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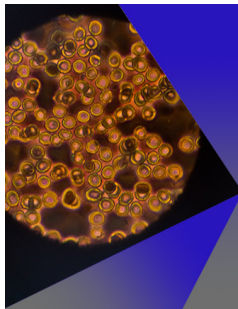
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Patrizio Ansalone,^{a)} E. S. Olivetti, A. Magni, A. Sola, and V. Basso

AFFILIATIONS

Istituto Nazionale di Ricerca Metrologica, Strada delle Cacce, 91, 10135 Torino, Italy

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^{a)} Author to whom correspondence should be addressed: p.ansalone@inrim.it

ABSTRACT

This paper employs a non-abelian gauge theory to derive the relation between a chiral crystal structure and the bulk magnetic DMI energy term. We apply the method to the B20 chiral compounds, in which the chirality develops along the diagonals of the cubic crystal, and we derive, in this framework, the corresponding isotropic Lifshitz invariant.

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I. INTRODUCTION

MnSi, FeGe, MnGe and Fe(Co)Si, belonging to the B20 crystal structure type, exhibit non-trivial magnetisation configurations. Most notably, magnetic structures are long-wavelength helical states^{1,2} or skyrmion states with a well-defined chirality.^{3–6} The interest in such magnetic states lies in the possibility to manipulate skyrmions as logic bits through the spin-transfer torque effect, driven by a low electric current density.^{7,8} Such chiral magnetic states are caused by energy terms called Lifshitz invariants, bilinear in the magnetisation and its first spatial partial derivative.^{3–7} In thin films and multilayers, the symmetry is broken at the interface between two metals, and at the interface between metals and ferromagnets due to the spin-orbit interaction. The so-called surface Dzyaloshinskii-Moriya interaction (DMI), give rise to the Lifshitz invariant term of the antisymmetric type, that stabilises Néel type skyrmions.^{9–14} A similar role is played by the presence of an external electric field.¹⁵ In bulk crystals, such as the non-centrosymmetric B20 compounds, the crystal possesses chirality in specific directions, and the relevant Lifshitz invariant term of diagonal type stabilises both Bloch-type skyrmions and helical states. The corresponding interaction is the so-called bulk DMI. This interaction should be related to the point group symmetry of the crystal structures; however, this connection is not always evident.^{16,17} This paper employs a non-abelian gauge theory to address the problem. The idea is to exploit the $SO(3)$ local gauge invariance of the micromagnetic energy under the action of a local rotation.^{15,18–20} By considering the case of the pure gauge field, the critical outcome of the theory is to substitute the traditional spatial derivative with

a gauge covariant derivative. In the micromagnetic energy functional, the substitution affects the exchange interaction term, which is usually proportional to the square of the space derivatives of the magnetisation vector. Therefore, if the substituted exchange term is expanded to recover the original term, one finds two additional energy terms: a DMI-like term and an anisotropy type term. We apply the theory to non-centrosymmetric crystals and exploit the Neumann's principle²¹ stating that the invariance of a crystal under the action of its own point group symmetry implies the invariance of its physical properties. In the specific case of B20 compounds with tetrahedral symmetry, we show that the corresponding energy term is the bulk DMI one. The structure of the paper is the following: in section II, we describe the chiral properties of the B20 compounds, in section III, we introduce the Lifshitz invariants and finally, in section IV, we present the gauge covariant derivative to be associated with the chiral tetrahedral point group symmetry.

II. CRYSTAL SYMMETRY

A. Chiral tetrahedral point group symmetry

Chiral crystals can occur in space groups (SGs) containing only proper symmetry elements (rotations, translations and roto-translations), i.e. the ones that do not contain any mirroring operation or inversion point. These space groups, called Sohncke groups, can be further divided into chiral SGs (i.e. the 11 pairs of SG which are in enantiomorphic relation) and non-chiral SGs.²² Achiral space

groups belonging to the Sohncke group contain a 2_1 rotation axis and produce chiral crystals only because the asymmetric unit is chiral: crystals of this type can thus be right-handed or left-handed without changing SG, which is the reason why the SG is classified as achiral. On the other hand, chiral SGs contain at least one screw axis different from the 2_1 axis, and they allow the chiral crystallisation even of achiral building blocks since the SG permits only a clockwise or an anticlockwise rotation. In this case, left-handed and right-handed crystals are classified under different SGs of one of the enantiomorphic pairs, e.g. $P3_1$ and $P3_2$. In the next section, we point out our attention to the cubic B20 structure type, in which well known chiral structures crystallise, such as the monosilicides and monogermanides of the transition metals (TM), among which MnSi, FeGe, MnGe and Fe(Co)Si exhibit magnetic ordering. The B20 structure is described by the space group $P2_13$ (#198 of the international tables for crystallography), which exhibits the tetrahedral symmetry of the point group 23, (i.e. the chiral tetrahedral point group), characterised by three orthogonal 2-fold rotation axes and four 3-fold axes, centred among the three orthogonal directions. All the twelve symmetry operators of the crystal class can be obtained by multiplying only two generating matrices representing the described rotations.²³ In Appendix, the two generators of an irreducible representation of the tetrahedral point group 23 (i.e. the subgroup of symmetries operations that leave one point fixed) are reported.

