Non-collinear magnetism: effects of symmetry and relativity

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Abstract

We give a brief review of the theory of non-collinear order in itinerant electron systems. The theory is an example of the use of the local density-functional approximation for first-principles calculations. We emphasize the role of symmetry arguments since they facilitate the calculations and make the physics of the problem transparent. We choose as examples spiral structures like those found experimentally in fcc Fe, the canted states of U_3P_4 and weak ferromagnetism in α-Fe_2O_3 and show that these different phenomena are explained by the theory.

1 Introduction

It was more than forty years ago that non-collinear magnetic structures were first discovered experimentally [1], yet this physical phenomenon was investigated theoretically almost entirely in the framework of model Hamiltonians, assuming localized atomic moments [1], in contrast to collinear magnets which were intensively studied using first-principles calculational schemes provided by the density functional theory [2, 3]. This is perhaps due to the fact that non-collinear magnetic order seemed rather exotic and rare. But it attracted renewed interest in the late seventies and beginning of the eighties when it became clear that Stoner theory, which explains ground-state properties quite well, fails to describe the temperature behaviour of itinerant magnets. The reason for this failure was found in the neglect of transverse fluctuations of the magnetization density that, if viewed as originating from well-formed atomic moments, is equivalent to neglecting fluctuations in the directions of atomic moments (see e.g. [4]).

Detailed investigations of particular non-collinear magnetic configurations were started by Heine and his group using the cluster recursion method applied to a simplified tight-binding Hamiltonian [5]. The line of this work was continued with the use of the KKR method for a periodic solid (see e.g. [6]). A thorough discussion of density functional theory for a non-collinear magnet was subsequently given in [7] and applied to investigate the ground-state electronic and magnetic structure of Mn_3Sn. It was the experimental discovery of a spiral magnetic structure in fcc Fe [8] that made Fe an interesting object for theoretical studies [9, 10]. The last years showed a boom in investigations of non-collinear magnetism. Thus, for instance, successful studies of disordered systems [11, 12, 13] as well as multilayers [14, 15] were reported and a noteworthy and interesting step was made in describing the spin dynamics in itinerant electron systems [16]. In spite of its rather short history the theory of non-collinear magnetism involves quite different methods and is applied to a multitude of different physical problems. In this brief review we

are not trying to discuss all aspects of the presently used first-principles studies of non-collinear magnets, but rather select aspects which possess interesting symmetry properties. In particular, we will expose the role of spin-orbit coupling. This relativistic interaction sometimes acts in a destructive, sometimes in a constructive, way in the formation of particular non-collinear magnetic structures.

2 Kohn-Sham Hamiltonian of a non-collinear magnet

The derivation of the Kohn-Sham Hamiltonian for non-collinear magnets follows the standard procedure of density functional theory. In this case the total energy is considered as a functional of the two-dimensional density matrix and all single-particle wave functions are consequently treated as two-component spinor functions [7]. After variation of the functional with respect to the components of the spinor function one obtains equations that describe a magnetization continuously varying in space. For practical calculations it is common to use the atomic sphere approximation for the magnetization direction, i.e. the direction of the magnetization is supposed to be constant within the atomic sphere of every atom and different for different atoms. The scalar-relativistic Hamiltonian of a non-collinear magnet then takes the form

$$\hat{\mathbf{H}}_{sc}(\mathbf{a}_\nu, \mathbf{e}_\nu) = \sum_\nu \mathbf{U}^+(\theta_\nu, \phi_\nu) \begin{pmatrix} H_{sc}^{\nu\uparrow}(\mathbf{r}_\nu) & 0 \\ 0 & H_{sc}^{\nu\downarrow}(\mathbf{r}_\nu) \end{pmatrix} \mathbf{U}(\theta_\nu, \phi_\nu) \quad . \tag{1}$$

Here $\mathbf{a}_\nu$ are atomic positions and $\mathbf{e}_\nu$ directions of atomic moments, $\mathbf{U}(\theta_\nu, \phi_\nu)$ is the standard spin-$\frac{1}{2}$-rotation matrix, which describes the transformation between a global and a local coordinate system of the νth atom, whose spin orientation is given by the polar angles θ_ν and ϕ_ν with respect to the z-axis of the global system. The quantities $H_{sc}^{\nu\uparrow}(\mathbf{r}_\nu)$ and $H_{sc}^{\nu\downarrow}(\mathbf{r}_\nu)$ are the standard atomic scalar-relativistic Hamiltonians (spin up, spin down) [17] in the local frame of reference for the atom at site ν. They contain the mass-velocity, the Darwin term and the effective one-particle potential which, as usual, is given by functional derivatives of the total energy and is spin-diagonal in the local frame of this atom.

