be qualitatively described on the basis of this concept. The Fermi level position is such that this part of the spectrum is involved in the optical transitions and is responsible for the stability of the peak on the experimental curves.

At the same time, the spectrum of the spiral configuration has regions sensitive to the magnetic structure. Here a substantial distortion of the ferromagnetic bands is observed. This distortion leads, in particular, to alteration of the Fermi-surface characteristics. Obviously, this part of the spectrum should lead to a substantial variation of many physical characteristics, such as kinetic coefficients and total electron energy.

Thus, the regions of the spectrum that respond in different ways to changes in magnetic structure determine the behaviour of the crystal in different experiments.

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