B. B20 chiral crystals

The B20 structure compounds were synthesised for a few transition metals (TMs) with group 14 elements (especially Si or Ge). The unit cell contains 4 TM atoms and 4 Si(Ge) atoms placed in a tetrahedral position along the cube body diagonal. By looking at the crystal from different perspectives (Fig. 1), one can notice the peculiar features related to the crystal chirality: i) the $(11\bar{2})$ projection reveals that atoms of both species are placed on (111) planes in alternating dense and sparse layers; ii) from the (111) projection, one can see that both TM and Si (or Ge) atoms form helical structures of opposite handedness, with an axis parallel to one of the cube diagonals, and iii) each helix involves only one atom for each of the dense layers, while atoms of the sparse layers do not participate to any of the helices. By looking at the TM species, only one can classify the chirality of the crystal. The specular crystal with opposite chirality can also occur in the same space group since $P2_13$ is an achiral Sohncke SG.

B20 are therefore characterised by intrinsic handedness due to the crystal structure, with each atomic species forming helices of the characteristic period ($\sqrt{3}l_a$, being l_a the lattice parameter) in $\langle 111 \rangle$ directions. From the magnetic point of view, the magnetic moments helix that develops in B20 compounds with magnetic ordering may display the same handedness of the crystal chirality or not, depending on the composition of the specific compound,²⁴ and it typically shows a period of 1-2 orders of magnitude larger (10-230 nm),²⁵ revealing that the connection between atomic arrangement and magnetic configuration is not straightforward. However, the tetrahedral crystal symmetry has a definite role in determining the magnetic structure since the magnetic helicity has been observed to propagate along the cube body diagonals.²⁶

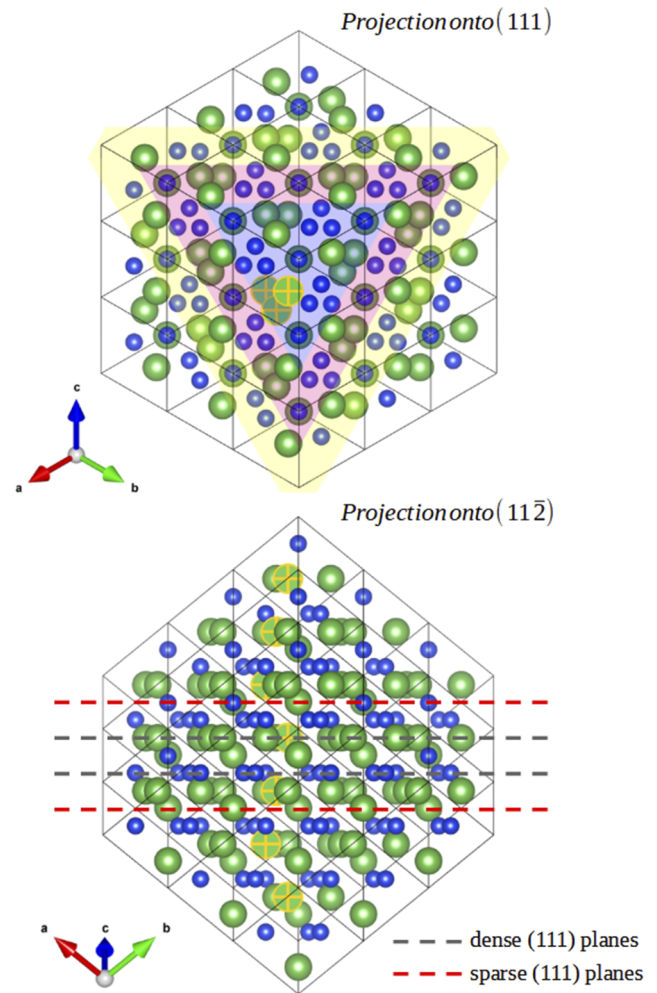


FIG. 1. A B20 crystal formed by $3 \times 3 \times 3$ unit cells viewed along $[111]$ or $[11\bar{2}]$ directions. The three topmost dense (111) planes containing TM atoms (green) are displayed in color. For example, the atoms involved in one of the right-handed helices of the TM species pointing in the $[111]$ direction have been highlighted with the yellow crosses. Such helices are present along each of the 4 cube body diagonals. The size of TM atoms has been slightly increased to better display the helix chirality. Pictures of the crystal structures have been produced with Vesta 3 software.²⁷

