Altermagnetism and magnetic groups with pseudoscalar electron spin

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We revise existing group-theoretical approaches for a treatment of nonrelativistic collinear magnetic systems with perfect translation invariance. We show that full symmetry groups of these systems, which contain elements with independent rotations in the spin and configuration spaces (spin groups), can be replaced by magnetic groups consisting of elements with rotations acting only on position vectors. This reduction follows from modified transformation properties of electron spin, which in the considered systems becomes effectively a pseudoscalar quantity remaining unchanged upon spatial operations but changing its sign due to an operation of antisymmetry. We introduce a unitary representation of the relevant magnetic point groups and use it for a classification of collinear magnets from the viewpoint of antiferromagnetism-induced spin splitting of electron bands near the center of the Brillouin zone. We prove that the recently revealed different altermagnetic classes correspond in a unique way to all nontrivial magnetic Laue classes, i.e., to the Laue groups containing the operation of antisymmetry only in combination with a spatial rotation. Four of these Laue classes are found to be compatible with a nonzero spin conductivity. Subsequent inspection of a simple model allows us to briefly address the physical mechanisms responsible for the spin splitting in real systems.

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I. INTRODUCTION

One of the most important characteristics of a solid from the viewpoint of magnetic properties is certainly its magnetic structure. A standard classification of various magnetic orders is based on the mutual arrangement of local magnetic moments and their orientation with respect to the atomic lattice [1]. This approach covers both traditional spin structures (ferromagnets, spin glasses, etc.) and more exotic orders, such as magnetic skyrmions [2,3]. In recent years, the close relation of magnetism and spintronics has given rise to a complementary approach to the varieties of magnetic solids, which is based on their electronic structure. This change of focus from the real space (local magnetic moments) to the reciprocal space (electronic spectra) has partly been motivated by new phenomena related to topological aspects of electron states [4–6] or by a momentum-dependent spin splitting of electron bands in collinear antiferromagnets [7–12]. The latter phenomenon, proposed theoretically by Pekar and Rashba in 1964 [13], has recently attracted considerable attention, especially due to the fact that the strength of this splitting can be sizable also in systems of light elements [14–17]. This contrasts the usual splitting due to spin-orbit interaction, which is mainly strong in systems containing heavy elements. The nonrelativistic origin of the antiferromagnetism-induced spin splitting, a large number of systems exhibiting this property, and its potential importance for further development of spintronics have led to a special term for this type of magnetic order, namely, altermagnetism, as introduced by Šmejkal *et al.* [17,18].

In the field of solid-state magnetism, group theory proved its usefulness several decades ago. Its standard tools include magnetic groups [19–21] which represent an extension of crystallographic groups by considering time reversal as an additional symmetry operation; the time reversal is a special case of an operation of antisymmetry or anti-identity contained in some elements of the magnetic groups [22,23]. The space-time symmetry in magnetic crystals has well-known consequences for shape restrictions of various vector or tensor quantities appearing as equilibrium properties [20,24] or linear response (transport) coefficients [25–28]. This involves, e.g., identification of magnetic point groups compatible with a net nonzero magnetic moment [19] or modification of the Onsager reciprocity relations for solids characterized by certain magnetic point groups [25]. These topics have been worked out in much detail; see Ref. [29] and references therein. Moreover, a scheme for labeling electron eigenvalues in magnetic crystals, based on irreducible representations of magnetic point and space groups, is available as well [21]. This scheme has recently been extended and used in the systematic search for new topological phases of magnetic materials [30–32]. The irreducible representations are also indispensable for an advanced analysis of complex magnetic structures [33,34].

From the viewpoint of electronic structures, treated within effective one-electron Pauli or Dirac equations, elements of the magnetic groups act simultaneously on internal degrees of freedom of electron (spin) and on the electron position vector. For specific problems, spin groups as an extension of the magnetic groups were introduced [35,36]. Elements of the spin groups are featured by independent rotations in the spin and configuration spaces. The spin groups are relevant, e.g., for systems without spin-orbit interaction; a very recent application of the spin groups deals with the spin splitting of electron

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states in collinear antiferromagnets [17]. Undoubtedly, the spin groups comprise all symmetry elements of nonrelativistic collinear magnets and their use is thus fully justified. Nevertheless, one should mention that this extension of theoretical formalism is accompanied by a substantial increase in the number of all possible groups: there are 32 crystallographic point groups, which lead to 122 magnetic point groups [25] and to 598 nontrivial spin point groups [36]. Moreover, inclusion of the translational invariance of crystals leads to a further extension of the group formalism by considering the space groups in addition to their point counterparts; this route has recently been followed with magnetic groups in Refs. [14,15] and with spin groups in Ref. [37].

The more sophisticated formalism of the spin groups as compared with that of the magnetic groups obviously contradicts the simpler theoretical and numerical electronic-structure techniques for nonrelativistic collinear magnets as compared with those for general magnetic crystals. The main purpose of this paper is to reconsider the group-theoretical framework for the electronic structure of nonrelativistic collinear magnets from the viewpoint of magnetic groups. We suggest that an alternative treatment of these systems can be formulated by replacing the vector spin operator by a pseudoscalar spin quantity, which leads to magnetic groups modified as compared to those with the standard vector spin. Such an approach has been mentioned implicitly in the literature [14,16], but its systematic description is not available. In this work, we derive a general unitary infinite-dimensional representation of the modified magnetic point groups which does not rely on any particular model of the electronic structure. We apply the developed formalism to investigation of the spin splitting of electronic states near the center of the Brillouin zone (BZ) of nonrelativistic crystalline collinear magnets. We also study a connection between the spin splitting and spin conductivity, which has recently lead to a prediction of efficient spin-current generation [16] and giant tunneling magnetoresistance [38,39]. Moreover, the obtained results allowed us to briefly address the physical mechanisms responsible for the appearance of this spin splitting in real materials.