Note that the scalar-relativistic Hamiltonian possesses the same symmetry properties as the non-relativistic Hamiltonian which is obtained from the former by neglecting the mass-velocity and Darwin terms. Therefore the symmetry aspects discussed in this paper will be equally valid for both cases. Our calculations were carried out with the scalar-relativistic Hamiltonian.

A substantial part of the discussion will be devoted to the role of spin-orbit coupling which we will write in the form

$$\hat{\mathbf{H}}_{so} = \sum_\nu \mathbf{U}^+(\theta_\nu, \phi_\nu) \left\{ \sum_\alpha M_\alpha \sigma_\alpha \hat{l}_\alpha \right\} \mathbf{U}(\theta_\nu, \phi_\nu). \tag{2}$$

Here σ_α and $\hat{l}_\alpha$ are the Cartesian components of the Pauli spin matrices and the angular momentum, respectively, in the local system and the coefficients M can be found in Ref. [18].

The purpose of our work is the first-principles determination of the magnetic structure of a crystal. The basic steps to achieve this can be summarized as follows [7]: in each iteration step the eigenstates $\begin{pmatrix} \psi_1(\mathbf{r}) \\ \psi_2(\mathbf{r}) \end{pmatrix}_i$ of the Hamiltonian $\hat{\mathbf{H}}_{sc}$ in the scalar-relativistic or $\hat{\mathbf{H}}_{sc} + \hat{\mathbf{H}}_{so}$ in the relativistic case are calculated which enables us to determine the two-dimensional density matrix of the system:

$$\rho(\mathbf{r}) = \sum_{i\ occ} \begin{pmatrix} \psi_1(\mathbf{r})^* \psi_1(\mathbf{r}) & \psi_1(\mathbf{r})^* \psi_2(\mathbf{r}) \\ \psi_2(\mathbf{r})^* \psi_1(\mathbf{r}) & \psi_2(\mathbf{r})^* \psi_2(\mathbf{r}) \end{pmatrix}_i \tag{3}$$

where the sum runs over all occupied states. The density matrix contains information on the charge density, the directions of the atomic magnetic moments and the magnetization, all of which are necessary to redetermine the Hamiltonian for the next iteration step. The iterations are repeated until full self-consistency is achieved. The new degrees of freedom connected with the variation of the direction of the magnetic moments make the problem numerically more involved than in the case of a collinear magnetic state.

3 Generalization of the symmetry basis

Traditionally the symmetry properties of non-relativistic Hamiltonians are described in terms of ordinary irreducible representations of the relevant space group whereas for the relativistic problem the so-called double-valued irreducible representations are used. However, this difference in the type of representation merely reflects the difference in the choice of the functions subjected to the transformation. In the relativistic case the transformed function is always a spinor function whereas it is a scalar wave function in the non-relativistic case for which, correspondingly, only the transformation properties in real space need be considered.

It is the spinor form of the wave function that is of prime importance for the case of non-collinear magnetism. Hence, as in the relativistic case, one must use the double-valued irreducible representation. Still there is a subtle difference in the symmetry properties of the problem depending on whether or not the spin-orbit coupling is retained in the Hamiltonian. To describe this properly one introduces a generalized set of operators which allows an independent transformation of the spin and space variables [19]. For the group of such operators we will use the term spin-space group (SSG).

We define the action of an operator of the SSG on a two-component spinor function as follows

$$\{\alpha_S|\alpha_R|\mathbf{t}\}\ \psi(\mathbf{r}) = U(\alpha_S)\ \psi(\{\alpha_R|\mathbf{t}\}^{-1}\mathbf{r}) \tag{4}$$

where ψ is a two-component spinor function, $\mathbf{U}$ is the spin-$\frac{1}{2}$-rotation matrix, α_S and α_R are, respectively, spin and space rotations, and $\mathbf{t}$ is a space translation. Operators of the usual space group are those with $\alpha_S = \alpha_R$.