III. LIFSHITZ INVARIANTS

The DMI-like energy term is described by the Lifshitz invariants $\mathcal{L}_{ijk} = m_k \partial_i m_j - m_j \partial_i m_k$ and, because of the antisymmetry $\mathcal{L}_{ijk} = -\mathcal{L}_{ikj}$, is written as

$$u_{\text{DMI}} = -\epsilon_{lkj} T_{il} (m_k \partial_i m_j - m_j \partial_i m_k), \quad (1)$$

where T_{il} is a matrix with 3×3 components that we can subdivide into an antisymmetrical, a symmetrical, and a diagonal parts $T_{il} = T_{A,il} + T_{S,il} + T_{D,il}$. The antisymmetrical part $T_{A,il} = -T_{A,li}$ can

be written as $T_{A,il} = \epsilon_{ilk} T_{A,k}$ where $T_{A,k}$ are components of a vector. These antisymmetric terms

$$u_{\text{DMI}} = -2T_A \cdot [\mathbf{m}(\nabla \cdot \mathbf{m}) - (\mathbf{m} \cdot \nabla)\mathbf{m}] \quad (2)$$

correspond to the so-called surface DMI terms and stabilise magnetic structures with a Néel type chirality. This can be seen, for example by choosing $T_k = T_z$, $\partial_i = \partial_x$ and $m_y = 0$. In this case, the minimum energy configuration, considering the competition with the exchange energy $A(\partial_i m_j)^2$, corresponds to a spiral state with wave-number $q_x = T_z/A$, therefore a positive rotation around the y -axis, if $T_z > 0$ (Fig.2 top). The symmetric terms correspond to an anisotropic modification of the previous terms and will not be considered here. The diagonal part of the tensor gives rise to the bulk DMI energy terms.

The energy term is written as

$$u_{\text{DMI}} = -2T_{ii}(\mathbf{m} \times \partial_i \mathbf{m})_i \quad (3)$$

Such a compact form is expanded as follows:

$$\begin{cases} -2T_{xx}(m_z \partial_x m_y - m_y \partial_x m_z) \\ -2T_{yy}(m_x \partial_y m_z - m_z \partial_y m_x) \\ -2T_{zz}(m_y \partial_z m_x - m_x \partial_z m_y) \end{cases} \quad (4)$$

In a material with an easy axis anisotropy along the z direction, the terms T_{xx} and T_{yy} produce a Bloch type chirality. For example,

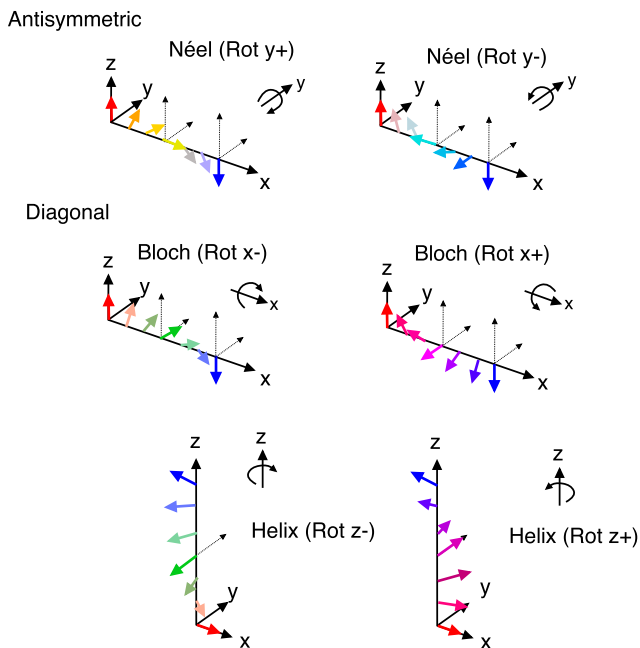


FIG. 2. Static configurations stabilised by the Lifshitz invariants of the DMI represented along one representative axis. Top: the so-called surface DMI term generates the Néel type chirality, i.e. the antisymmetric Lifshitz invariants. Middle and bottom: Bloch type chirality (middle) and helix (bottom) stabilised by the bulk DMI, i.e. the diagonal Lifshitz invariants.

choosing T_{xx} , $\partial_i = \partial_x$ and $m_x = 0$ the corresponding stable state is a spiral state with $q_x = T_{xx}/A$ (Fig.2 middle). Then $T_{xx} > 0$ produces a negative rotation around the x -axis. In a material with a hard axis anisotropy along the z direction, the term T_{zz} produces a helical state. For those with $\partial_i = \partial_z$ and $m_z = 0$ the stable state is a helical state with $q_z = -T_{zz}/A$ corresponding to a negative rotation around the z -axis for $T_{zz} > 0$ (Fig.2 bottom).