II. FORMALISM

A. Pseudoscalar electron spin

Electrons are charged fermions of spin $1/2$. In one-particle approximations for many-electron spin-polarized systems, the Pauli exclusion principle and the Coulomb interaction between the electrons give rise to a vector exchange field coupled to the vector spin operator in the Zeeman term of an effective one-electron Hamiltonian. The additional spin-orbit interaction and/or the noncollinear spin structure (and, consequently, the noncollinear exchange field) lead to coupled equations for the electron wave functions in the two spin channels (spin-up and spin-down channels) of the Pauli equation as a nonrelativistic limit of the Dirac equation [40]. Transformations of the wave functions, comprised in the magnetic space and point groups, thus take the vector nature of the electron spin, of the exchange field, and of the electron position vector fully into account. Transformation properties of the spin and of the exchange field are the same as those of the angular orbital momentum $\mathbf{r}\times\mathbf{p}$, where $\mathbf{r}$ is the position vector and $\mathbf{p}$ is the electron momentum.

The situation simplifies substantially for systems with neglected spin-orbit interaction and with collinear exchange fields, leading thus to collinear spin structures. The wave function amplitudes are $\langle \mathbf{r}s|\psi\rangle = \psi_s(\mathbf{r})$, where s denotes the spin index ($s=1$ for spin-up channel, $s=-1$ for spin-down channel). The Hamiltonian can be written (in atomic units with $\hbar=1$ and with the electron mass $m=1/2$) as

$$H(\mathbf{r}) = -\Delta + V(\mathbf{r}), \tag{1}$$

where the kinetic energy term is spin independent, whereas the local potential $V(\mathbf{r})$ is spin dependent but diagonal in the spin index: $\langle s|V(\mathbf{r})|s'\rangle = \delta_{ss'}V_s(\mathbf{r})$. This leads to two eigenvalue problems with eigenvalues E_s,

$$-\Delta\psi_s(\mathbf{r}) + V_s(\mathbf{r})\psi_s(\mathbf{r}) = E_s\psi_s(\mathbf{r}), \tag{2}$$

to be solved separately in each spin channel ($s=\pm1$). If we introduce a spin operator σ such that $\langle s|\sigma|s'\rangle = s\delta_{ss'}$, a spin-averaged potential $\bar{V}(\mathbf{r}) = [V_+(\mathbf{r}) + V_-(\mathbf{r})]/2$, and an exchange field $B(\mathbf{r}) = [V_+(\mathbf{r}) - V_-(\mathbf{r})]/2$, the Hamiltonian (1) can be rewritten as

$$H(\mathbf{r}) = -\Delta + \bar{V}(\mathbf{r}) + B(\mathbf{r})\sigma. \tag{3}$$

The direction of the spin quantization axis is irrelevant, the Hamiltonian $H(\mathbf{r})$ describes motion in two uncoupled spin channels with local potentials $V_s(\mathbf{r})$, $s=\pm1$, and the defined spin σ and exchange field $B(\mathbf{r})$ can be treated as scalar quantities.

In magnetic crystals, the Hamiltonian $H(\mathbf{r})$ is translationally invariant, so that $V(\mathbf{r}) = V(\mathbf{r}+\mathbf{T})$ for all $\mathbf{r}$ and for all primitive translation vectors $\mathbf{T}$ (vectors of the Bravais lattice), which implies the same condition for $V_s(\mathbf{r})$, $s=\pm1$, $\bar{V}(\mathbf{r})$, and $B(\mathbf{r})$. Let us consider further symmetry elements of the system. In ferromagnets, the two potentials $V_s(\mathbf{r})$ are mutually different since $V_+(\mathbf{r})$ is on average more (or less) attractive than $V_-(\mathbf{r})$. The system is thus invariant only with respect to ordinary rotations (combined optionally with nonprimitive translations) that belong to the crystallographic point group. These rotations will be denoted by a symbol α, which is a real 3×3 orthogonal matrix, $\alpha \equiv \{\alpha_{\mu\nu}\}$, where the subscripts μ and ν denote the Cartesian index ($\mu,\nu\in\{x,y,z\}$); the rotations α can be both proper and improper (accompanied by space inversion).

In antiferromagnets, both spin channels are mutually equivalent, which points to a presence of more general symmetry elements as compared to ferromagnets. These elements of the system point group will be denoted as (α,η), where the extra parameter η acquires two values, namely, $\eta=1$ for symmetry elements not changing the spin channels, and $\eta=-1$ for symmetry elements with mutual interchange of both spin channels. All these elements form the magnetic point group $\mathcal{P}_\mathrm{M}$ of the system with a group multiplication rule

$$(\alpha_1,\eta_1)(\alpha_2,\eta_2) = (\alpha_1\alpha_2, \eta_1\eta_2). \tag{4}$$

Strictly defined, $(\alpha,\eta)\in\mathcal{P}_\mathrm{M}$ means that a translation vector $\mathbf{t}$ (either null or nonprimitive) exists such that

$$V_s(\mathbf{r}) = V_{\eta s}(\alpha\mathbf{r}+\mathbf{t}) \tag{5}$$

holds for all $\mathbf{r}$ and for both values of s ($s = \pm 1$). Hence the group elements $(\alpha, 1)$ correspond to usual rotations, whereas the group elements $(\alpha, -1)$ correspond to rotations combined with the spin-channel interchange, which plays a role of the operation of antisymmetry of the magnetic group [21]. Note that the spin-channel interchange does not change only the sign of the spin channel ($s \to -s$), but it changes the sign of the exchange field as well [$B(\mathbf{r}) \to -B(\mathbf{r})$]. The electron spin and the exchange field thus behave like pseudoscalar quantities changing their signs due to the operation of antisymmetry. In antiferromagnets, the regions of positive and negative values of the exchange field $B(\mathbf{r})$ represent an analogy to white and black regions, respectively, of two-color figures with a symmetry group extended by inclusion of an operation of antisymmetry (interchange of colors), as introduced by Shubnikov [22,23]. However, the group $\mathcal{P}_\mathrm{M}$ defined by Eq. (5) reflects the symmetry of both local potentials $V_s(\mathbf{r})$ ($s = \pm 1$), not only of their difference (the exchange field), in full compatibility with the density functional theory of nonrelativistic collinear magnets [41]. This means that the presence and positions of nonmagnetic atoms in the system have to be taken into account in a reliable symmetry analysis.