One easily proves that a transformation of the scalar-relativistic Hamiltonian (i.e. not including spin-orbit coupling) of a non-collinear magnet with the operations (4) leaves the form of the Hamiltonian invariant, i.e.

$$\hat{\mathbf{H}}_{sc}(\mathbf{a}'_\nu, \mathbf{e}'_\nu) = \{\alpha_\mathbf{S}|\alpha_\mathbf{R}|\mathbf{t}\}\hat{\mathbf{H}}_\mathbf{sc}(\mathbf{a}_\nu, \mathbf{e}_\nu)\{\alpha_\mathbf{S}|\alpha_\mathbf{R}|\mathbf{t}\}^{-1} \tag{5}$$

where $\mathbf{a}_\nu$ are atomic positions and $\mathbf{e}_\nu$ directions of atomic moments corresponding to the untransformed Hamiltonian. From (5) it follows that two magnetic crystals with atomic positions connected by the relation $\mathbf{a}'_\nu = \alpha_\mathbf{R}\mathbf{a}_\nu + \mathbf{t}$, and directions of magnetic moment connected by $\mathbf{e}'_\nu = \alpha_\mathbf{S}\mathbf{e}_\nu$, are equivalent in the scalar-relativistic case.

However, a transformation of the spin-orbit coupling term with an SSG operator does not reproduce the form of this term. Only when α_S=α_R do we restore the form-invariance of the Hamiltonian and find equivalent magnetic crystals:

$$\{\alpha_\mathrm{R}|\alpha_\mathrm{R}|\mathbf{t}\}\ \hat{\mathbf{H}}_\mathrm{so}(\mathbf{a}_\nu, \mathbf{e}_\nu)\ \{\alpha_\mathrm{R}|\alpha_\mathrm{R}|\mathbf{t}\}^{-1} = \hat{\mathbf{H}}_\mathrm{so}(\mathbf{a}'_\nu, \mathbf{e}'_\nu) \tag{6}$$

In many cases we are interested in the symmetry properties of one particular magnetic configuration and not in establishing the equivalence of different magnetic configurations. In this case the atomic positions and corresponding atomic moments must be the same before and after the transformation and the equations (5,6) reduce to commutating Hamiltonian and symmetry operators.

In what follows we will show how symmetry arguments help us to make calculations and facilitate to analyze the calculational results for a number of different physical problems.

4 Incommensurate spiral structure

A spiral magnetic structure is defined by

$$\mathbf{m}_n = m\ (\cos(\mathbf{q}\cdot\mathbf{R}_n)\sin\vartheta, \sin(\mathbf{q}\cdot\mathbf{R}_n)\ \sin\vartheta, \cos\vartheta) \tag{7}$$

where $\mathbf{m}_n$ is the magnetic moment of the n-th atom and m, $(\mathbf{q}\cdot\mathbf{R}_n)$, ϑ are polar coordinates.

An apparent difficulty for first-principles calculation of a spiral structure is the loss of periodicity with respect to lattice translations non-orthogonal to $\mathbf{q}$. One should notice, however, that in formula (7) all atoms of the spiral structure are equivalent, in particular, because of the equal

length of all atomic moments. But atoms can be equivalent only if they are connected by a symmetry transformation. A solution of the problem is suggested by using the operators of the SSG.

Indeed, transformations combining a lattice translation $\mathbf{R}_n$ and a spin rotation about the z axis by an angle $\mathbf{qR}_n$ leave the spiral structure invariant. The corresponding operators $\{\mathbf{qR}_n|\varepsilon|\mathbf{R}_n\}$ commute with the Hamiltonian of the spiral structure and therefore supply a symmetry transformation of the Hamiltonian. Here ε denotes the identity operation. These generalized translations form an Abelian group isomorphic to the group of ordinary space translations by vectors $\mathbf{R}_n$. Therefore the irreducible representations of both groups coincide and for the eigenfunctions of the Hamiltonian (1) there exists a generalized Bloch theorem [20]

$$\{\mathbf{qR}_n|\varepsilon|\mathbf{R}_n\}\psi_k(\mathbf{r}) = exp(-i\mathbf{kR}_n)\psi_k(\mathbf{r}) \tag{8}$$

where the vectors $\mathbf{k}$ lie in the first Brillouin zone which is defined in the usual way by the vectors $\mathbf{qR}_n$. These properties permit to restrict our considerations of real space to a chemical unit cell, not a supercell.