By considering the case with all the coefficients equal each others, i.e. $T_{xx} = T_{yy} = T_{zz} = T$, the sum of the three diagonal terms give rise to the isotropic bulk DMI energy density that is written as

$$u_{\text{DMI}} = -2T\mathbf{m} \cdot (\nabla \times \mathbf{m}) \quad (5)$$

The bulk DMI terms generated by the diagonal part of the tensor of the Lifshitz invariants are those expected due to the chiral properties of the crystal. Nevertheless, as the description in terms of the invariants is thoroughly phenomenological, the coefficients should be derived based on the specific symmetries possessed by the crystal.

IV. GAUGE, POINT GROUP SYMMETRY AND NEUMANN'S PRINCIPLE

The purpose of this section is to introduce a non-abelian gauge field \mathcal{A}_i with values in the non-abelian $SO(3)$ -group (i.e. the group of the rotation in the Euclidean space). Such a non-abelian gauge field imposes a modification in the definition of the partial derivatives that occur in the exchange energy term of the classical micromagnetic energy. With this method and the Neumann's principle, we directly found the relationship among the gauge covariant derivative, the point group symmetry of the material, and the Lifshitz invariants. Firstly, the gauge covariant derivative is introduced through the general concept of non-abelian gauge fields as in Refs. 15 and 28-31

$$\mathcal{D}_i \mathbf{m} = \partial_i \mathbf{m} - \mathcal{A}_i \times \mathbf{m}. \quad (6)$$

Secondly, the non-abelian gauge field \mathcal{A}_i transforms according to the following rule $\mathcal{A}_i \rightarrow \mathcal{R}^T \mathcal{A}_i \mathcal{R} + \mathcal{R}^T \partial_i \mathcal{R}$, with \mathcal{R} an element of the $SO(3)$ -group³² represented as

$$\begin{aligned} \mathcal{R}_{lk}(\psi, \mathbf{n}) &= \exp(\psi \hat{\mathbf{n}} \cdot \boldsymbol{\Sigma}) \\ &= n_l n_k + (\delta_{lk} - n_l n_k) \cos \psi - \epsilon_{lki} n_i \sin \psi, \end{aligned} \quad (7)$$

where ψ is the rotation angle, and \mathbf{n} the rotation axis. Moreover, we assume the following relation $J_l = i\Sigma_l$ where J_l matrices are the generators of the Lie algebra of the $SO(3)$ -group, $[J_l, J_k] = i\epsilon_{lki} J_i$. However, we limit our attention to the vacuum state of the system, classically a pure gauge field configuration (i.e. $\mathcal{A}_i \rightarrow \mathcal{R}^T \partial_i \mathcal{R}$). Hence the pure gauge covariant derivative assumes the following form

$$\mathcal{D}_i \mathbf{m} = \partial_i \mathbf{m} - \partial_i \psi \times \mathbf{m}, \quad (8)$$

where ψ is an axis of rotation whose module quantifies the rotation angle around itself. Finally, the micromagnetic energy, in a

gauge-invariant fashion, taking into account the generalised exchange interaction, it is written as follows

$$\begin{aligned}
 u(\mathbf{m}, \partial_i \mathbf{m}, \partial_i \psi) &= A \mathcal{D}_i \mathbf{m} \cdot \mathcal{D}_i \mathbf{m} \\
 &= A [\partial_i \mathbf{m} \cdot \partial_i \mathbf{m} - 2(\mathbf{m} \times \partial_i \mathbf{m}) \cdot \partial_i \psi \\
 &\quad + (\partial_i \psi \times \mathbf{m}) \cdot (\partial_i \psi \times \mathbf{m})] \quad (9)
 \end{aligned}$$