The magnetic point groups $\mathcal{P}_\mathrm{M}$ derived from crystallographic point groups $\mathcal{P}$ can be split into three categories (a), (b), and (c) [25] or, alternatively, into three types I, II, and III [21] [whereby the categories (a), (b), and (c) correspond to the types II, I, and III, respectively]. The category (a) comprises all 32 groups $\mathcal{P}$ to which the operation of antisymmetry is added (so that the pure operation of antisymmetry is an element of $\mathcal{P}_\mathrm{M}$). The groups of the category (b) do not involve the operation of antisymmetry at all (neither as a separate element nor in a combination with a rotation); all these groups are thus equivalent to all bare 32 groups $\mathcal{P}$. The groups $\mathcal{P}_\mathrm{M}$ of the category (c) contain the operation of antisymmetry only in a combination with a nontrivial rotation; there are 58 groups in this category. Each group $\mathcal{P}_\mathrm{M}$ of the category (c) can be constructed from a parent group $\mathcal{P}$ by taking its subgroup $\mathcal{S}$ of index two. All elements $\alpha \in \mathcal{S}$ then enter the group $\mathcal{P}_\mathrm{M}$ as $(\alpha, 1)$, i.e., without the operation of antisymmetry, whereas all elements $\alpha \in \mathcal{P}$ and $\alpha \notin \mathcal{S}$ give rise to elements containing the operation of antisymmetry, $(\alpha, -1) \in \mathcal{P}_\mathrm{M}$. Loosely speaking, the group $\mathcal{S}$ can be identified with a subgroup of $\mathcal{P}_\mathrm{M}$ containing all elements of $\mathcal{P}_\mathrm{M}$ without the operation of antisymmetry. For the magnetic point groups $\mathcal{P}_\mathrm{M}$ defined by Eq. (5), the three mentioned categories are unambiguously related to basic types of collinear nonrelativistic magnets: ferromagnets and ferrimagnets possess $\mathcal{P}_\mathrm{M}$ of category (b), whereas antiferromagnets are featured by $\mathcal{P}_\mathrm{M}$ of category (a) or (c). This simple classification contrasts with that based on the standard magnetic groups applied to general magnets (with spin-orbit coupling and/or with noncollinear orders), where the magnetic point groups of ferromagnets and ferrimagnets belong to categories (b) and (c) while those of antiferromagnets belong to categories (a), (b), and (c).

The magnetic point group $\mathcal{P}_\mathrm{M}$ defined by Eq. (5) can differ from the standard magnetic point group of the same collinear system. The latter group reflects the vector nature of the involved quantities and it depends on the direction of the exchange field and magnetic moments. Moreover, the operation of antisymmetry contained in elements of the standard magnetic groups denotes the time reversal leading to the sign change of the spin, exchange field, and magnetic moments. The modification of the magnetic groups owing to the pseudoscalar nature of the involved quantities can lead to additional spatial operations contained in the group elements, while the operation of antisymmetry has to be identified with the spin-channel interchange according to Eq. (5). More details about the relation of both kinds of magnetic point groups can be found in the Supplemental Material [42] and examples of these groups for selected systems are presented in Sec. III A.

Let us note that the symmetry operations of the introduced modified magnetic groups rest on the neglect of all interactions leading to a coupling of the spin-up and spin-down channels of the one-electron Hamiltonian. In the case of collinear ferromagnets and ferrimagnets, this means the neglect of spin-orbit interaction and of its well-known consequences, such as the anisotropic magnetostriction often responsible for reduced symmetry of the lattice in the magnetically ordered phase as compared to that in the paramagnetic phase [43,44]. This approximate approach resulted in important theoretical concepts, including the half-metallic magnetism [45] or the symmetry-induced spin filtering in Fe|MgO|Fe magnetic tunnel junctions [46]. For antiferromagnets, this approach also neglects a weak noncollinearity of the magnetic moments in noncentrosymmetric systems owing to the Dzyaloshinskii-Moriya interaction [47,48]. The symmetry analysis of nonrelativistic collinear antiferromagnets has recently been carried out in several theoretical studies using the spin groups [17,18,37]. These and similar studies are devoted not only to systems of very light elements, such as MnF_2 [14], CuF_2 [17], Mn_5Si_3 [39], or NiO [15,49], but also to systems with heavier elements, such as RuO_2 [16,38], KRu_4O_8 [17], $FeSb_2$ [12], CrSb and MnTe [16,17], La_2CuO_4 [17], and AMnBi$_2$ (A = Ca, Sr) [37]. A comparison of theoretical results of the above approximate treatment with those of a more accurate description (with spin-orbit interaction switched on), supported by *ab initio* electronic structure calculations, enables one to identify the origin of unusual properties of altermagnetic materials [17,18].

The magnetic group introduced according to Eq. (5) contains only symmetry elements for invariance of the pair of potentials $V_s(\mathbf{r})$ ($s = \pm 1$). However, the full group for invariance of the Hamiltonian, given by Eq. (1), is inevitably bigger; two additional symmetry operations have to be considered. First, it is the spin operator σ which obviously commutes with the Hamiltonian $H(\mathbf{r})$. This symmetry reflects invariance with respect to arbitrary rotations in the spin space around the axis parallel to the direction of all magnetic moments of the collinear magnet. Second, the Hamiltonian eigenvalue problem (2) is invariant with respect to complex conjugation of the wave functions: $\psi_s(\mathbf{r}) \to \psi_s^*(\mathbf{r})$. This symmetry reflects real values of the potentials $V_s(\mathbf{r}) = V_s^*(\mathbf{r})$ and it corresponds to time reversal for effective particles of spin zero [6,50,51] moving in both decoupled spin channels. A closer inspection of a relation between the introduced magnetic groups and the spin groups of the studied systems (see Supplemental Material [42]) proves that no further independent symmetry operations exist. In the following, none of both mentioned additional symmetries (present in all collinear nonrelativistic magnets)

is included in the magnetic point group $\mathcal{P}_{\rm M}$; however, their possible effect on the results of the performed analysis is properly taken into account.