Generalizations of modern methods employing density functional theory to the case of spiral structures were done in Refs. [21] (for KKR, APW and tight binding methods), [9] (for the LMTO method), [10] (for the ASW method). This approach was successfully applied to the description of the ground state of fcc-Fe [9, 10] which was experimentally observed to have a spiral magnetic structure [8].

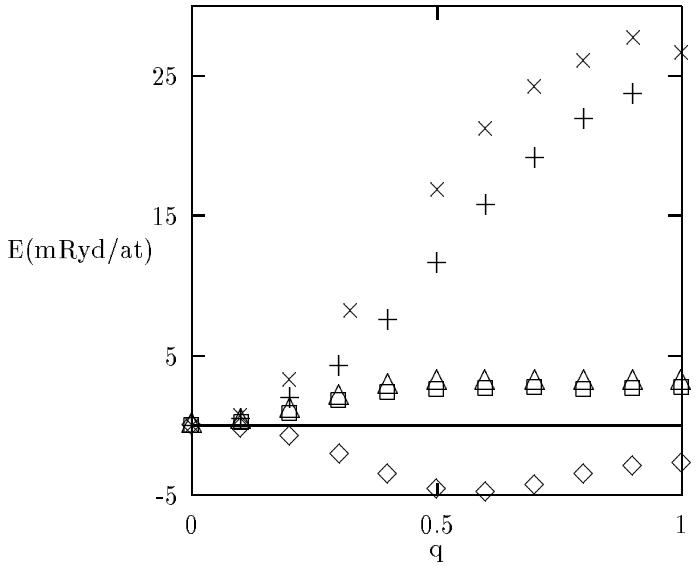


Figure 1: The total energy as a function of q for the (001) direction. $\diamond$ - fcc-Fe; + - bcc-Fe; $\square$ - fcc-Co; $\times$ - hcp-Co; $\triangle$ - Ni.

In Fig. 1 we show the results of calculations for the q-dependence of the total energy for a number of transition metals [22]. In full agreement with experiment for all metals, excluding the case of fcc-Fe, the ground state was found to be ferromagnetic which is the case of q=0. In fcc-Fe the minimum of the total energy occurs at a finite value of q, i.e. the ground state is spiral.

We complete this section with a discussion of the role of spin-orbit coupling in a spiral structure. The symmetry analysis of the previous section shows that spin-orbit coupling does not allow a separate transformation of the spin and space variables. This means the generalized translations do not apply here and we must conclude that spin-orbit coupling is destructive for the spiral structure. Indeed, experimental evidence seems to be in favour of our point of view since spiral structures are not observed in cases where the spin-orbit coupling is strong in the valence states. In particular, no spiral structures are observed in the U compounds where the U 5f electrons are itinerant and where the spin-orbit coupling is of the same order of magnitude as the exchange splitting. In contrast to this is the strong spin-orbit coupling for the core states which does not

lead to an increase of the magnetic anisotropy and therefore seems not to be an obstacle for the use of the generalized symmetry. Thus, in our opinion, the observation of spiral structures in 4f elements [1] is an argument in favour of treating the 4f states as core states.

5 Non-collinear magnetic structures in U_3P_4

Although no spiral structure was observed in U compounds there were many very different non-collinear magnetic configurations reported. To keep the length of this review acceptable we restrict the discussion to the first-principles study [23] of one interesting case namely to that of U_3P_4 [24]. The magnetic moments of the individual atoms in U_3P_4 do not compensate but rather possess a ferromagnetic component along the (111)-axis and the angles between the magnetic moments and the (111) axis seem to assume some accidental value. When calculations were started aligning all magnetic moments along the easy (111) axis then the scalar-relativistic and the relativistic Hamiltonians lead to drastically different results. Free to rotate, the magnetic moments deviate from the initial parallel directions in the relativistic case but stay parallel in the scalar-relativistic case. To appreciate the difference between these two cases we formulate the following nearly self-evident statement: "*The symmetry of the initial Kohn-Sham Hamiltonian must be preserved during calculations*". This means on the one hand that if the combined symmetry of the crystal and magnetic structure is so high that a deviation of magnetic moments from the initial directions leads to perturbing the invariance of the Hamiltonian with respect to at least one symmetry operator this deviation cannot take place. On the other hand, if a deviation of the magnetic moments from the initial directions is allowed by all symmetry operations present, then there are no symmetry reasons for keeping the initial magnetic configuration and the magnetic moments will start to rotate tending to assume the state of lowest total energy. This simulated annealing of magnetic moments will continue until the "accidental" - from a symmetry point of view - ground state magnetic structure will be found by the system.