We now focus our attention on a DMI-like term in the second row of the Eq.(9)

$$\begin{aligned}
 -2(\mathbf{m} \times \partial_i \mathbf{m}) \cdot \partial_i \psi &= -\epsilon_{ijk} \partial_i \psi_l (m_k \partial_i m_j - m_j \partial_i m_k) \\
 &= -\epsilon_{ijk} \partial_i \psi_l \mathcal{L}_{ijk} \quad (10)
 \end{aligned}$$

where \mathcal{L}_{ijk} is the Lifshitz invariant. The coefficient $\partial_i \psi_l$ corresponds to the T_{il} of the section III. By choosing as axes of rotation the four diagonal of the B20 crystal where the chirality develops, one can obtain the corresponding energy of the bulk DMI type. The phenomenological constitutive properties of the B20 crystal regarding the DMI-like energy term are described by the matrix T_{il} . The crystal B20 is invariant under the action of an irreducible representation of the generators of the point group symmetry 23, $\mathcal{R}^{(\alpha)}(\mathbf{n}, \psi) = \mathcal{R}_{lk}^{(\alpha)}(\mathbf{n}, \psi) \mathbf{e}^l \otimes \mathbf{e}^k$. The Neumann's principle applied to the DMI-tensor is

$$T_{il} = |\mathcal{R}^{(\alpha)}(\mathbf{n}, \psi)| \mathcal{R}_{ir}^{(\alpha)}(\mathbf{n}, \psi) T_{rs} \mathcal{R}_{sl}^{(\alpha)}(\mathbf{n}, \psi) \quad (11)$$

By solving the linear system Eq.(11) (see Appendix) we obtain the bulk DMI-like energy term, and the permitted coefficients of the matrix T_{il} are only diagonal terms with equal values.

V. DISCUSSION AND CONCLUSIONS

Starting from general considerations about the irreducible representation of point group symmetry of the B20 structure, we have provided a detailed construction of a non-abelian gauge theory applied to this class of crystals. The presented results give an insight into the relationship between the Lifshitz invariants and the gauge covariant derivative, providing a connection between the partial derivatives of the local rotation $\partial_i \psi_l$ and the DMI tensor T_{il} by using the Neumanns' principle. The construction shown can easily extend beyond the tetrahedral point group symmetry 23 to other ones. Moreover, this model may be extended by adding permitted magnetocrystalline anisotropy, although further analysis within this framework will be required to include, for example, the fourth-order magnetocrystalline anisotropy term.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

DATA AVAILABILITY

The data that support the findings of this study are available within the article.

APPENDIX

We derive the DMI-tensor explicitly for a cubic crystal with the point group symmetry 23 (i.e. the chiral tetrahedral point group). An irreducible representation of the tetrahedral point group consists of two linearly independent elements able to generate the whole symmetry class of the crystal constituted by 12 elements. Moreover, since the tetrahedral group 23 is the rotation symmetry group of the regular tetrahedron, we use the same notation for the rotation matrices specifying the direction \mathbf{e}_z , $\mathbf{n} = -\frac{1}{\sqrt{3}}(1, 1, 1)^T$, and the angles of rotation:

$$\begin{aligned}
 \mathcal{R}_{lk}^{(1)}(\mathbf{e}_z, \pi) &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \\
 \mathcal{R}_{lk}^{(2)}\left(\mathbf{n}, \frac{2}{3}\pi\right) &= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}. \quad (A1)
 \end{aligned}$$

Now we apply the Neumanns' principle,²¹ and we explicitly compute the components of the DMI-tensor T ,

$$\begin{aligned}
 T &= \mathcal{R}^{(1)}(\mathbf{e}_z, \pi) T \mathcal{R}^{\tau(1)}(\mathbf{e}_z, \pi) \\
 &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\
 &= \begin{pmatrix} T_{11} & T_{12} & -T_{13} \\ T_{21} & T_{22} & -T_{23} \\ -T_{31} & -T_{32} & T_{33} \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{pmatrix}. \quad (A2)
 \end{aligned}$$

$$\begin{aligned}
 T &= \mathcal{R}^{(2)}\left(\mathbf{n}, \frac{2}{3}\pi\right) T \mathcal{R}^{(2)\tau}\left(\mathbf{n}, \frac{2}{3}\pi\right) \\
 &= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} T_{11} & T_{12} & 0 \\ T_{21} & T_{22} & 0 \\ 0 & 0 & T_{33} \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \\
 &= \begin{pmatrix} T_{22} & 0 & T_{21} \\ 0 & T_{33} & 0 \\ T_{21} & 0 & T_{11} \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} & 0 \\ T_{21} & T_{22} & 0 \\ 0 & 0 & T_{33} \end{pmatrix} \quad (A3)
 \end{aligned}$$

In order to fulfil both constraints in Eqs.(A2) and (A3) the DMI-tensor is defined as follows

$$T_{il} = \begin{pmatrix} T & 0 & 0 \\ 0 & T & 0 \\ 0 & 0 & T \end{pmatrix}. \quad (\text{A4})$$

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