B. Hamiltonians and resolvents in reciprocal space

In the analysis of spin splitting of the eigenvalues of the real-space Hamiltonian (1), we employ the Bloch theorem, transform the original $H(\mathbf{r})$ into a $\mathbf{k}$-dependent Hamiltonian $\tilde{H}(\mathbf{k})$, where $\mathbf{k}$ denotes a reciprocal-space vector, and focus on a neighborhood of the center of BZ, i.e., on $\mathbf{k} \to \mathbf{0}$. The Hamiltonians $\tilde{H}(\mathbf{k})$ for different $\mathbf{k}$ vectors are defined on different Hilbert spaces. However, we represent each $\tilde{H}(\mathbf{k})$ by a matrix in an orthonormal basis $\{|\mathbf{G}s\rangle\}$, where $\mathbf{G}$ runs over all lattice vectors of the reciprocal lattice and s runs over both spin channels, $s = \pm 1$. The basis vectors are chosen as $|\mathbf{G}s\rangle = |\mathbf{G}\rangle \otimes |s\rangle$, where $|\mathbf{G}\rangle$ describes a plane wave, $\langle \mathbf{r}|\mathbf{G}\rangle \sim \exp[i(\mathbf{k}-\mathbf{G})\cdot\mathbf{r}]$, and where $|s\rangle$ denotes the basis vector in the two-dimensional spin space. This plane-wave basis is used in a formulation of the nearly free electron model [6,52]; however, it leads to accurate eigenvalues as long as the full infinite basis set $\{|\mathbf{G}s\rangle\}$ is employed. With this matrix representation, all Hamiltonians can be considered as defined on the same Hilbert space $\mathcal{H}$ (corresponding to $\mathbf{k} = \mathbf{0}$). The particular form of $\tilde{H}(\mathbf{k})$ is given in Appendix A. Its full dependence on $\mathbf{k}$ is confined to a few terms,

$$\tilde{H}(\mathbf{k}) = h + U(\mathbf{k}), \quad U(\mathbf{k}) = \sum_{\mu} J_\mu k_\mu + \sum_{\mu_1\mu_2} L_{\mu_1\mu_2} k_{\mu_1} k_{\mu_2}. \tag{6}$$

The first term h refers to the Hamiltonian for $\mathbf{k} = \mathbf{0}$ and the operator $U(\mathbf{k})$, consisting of terms that are linear and quadratic in $\mathbf{k}$, can be considered for $\mathbf{k} \to \mathbf{0}$ as a small perturbation added to the reference Hamiltonian h. The operators J_μ coincide with components of a velocity operator and the operators $L_{\mu_1\mu_2}$ are symmetric in their indices, $L_{\mu_1\mu_2} = L_{\mu_2\mu_1}$. The latter is equal to $L_{\mu_1\mu_2} = I\delta_{\mu_1\mu_2}$, where I is the unit operator in $\mathcal{H}$.

The spin-resolved eigenvalues $E_s^{(n)}(\mathbf{k})$, where n denotes the band index, depend on the matrix elements of $\tilde{H}(\mathbf{k})$ in a complicated manner. Moreover, a thorough analysis of the spin splitting requires a reliable identification of the spin pairs of eigenvalues, which is not always straightforward owing to band crossing [49]. In order to avoid these problems, we turn to techniques developed earlier for shapes of various tensor quantities due to the point-group symmetry of the system [24–26]. For this purpose, we focus on spin-resolved Bloch spectral functions $A_s(\mathbf{k}, E) = \sum_n \delta[E - E_s^{(n)}(\mathbf{k})]$, where E denotes an energy variable. Let us note that the Bloch spectral functions substitute the energy bands in strongly correlated systems [9]. The spin splitting of the system eigenvalues is reflected by nonzero values of the difference $A_+(\mathbf{k}, E) - A_-(\mathbf{k}, E) = \sum_s sA_s(\mathbf{k}, E)$. The Bloch spectral functions are closely related to the resolvent $G(\mathbf{k}, E \pm i\varepsilon)$ of the Hamiltonian $\tilde{H}(\mathbf{k})$, defined for $\varepsilon > 0$ by [53]

$$G(\mathbf{k}, E \pm i\varepsilon) = [(E \pm i\varepsilon)I - \tilde{H}(\mathbf{k}]^{-1}. \tag{7}$$

This yields explicit relations involving the quantity $\sum_s sA_s(\mathbf{k}, E)$:

$$\mathrm{Tr}[\sigma G(\mathbf{k}, E \pm i\varepsilon)] = \int_{-\infty}^{+\infty} \frac{1}{E \pm i\varepsilon - E'} \sum_s sA_s(\mathbf{k}, E')dE',$$

$$\sum_s sA_s(\mathbf{k}, E) = -\frac{1}{\pi}\mathrm{Im}\mathrm{Tr}[\sigma G(\mathbf{k}, E + i0)], \tag{8}$$

where Im denotes the imaginary part and the trace Tr refers to the Hilbert space $\mathcal{H}$. In the following, we thus examine the properties of $\mathrm{Tr}[\sigma G(\mathbf{k}, E \pm i\varepsilon)]$ for small $\mathbf{k}$ vectors.

Let us denote the resolvent of the reference Hamiltonian h as $g(E \pm i\varepsilon)$ and let us employ it in evaluation of the $\mathbf{k}$-dependent resolvent $G(\mathbf{k}, E \pm i\varepsilon)$. For brevity, we omit the energy arguments of both resolvents. The infinite Born series corresponding to Eq. (6),

$$G(\mathbf{k}) = g + \sum_{N\geqslant 1} [gU(\mathbf{k})]^N g, \tag{9}$$

can be rearranged into the Taylor series

$$G(\mathbf{k}) = g + \sum_{N\geqslant 1} \sum_{\mu_1\mu_2\ldots\mu_N} gW^{(N)}_{\mu_1\mu_2\ldots\mu_N} g k_{\mu_1} k_{\mu_2} \ldots k_{\mu_N}, \tag{10}$$