These general statements will help us to explain the behaviour of magnetic moments in U_3P_4. We start with the scalar-relativistic case. As was shown in Sect. 3 the symmetry basis of a scalar-relativistic problem is formed by the spin-space group, i.e. separate transformations of the spin and space variables are allowed. We can formulate the result in a very general way: starting the scalar-relativistic calculation with a collinear configuration we will never obtain a deviation of magnetic moments from the initial direction. Indeed, independent of the crystal structure any spin rotation by an arbitrary angle ϕ about the direction of the magnetic moments $\{C_\phi|\varepsilon|0\}$ is a symmetry operation. This group of symmetry operations gives the symmetry basis for treating the spin projection of an electron state as a good quantum number [19]. Deviations of any magnetic moment from this direction would destroy the symmetry with respect to operations $\{C_\phi|\varepsilon|0\}$ and are therefore forbidden.

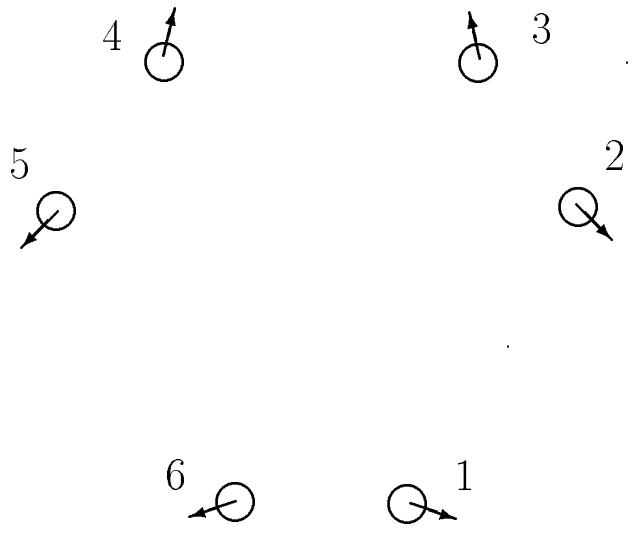


FIG. 2. Projection of the atomic positions and magnetic moments of the U atoms in U_3P_4 onto the (111) plane.

The situation changes drastically in the presence of SOC because of the reduction of the symmetry basis from the SSG to the usual space groups which transforms spin and space variables in an identical way i.e. $\alpha_S=\alpha_R$ in Sec.3. This means that the question of stability of a magnetic structure cannot be answered without analysis of the particular crystal structure. Therefore we note that U_3P_4 has a bcc lattice with a basis formed by two formula units, i.e. the unit cell consists of six U and eight P atoms. The crystal structure is rather complicated and need not be discussed here in detail. Instead, to illustrate the important symmetry properties it is sufficient to consider the simple picture of Fig. 2 where the projections onto the (111) plane of the positions of the six U atoms are shown. Let us assume that initially all magnetic moments are parallel to the (111) axis which is perpendicular to the plane of the paper. Then the following operations leave the magnetic and crystal structures invariant: the rotations by 120° and 240° about the (111) axis and the reflections in the planes containing the (111) axis accompanied by time reversal. Of importance is the observation that none of these operations leaves the position of any particular atom unchanged. Because of this, symmetry imposes no restrictions on the direction of the magnetic moment of a particular atom but only on the orientation of the atomic moments relative to each other and to the crystal lattice. The deviation of the moments from the (111) axis resulting in a non-collinear magnetic configuration does not change the symmetry of the crystal. Therefore, the ferromagnetic (θ=0) structure, from a point of view of symmetry, is not isolated from structures possessing a non-zero θ. In Fig. 2 we show the projections of the magnetic moments on the (111) plane which are obtained in the self-consistent calculation; these calculated deviations from the (111) axis evidently do not destroy the symmetry of the atomic configuration.

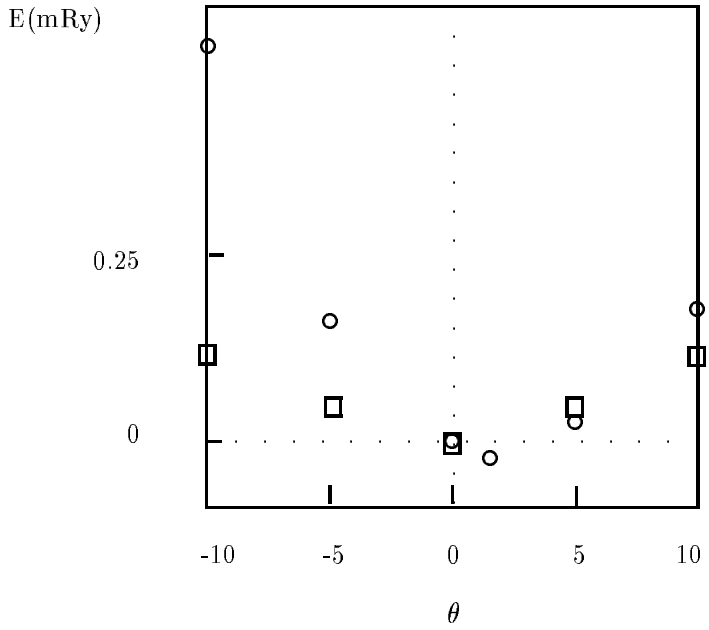


FIG. 3 Total energy of U_3P_4 as a function of angle θ. Circles show the points calculated with and squares without SOC.

More understanding of the system's behaviour can be gained with the help of Fig. 3 which shows the result for total energies when the directions of the magnetic moments are constrained to some values of angle θ near equilibrium (θ is the deviation of magnetic moments from the (111) direction). (During the variation of the magnetic structure we keep each moment in the plane containing the ground state direction of this moment and the (111) axis.) Fig. 3 shows that scalar-relativistic calculations give a total-energy curve symmetric with respect to a change of the sign of θ. This means an extremum of the total energy for the ferromagnetic configuration, θ=0, is predetermined by symmetry. In the relativistic case, however, the total energy as a function of θ is not symmetric about θ=0. In fact, for reasons of symmetry no extremum of the total energy at θ=0 is expected. As a result, the position of the extremum of the the total energy curve as a function of θ is "accidental" i.e. not determined by the symmetry of the problem.

The deviation of the magnetic moments from parallel directions in the case of U_3P_4 which

are caused by symmetry properties of the crystal and magnetic structures reminds us of the effect of weak ferromagnetism in Fe_2O_3, connected with the names Dzialoshinski and Moriya. We therefore show in the next Sect. that our symmetry analysis together with the method of calculation also explains this interesting case.

6 First principles study of weak ferromagnetism in Fe_2O_3

The phenomenon of weak ferromagnetism has been known for more than forty years (see e.g. [25]). It is characterized by a small net magnetic moment resulting from a collection of atomic magnetic moments that nearly cancel each other, one of the best known examples being α-Fe_2O_3. It has traditionally been discussed in terms of a model Hamiltonian of localized atomic moments of the form

$$H = I_{ij}\mathbf{S}_i\mathbf{S}_j + \mathbf{d}_{ij}[\mathbf{S}_i \times \mathbf{S}_j] + K_x S_x^2 + K_y S_y^2 + K_z S_z^2 \qquad (9)$$

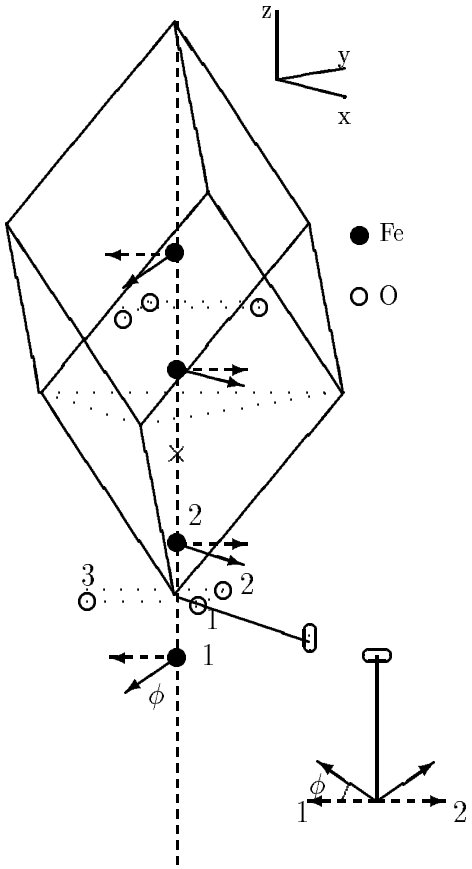
This Hamiltonian was suggested by Dzialoshinski [26] on the basis of phenomenological arguments. Moriya [27] showed that Dzialoshinski's explanation can be given a microscopic footing by means of Anderson's perturbation approach to magnetic superexchange. The first term of the Hamiltonian (9), the symmetric exchange, is supposed to lead to a compensated magnetic configuration. The next two terms, the anisotropic exchange and the magneto-crystalline anisotropy terms,respectively, can lead to a small ferromagnetic moment in an otherwise antiferromagnetic crystal. α-Fe_2O_3 is a classical example of a weak ferromagnet where the antisymmetrical exchange plays a key role.