where the operators $W^{(N)}_{\mu_1\mu_2\ldots\mu_N}$ are fully symmetric in the indices $\mu_1, \ldots, \mu_N$. The first four members of the infinite sequence $W^{(N)}_{\mu_1\mu_2\ldots\mu_N}$, $N = 1, 2, \ldots$, are equal to

$$\begin{aligned}
W^{(1)}_{\mu} &= J_\mu, \quad W^{(2)}_{\mu_1\mu_2} = L_{\mu_1\mu_2} + \tfrac{1}{2}\big(J_{\mu_1} g J_{\mu_2} + J_{\mu_2} g J_{\mu_1}\big), \\
W^{(3)}_{\mu_1\mu_2\mu_3} &= \tfrac{1}{6}\big(J_{\mu_1} g L_{\mu_2\mu_3} + L_{\mu_1\mu_2} g J_{\mu_3} + J_{\mu_1} g J_{\mu_2} g J_{\mu_3} + \cdots\big), \\
W^{(4)}_{\mu_1\mu_2\mu_3\mu_4} &= \tfrac{1}{24}\big(L_{\mu_1\mu_2} g L_{\mu_3\mu_4} + J_{\mu_1} g J_{\mu_2} g L_{\mu_3\mu_4} \\
&\quad + J_{\mu_1} g L_{\mu_2\mu_3} g J_{\mu_4} + L_{\mu_1\mu_2} g J_{\mu_3} g J_{\mu_4} \\
&\quad + J_{\mu_1} g J_{\mu_2} g J_{\mu_3} g J_{\mu_4} + \cdots\big),
\end{aligned} \tag{11}$$

where the dots denote terms obtained from the given ones by all permutations of the indices $\mu_1, \mu_2, \ldots$. The infinite series (10) leads to the following Taylor expansion of the quantity $F(\mathbf{k}) = \mathrm{Tr}[\sigma G(\mathbf{k})]$:

$$F(\mathbf{k}) = \mathrm{Tr}(\sigma g) + \sum_{N\geqslant 1} \sum_{\mu_1\mu_2\ldots\mu_N} T^{(N)}_{\mu_1\mu_2\ldots\mu_N} k_{\mu_1} k_{\mu_2} \ldots k_{\mu_N},$$

$$T^{(N)}_{\mu_1\mu_2\ldots\mu_N} = \mathrm{Tr}\big[\sigma g W^{(N)}_{\mu_1\mu_2\ldots\mu_N} g\big], \tag{12}$$

where the tensor components $T^{(N)}_{\mu_1\mu_2\ldots\mu_N}$ are fully symmetric in their indices. We will investigate the shape of the tensors $T^{(N)}$ due to the symmetry of the studied system; nonvanishing components $T^{(N)}_{\mu_1\mu_2\ldots\mu_N}$ correspond to spin splitting of energy bands near the BZ center.

C. Representation of magnetic point groups

Since the operators h, J_μ, $L_{\mu_1\mu_2}$, g, and $W^{(N)}_{\mu_1\mu_2\ldots\mu_N}$, involved in the expansions (6), (10), and (12), act in the Hilbert space $\mathcal{H}$ for zero $\mathbf{k}$ vector, the symmetry analysis can be carried out in terms of the magnetic point group $\mathcal{P}_{\rm M}$ of the system. For this purpose, one has to construct the corresponding representation of the group $\mathcal{P}_{\rm M}$ by means of operators $\mathcal{D}(\alpha, \eta)$ acting in the space $\mathcal{H}$ [21,54,55]. The spatial parts of the orthonormal basis vectors $|\mathbf{G}s\rangle$ for $\mathbf{k} = \mathbf{0}$ are given by $\langle \mathbf{r}|\mathbf{G}\rangle \sim \exp(-i\mathbf{G}\cdot\mathbf{r})$ and

we define the unitary operators $\mathcal{D}(\alpha,\eta)$ explicitly by

$$\mathcal{D}(\alpha,\eta)|\mathbf{G}s\rangle = |\alpha\mathbf{G},\eta s\rangle \exp(i\alpha\mathbf{G}\cdot\mathbf{t}), \tag{13}$$

where $\mathbf{t}$ denotes the translation vector involved in the invariance condition (5). Note that this definition naturally includes the rotation of the reciprocal lattice vectors ($\mathbf{G}\to\alpha\mathbf{G}$) and the sign change of the spin index ($s\to\eta s$) due to the operation of antisymmetry. The additional phase factor in Eq. (13) is consistent with a general rule for rotations and translations in a space of scalar functions of the position vector $\mathbf{r}$ [21,55]. Alternatively, one can show that Eq. (13) follows from a simple transformation of all basic kets $|\mathbf{r}s\rangle$ due to a combined effect of the rotation α, translation $\mathbf{t}$, and spin-channel interchange η, which yields $|\mathbf{r}s\rangle\to|\mathbf{r}'s'\rangle$, where $\mathbf{r}'=\alpha\mathbf{r}+\mathbf{t}$ and $s'=\eta s$; see, also, Eq. (32) in the Supplemental Material [42]. It can be proved that the introduced operators $\mathcal{D}(\alpha,\eta)$, given by Eq. (13), possess all properties of a representation; in particular, the operator counterpart of the group multiplication rule (4),

$$\mathcal{D}(\alpha_1,\eta_1)\mathcal{D}(\alpha_2,\eta_2)=\mathcal{D}(\alpha_1\alpha_2,\eta_1\eta_2), \tag{14}$$

holds for all elements $(\alpha_1,\eta_1)\in\mathcal{P}_{\rm M}$ and $(\alpha_2,\eta_2)\in\mathcal{P}_{\rm M}$ (for a proof, see Appendix A).

Let us briefly compare the present treatment of rotations and of the operation of antisymmetry according to Eq. (13) with other group-theoretical approaches. Elements of the spin groups contain two independent rotations, acting separately in the spin and configuration spaces [17,35,37], in contrast to the rotations of standard magnetic groups, acting simultaneously in both spaces [19,21]. However, the standard magnetic point groups applied to one-particle Hamiltonians for real electrons with spin 1/2 lead to double-valued representations [21,54,55]. Moreover, the operation of antisymmetry is identified with time reversal and the group elements containing the time reversal are represented by antiunitary operators, which calls for the use of corepresentations of these magnetic groups [21]. The present formalism does not employ any of these extensions of the group theory. The structure of the nonrelativistic Hamiltonian for collinear magnets (Sec. II A) allows one to confine the action of rotations only to the configuration space, while the operation of antisymmetry reduces to the interchange of the spin channels; see Eq. (5). As a consequence, the defined representation $\mathcal{D}(\alpha,\eta)$, given by Eq. (13), is single valued and all elements (α,η) of the modified magnetic point groups $\mathcal{P}_{\rm M}$ are represented by unitary operators, so that no corepresentations have to be considered. These features simplify the formalism substantially.

The introduced representation (13) leads to the following transformations of the involved operators. For each element $(\alpha,\eta)\in\mathcal{P}_{\rm M}$ and with abbreviation $\mathcal{D}(\alpha,\eta)=D$, we get

$$\begin{aligned}
D^{-1}hD&=h,\quad D^{-1}gD=g,\quad D^{-1}\sigma D=\eta\sigma,\\
D^{-1}J_\mu D&=\sum_\nu \alpha_{\mu\nu}J_\nu,\\
D^{-1}L_{\mu_1\mu_2}D&=\sum_{\nu_1\nu_2}\alpha_{\mu_1\nu_1}\alpha_{\mu_2\nu_2}L_{\nu_1\nu_2},\\
D^{-1}W^{(N)}_{\mu_1\mu_2\ldots\mu_N}D&=\sum_{\nu_1\nu_2\ldots\nu_N}\alpha_{\mu_1\nu_1}\alpha_{\mu_2\nu_2}\ldots\alpha_{\mu_N\nu_N}W^{(N)}_{\nu_1\nu_2\ldots\nu_N}.
\end{aligned} \tag{15}$$

The proof of these relations is sketched in Appendix A and their physical meaning is obvious: the Hamiltonian h and the resolvent g are invariant with respect to the action of all group elements, the velocity operators J_μ are components of a vector operator, the operators $L_{\mu_1\mu_2}$ and $W^{(N)}_{\mu_1\mu_2\ldots\mu_N}$ are components of tensor operators of rank 2 and N, respectively, and the spin σ changes its sign due to the operation of antisymmetry, but remains unchanged by pure spatial rotations, in full agreement with its pseudoscalar nature discussed in Sec. II A.

The time reversal mentioned in the last paragraph of Sec. II A has to be represented by an antiunitary operator. We denote it by $\mathcal{T}$ and define it explicitly by

$$\mathcal{T}|\mathbf{G}s\rangle = |-\mathbf{G},s\rangle, \tag{16}$$

so that $\mathcal{T}$ changes the sign of the reciprocal lattice vector $\mathbf{G}$, but leaves the spin index s unchanged. We have thus $\mathcal{T}^2=I$ and obtain the following transformation rules:

$$\begin{aligned}
\mathcal{T}h\mathcal{T}&=h,\quad \mathcal{T}g\mathcal{T}=g^+,\quad \mathcal{T}\sigma\mathcal{T}=\sigma,\\
\mathcal{T}J_\mu\mathcal{T}&=-J_\mu,\quad \mathcal{T}L_{\mu_1\mu_2}\mathcal{T}=L_{\mu_1\mu_2},\\
\mathcal{T}W^{(N)}_{\mu_1\mu_2\ldots\mu_N}\mathcal{T}&=(-1)^N\big[W^{(N)}_{\mu_1\mu_2\ldots\mu_N}\big]^+,
\end{aligned} \tag{17}$$

where M^+ denotes the Hermitian conjugate of an operator M. Note especially the unchanged sign of the spin operator σ, which reflects the fact that the time reversal treats each separate spin channel as a subspace for a particle of spin zero. The sign $(-1)^N$ in the transformation of operators $W^{(N)}_{\mu_1\mu_2\ldots\mu_N}$ is due to the velocities J_μ in their definition (11).

D. Shape analysis of the studied tensors

The invariance of the system with respect to the time reversal (17) has an obvious consequence for the studied tensors $T^{(N)}$. We get from Eq. (12) for N odd:

$$\begin{aligned}
T^{(N)}_{\mu_1\mu_2\ldots\mu_N}&=-\mathrm{Tr}\big\{\mathcal{T}\sigma\mathcal{T}\mathcal{T}g^+\mathcal{T}\mathcal{T}\big[W^{(N)}_{\mu_1\mu_2\ldots\mu_N}\big]^+\mathcal{T}\mathcal{T}g^+\mathcal{T}\big\}\\
&=-\mathrm{Tr}\big\{gW^{(N)}_{\mu_1\mu_2\ldots\mu_N}g\sigma\big\}=-T^{(N)}_{\mu_1\mu_2\ldots\mu_N},
\end{aligned} \tag{18}$$

where we used the rule $\mathrm{Tr}(\mathcal{T}M\mathcal{T})=\mathrm{Tr}(M^+)$ that is valid for linear operators M. This means that the entire tensor $T^{(N)}$ vanishes identically for N odd, which is consistent with the eigenvalues of the considered systems being even functions of the $\mathbf{k}$ vector, $E^{(n)}_s(-\mathbf{k})=E^{(n)}_s(\mathbf{k})$.

Let us now examine the terms in the expansion (12) that are even in $\mathbf{k}$; we will employ the transformations given by Eq. (15). For the reference term $\mathrm{Tr}(\sigma g)$, for an arbitrary element $(\alpha,\eta)\in\mathcal{P}_{\rm M}$, and with abbreviation $\mathcal{D}(\alpha,\eta)=D$, we get

$$\mathrm{Tr}(\sigma g)=\mathrm{Tr}(D\eta\sigma D^{-1}DgD^{-1})=\eta\mathrm{Tr}(\sigma g). \tag{19}$$

This means that for $\mathcal{P}_{\rm M}$ of category (a) or (c), which contains elements $(\alpha,-1)$, the term $\mathrm{Tr}(\sigma g)$ vanishes and there is no spin splitting of the bands in the very center of the BZ. For ferromagnets and ferrimagnets, featured by $\mathcal{P}_{\rm M}$ of category (b), the eigenstates are obviously spin split for all $\mathbf{k}$ points. In the following, we thus confine ourselves to magnetic point groups of categories (a) and (c), i.e., to groups with some elements containing the operation of antisymmetry.