The unit cell of the α-Fe_2O_3 is shown in Fig. 4. We start our calculation with the magnetic moments of the Fe atoms directed along the y axis which corresponds to the experimental situation at temperatures below that where weak ferromagnetism occurs. As was discussed above, in the scalar-relativistic case any collinear structure will be stable during calculations. However with the spin-orbit coupling taken into account the magnetic moments start to move until that magnetic configuration is reached where the total energy is lowest. The directions of the moments thus calculated are shown in Fig. 4. by solid arrows. Canting of magnetic moments produces a small ferromagnetic component of about 0.002 μ_B per Fe atom. This estimate is in a quite good agreement with the experimental value. Our symmetry analysis easily explains this canting as follows. With the spin-orbit coupling taken into account only four symmetry operations are left in the group of the

FIG. 4 The unit cell of Fe_2O_3. Cross on the diagonal of the rombohedron shows the point of inversion. The solid line passing through the first oxygen atom indicates a twofold symmetry axis. The collinear (dashed arrow) and canted (solid arrow) directions of the Fe atoms are shown. The canting of the Fe moments in the xy plane is demonstrated differently in the lower right corner of the Figure.

Kohn-Sham Hamiltonian: the identity transformation,the 180°-rotation about the x-axis and these operations multiplied by the inversion. Inversion transforms the atoms of the upper Fe_2O_3 molecule into the atoms of the lower molecule, see Fig. 4 and, since the magnetic moments are axial vectors, they do not change under this transformation. Hence, the corresponding atoms of the two molecules must keep parallel moments and we may restrict our consideration to the lower molecule in Fig. 4 . The only condition imposed on the moments of the Fe atoms by symmetry is the transformation of the moment of atom 1 into that of atom 2 by a rotation through 180° about the x-axis (see Fig. 4). However to fulfill this condition it is not necessary for the atomic moments to be parallel to the y-axis nor to remain collinear. Correspondingly, in the simulated annealing process, the magnetic moments deviate from their collinear initial directions toward the direction of the x-axis (see Fig. 4) until an "accidental" self-consistent magnetic structure preserved during iterations will be achieved.

An essentially different type of weak ferromagnetism was observed in Mn_3Sn [28]. Its magnetic structure is triangular and almost antiferromagnetic. A small canting of the magnetic moments leading to a weak ferromagnetic component cannot be caused in this case by the antisymmetric exchange because the contributions from different atoms cancel perfectly. Here the effect is supposed to be caused by the magneto-crystalline anisotropy. We carried out first-principles calculations [30] and obtained also in this case a very good description of the weak ferromagnetism. Again, in the scalar-relativistic calculation the ground state appears to be antiferromagnetic. But with spin-orbit coupling taken into account some magnetic moments deviate destroying the



complete magnetic compensation. Thus our method is universal and describes both types of weak ferromagnetism in the same calculational scheme.

7 Conclusion

In this short review we have shown that the local density approximation to density functional theory supplies a reliable basis for first-principles studies of non-collinear magnetic configurations in crystals. We restricted our discussion to ordered non-collinear structures which allowed us to use symmetry arguments to both, make accurate calculations possible and to render the physics transparent. We have shown that a consequent development of the density functional theory allows to explain within the itinerant electron picture the physical phenomena which were traditionally discussed in terms of the model Hamiltonian of localized moments.

The shortage of space did not allow us to discuss even briefly our work on an essentially different role of the spin-orbit coupling in non-collinear magnetism in various other U compounds [23]. Furthermore, we did not discuss calculations of the q-dependent magnetic susceptibility [22] , nor the use of the methods of non-collinear magnetism to study effects of non-zero temperatures [6, 29] as well as the work of other groups like that of [4, 5, 11, 12, 13, 15, 16, 31] on different aspects of non-collinear magnetism. Neither could we give a reasonably complete list of references to the work of others. Still we hope to have succeeded in giving an impression of the present state of the local density functional theory of non-collinear magnetism and supply at least a few first references for those who will want to gain a deeper insight into this rapidly developing branch of the physics of itinerant magnetism.