Let us further discuss in detail the shape of the tensor $T^{(2)}_{\mu_1\mu_2}$, given by Eq. (12). For $(\alpha,\eta)\in\mathcal{P}_{\rm M}$ and with abbreviation

$\mathcal{D}(\alpha,\eta)=D$, we get

$$T^{(2)}_{\mu_1\mu_2} = \mathrm{Tr}\big(D\eta\sigma D^{-1}DgD^{-1}W^{(2)}_{\mu_1\mu_2}DgD^{-1}\big) = \eta\sum_{\nu_1\nu_2}\alpha_{\mu_1\nu_1}\alpha_{\mu_2\nu_2}\mathrm{Tr}\big(\sigma g W^{(2)}_{\nu_1\nu_2}g\big), \tag{20}$$

so that the condition for each element $(\alpha,\eta)\in\mathcal{P}_\mathrm{M}$ is

$$T^{(2)}_{\mu_1\mu_2} = \eta\sum_{\nu_1\nu_2}\alpha_{\mu_1\nu_1}\alpha_{\mu_2\nu_2}T^{(2)}_{\nu_1\nu_2}. \tag{21}$$

However, this approach does not account explicitly for the tensor symmetry, $T^{(2)}_{\mu_1\mu_2}=T^{(2)}_{\mu_2\mu_1}$. In order to include this property, one has to modify the condition (21) to

$$T^{(2)}_{\mu_1\mu_2} = \frac{1}{2}\eta\sum_{\nu_1\nu_2}\big(\alpha_{\mu_1\nu_1}\alpha_{\mu_2\nu_2}+\alpha_{\mu_2\nu_1}\alpha_{\mu_1\nu_2}\big)T^{(2)}_{\nu_1\nu_2}. \tag{22}$$

The validity of the last condition for all group elements then leads to the final condition on the shape of the tensor $T^{(2)}_{\mu_1\mu_2}$ as

$$T^{(2)}_{\mu_1\mu_2} = \sum_{\nu_1\nu_2}Q^{(2)}_{\mu_1\mu_2,\nu_1\nu_2}T^{(2)}_{\nu_1\nu_2},$$

$$Q^{(2)}_{\mu_1\mu_2,\nu_1\nu_2} = \frac{1}{2|\mathcal{P}_\mathrm{M}|}\sum_{(\alpha,\eta)}^{\mathcal{P}_\mathrm{M}}\eta\big(\alpha_{\mu_1\nu_1}\alpha_{\mu_2\nu_2}+\alpha_{\mu_2\nu_1}\alpha_{\mu_1\nu_2}\big), \tag{23}$$

where the last sum runs over all elements (α,η) of the magnetic point group $\mathcal{P}_\mathrm{M}$ and where $|\mathcal{P}_\mathrm{M}|$ denotes its order (number of group elements). It can be shown that the introduced superoperator $Q^{(2)}_{\mu_1\mu_2,\nu_1\nu_2}$ is a projector in a nine-dimensional vector space, i.e., it is symmetric, $Q^{(2)}_{\mu_1\mu_2,\nu_1\nu_2}=Q^{(2)}_{\nu_1\nu_2,\mu_1\mu_2}$, and idempotent,

$$\sum_{\lambda_1\lambda_2}Q^{(2)}_{\mu_1\mu_2,\lambda_1\lambda_2}Q^{(2)}_{\lambda_1\lambda_2,\nu_1\nu_2} = Q^{(2)}_{\mu_1\mu_2,\nu_1\nu_2}. \tag{24}$$

Consequently, the number $q^{(2)}$ of independent nonzero components of the tensor $T^{(2)}_{\mu_1\mu_2}$ can easily be obtained as the trace of the projector $Q^{(2)}_{\mu_1\mu_2,\nu_1\nu_2}$, namely,

$$q^{(2)} = \sum_{\mu_1\mu_2}Q^{(2)}_{\mu_1\mu_2,\mu_1\mu_2}. \tag{25}$$

The shape of the tensor $T^{(2)}_{\mu_1\mu_2}$, given by Eq. (23), was derived by considering only the elements of the group $\mathcal{P}_\mathrm{M}$; it can easily be shown that inclusion of both additional symmetries, mentioned in the end of Sec. II A, has no influence on the obtained result. This follows from the commutation of the spin operator σ with operators h, g, and $W^{(2)}_{\mu_1\mu_2}$, as well as from the obvious modification of Eq. (18) for N even.

The derived shape of the tensor $T^{(2)}_{\mu_1\mu_2}$ is closely related to spin conductivity. The latter property, defined as the linear response of a spin current to an external electric field, is usually quantified by a tensor $\sigma^{\lambda}_{\mu_1\mu_2}$, where the Cartesian index λ refers to the spin polarization of the spin current, μ_1 corresponds to the direction of the spin-current flow, and μ_2 to the direction of the electric field [16,26]. In nonrelativistic collinear magnets, the two-current model of electron transport is valid [56], the original tensor reduces to $\sigma^{\lambda}_{\mu_1\mu_2}=n_\lambda\tilde{\sigma}_{\mu_1\mu_2}$, where $(n_x,n_y,n_z)=\mathbf{n}$ is a unit vector parallel to all magnetic moments, and the shape of the tensor $\tilde{\sigma}_{\mu_1\mu_2}$ coincides with that of $T^{(2)}_{\mu_1\mu_2}$; see Appendix B. This fact points to a close relation between the spin splitting of the electronic band structure and the spin conductivity, which is one of the central properties in spintronics.