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References

[1] F. Keffer, in *Encyclopedia of Physics*, vol. 18/2, edited by H.P.J. Wijn (Springer, Berlin, 1966).

[2] J. Kübler and V. Eyert, in *Electronic and Magnetic Properties of Metals and Ceramics*, edited by K.H.J. Buschow (VCH-Verlag, Weinheim, 1992), p. 1.

[3] J.B. Staunton, *Rep. Prog. Phys.* **57** 1289 (1994)

[4] B.L. Györffy, A.J. Pindor, J. Staunton, G.M. Stocks, and H. Winter, *J.Phys. F* **15**, 1337 (1985).

[5] M.V. You, and V. Heine , *J.Phys. F* **12**, 177 (1982).

[6] L.M. Sandratskii, and P.G. Guletskii, *J. Magn. Magn. Mater.* **79**, 306 (1989).

[7] J. Sticht, K.H. Höck, and J. Kübler, *J. Phys.: Condens. Matter* **1**, 8155 (1989).

[8] Y. Tsunoda, *J. Phys. Condens. Matter* **1**, 10427 (1989).

[9] O.N. Mryasov, A.I. Liechtenstein, L.M. Sandratskii, and V.A. Gubanov, *J. Phys.: Condens. Matter* **3**, 7683 (1991).

[10] M. Uhl, L.M. Sandratskii, and J. Kübler, *Magn. Magn. Mater.* **103**, 314 (1992).

[11] R. Lorenz, J. Hafner, S.S. Jaswal and D.J. Sellmyer, *Phys. Rev. Lett.* **74**, 3688 (1995).

[12] M. Liebs, K. Hummer, Fähnle, *Phys. Rev.B*, **51**, 8664 (1995).

[13] A.V. Smirnov and A.M. Bratkovsky, *Europhys. Lett.*, **33**, 527 (1996).

[14] A. Vega, D. Stoeffler, H. Dreysse and C. Demangeat, *Europhys. Lett.* **31**, 561 (1995).

[15] V. Drchal, J. Kudrnovsky, I. Turek and P. Weinberger, preprint

[16] V. P. Antropov, M. I. Katsnelson, M. van Schilfgaarde and B. N. Harmon, *Phys. Rev. Lett.* **75**, 729 (1995).

[17] D.D. Koelling and B.N. Harmon *J. Phys.C*, **10** 3107 (1977).

[18] L.M. Sandratskii , J. Kübler, P. Zahn and I. Mertig, *Phys. Rev.B*, **50** 15834 (1994).

[19] L.M. Sandratskii, *J. Phys.: Cond. Matter* **3**, 8565 (1991); **3**, 8587 (1991).

[20] C. Herring, in:*Magnetism IV*, Chapt. V and XIII, eds. G. Rado, H. Suhl, Academic Press, New York, London 1966.

[21] L.M. Sandratskii, *Phys. Status Solidi b* **135** , 167 (1986).

[22] L.M. Sandratskii, J. Kübler, *J. Phys. Condens. Matter*, **4**, 6927 (1992).

[23] L.M. Sandratskii and J. Kübler, *Phys. Rev. Lett.* **75** (1995) 946, *Physica B* (in press).

[24] P. Burlet, J. Rossat-Mignod, R. Troc and Z. Henkie, *Solid State Commun.* **39**, 745 (1981).

[25] L. Néel and R. Pauthenet C.R. *Acad. Sci.*, Paris 234, 2172 (1952).

[26] I.J. Dzialoshinski, *Phys. Chem. Solids*, **4** (1958) 241.

[27] T. Moriya, *Phys. Rev.*, **120** (1960) 91.

[28] S. Tomiyoshi and Y. Yamaguchi, *J. Phys. Soc. Japan* **51**, 2478 (1982).

[29] M. Uhl, L.M. Sandratskii and J. Kübler, *Phys. Rev.B* **50** (1994) 291.

[30] L.M. Sandratskii and J. Kübler, to be published

[31] A.I. Liechtenstein, M.I. Katsnelson, V.P. Antropov, V.A. Gubanov, *J. Magn. Magn. Mater.* **67**, 65 (1987).