We turn finally to the case of a general even N. In full analogy with Eq. (21) for $N=2$, the condition on the tensor $T^{(N)}_{\mu_1\mu_2\ldots\mu_N}$ can be written for each $(\alpha,\eta)\in\mathcal{P}_\mathrm{M}$ as

$$T^{(N)}_{\mu_1\mu_2\ldots\mu_N} = \eta\sum_{\nu_1\nu_2\ldots\nu_N}\alpha_{\mu_1\nu_1}\alpha_{\mu_2\nu_2}\ldots\alpha_{\mu_N\nu_N}T^{(N)}_{\nu_1\nu_2\ldots\nu_N}. \tag{26}$$

Explicit inclusion of the tensor symmetry (invariance of $T^{(N)}_{\mu_1\mu_2\ldots\mu_N}$ with respect to all permutations of the indices) leads to a modified condition of the form

$$T^{(N)}_{\mu_1\mu_2\ldots\mu_N} = \frac{1}{N!}\eta\sum_{\nu_1\nu_2\ldots\nu_N}\mathrm{per}(\tilde{\alpha}^{\mu_1\mu_2\ldots\mu_N,\nu_1\nu_2\ldots\nu_N})T^{(N)}_{\nu_1\nu_2\ldots\nu_N}, \tag{27}$$

where the symbol $\mathrm{per}(C)$ denotes the permanent of a square matrix C and where $\tilde{\alpha}^{\mu_1\mu_2\ldots\mu_N,\nu_1\nu_2\ldots\nu_N}$ denotes a square $N\times N$ matrix with elements

$$\{\tilde{\alpha}^{\mu_1\mu_2\ldots\mu_N,\nu_1\nu_2\ldots\nu_N}\}_{ij}=\alpha_{\mu_i\nu_j}\quad\text{for } i,j\in\{1,2,\ldots,N\}. \tag{28}$$

The final condition on the tensor shape is

$$T^{(N)}_{\mu_1\mu_2\ldots\mu_N} = \sum_{\nu_1\nu_2\ldots\nu_N}Q^{(N)}_{\mu_1\mu_2\ldots\mu_N,\nu_1\nu_2\ldots\nu_N}T^{(N)}_{\nu_1\nu_2\ldots\nu_N},$$

$$Q^{(N)}_{\mu_1\mu_2\ldots\mu_N,\nu_1\nu_2\ldots\nu_N} = \frac{1}{N!\,|\mathcal{P}_\mathrm{M}|}\sum_{(\alpha,\eta)}^{\mathcal{P}_\mathrm{M}}\eta\,\mathrm{per}(\tilde{\alpha}^{\mu_1\mu_2\ldots\mu_N,\nu_1\nu_2\ldots\nu_N}), \tag{29}$$

and the number $q^{(N)}$ of independent nonzero components of the tensor $T^{(N)}_{\mu_1\mu_2\ldots\mu_N}$ equals

$$q^{(N)} = \sum_{\mu_1\mu_2\ldots\mu_N}Q^{(N)}_{\mu_1\mu_2\ldots\mu_N,\mu_1\mu_2\ldots\mu_N}. \tag{30}$$

The last two equations represent the main result of this section.

Evaluation of the projection superoperator $Q^{(N)}_{\mu_1\mu_2\ldots\mu_N,\nu_1\nu_2\ldots\nu_N}$ for selected groups $\mathcal{P}_\mathrm{M}$ was straightforward, based on the known group elements (α,η) and rotation matrices $\alpha=\{\alpha_{\mu\nu}\}$. The identification of nonvanishing components of the tensor $T^{(N)}_{\mu_1\mu_2\ldots\mu_N}$ and the linear dependences among them were derived from the identification of nonzero rows of the superoperator $Q^{(N)}_{\mu_1\mu_2\ldots\mu_N,\nu_1\nu_2\ldots\nu_N}$ and from the linear dependences among them. The success of this simple approach rests on the adopted orientation of rotation axes and mirror planes of the considered point groups with respect to the Cartesian coordinate system (for details, see Appendix C). However, the number $q^{(N)}$ is insensitive to this orientation.

III. RESULTS AND DISCUSSION

A. Magnetic point groups of selected systems

As mentioned in Sec. II A, the replacement of the original vector spin, exchange field, and local magnetic moments by their pseudoscalar counterparts (accompanied also by switching off spin-orbit interaction) leads to modified magnetic point groups for real systems (see Supplemental Material [42]). As an illustration, we present in Table I the standard and modified magnetic point groups $\mathcal{P}_\mathrm{M}$ for three elemental ferromagnets

TABLE I. Directions of magnetic moments (**n**), standard magnetic point groups (st-MPG), and modified magnetic point groups (mod-MPG) with pseudoscalar spin for selected collinear magnetic systems. The parentheses at the group symbols contain the group orders.

System	**n**	st-MPG	mod-MPG
Fe	(001)	$4/mm'm'$ (16)	$m\bar{3}m$ (48)
Co	(0001)	$6/mm'm'$ (24)	$6/mmm$ (24)
Ni	(111)	$\bar{3}m'$ (12)	$m\bar{3}m$ (48)
FeO	(111)	$\bar{3}m1'$ (24)	$\bar{3}m1'$ (24)
Mn_2Au	(100), (110)	$m'mm$ (8)	$4/m'mm$ (16)
RuO_2	(001)	$4'/mm'm$ (16)	$4'/mm'm$ (16)
RuO_2	(100), (110)	$m'm'm$ (8)	$4'/mm'm$ (16)
MnTe	$(11\bar{2}0)$	mmm (8)	$6'/m'm'm$ (24)
MnTe	$(1\bar{1}00)$	$m'm'm$ (8)	$6'/m'm'm$ (24)

TABLE II. Nontrivial magnetic Laue groups (MLG) (in parentheses is the subgroup $\mathcal{S}$ of all elements without the operation of antisymmetry), the lowest rank N of a nonvanishing symmetric tensor $T^{(N)}$, the nature B or P of the leading term in the Taylor expansion of $F(\mathbf{k})$, and the number $q^{(N)}$ of independent nonzero components of the tensor $T^{(N)}$.

MLG ($\mathcal{S}$)	N	B/P	$q^{(N)}$
$m'm'm$ $(2/m)$	2	P	1
$2'/m'$ $(\bar{1})$	2	B	2
$4'/m$ $(2/m)$	2	P	2
$4'/mm'm$ (mmm)	2	P	1
$\bar{3}m'$ $(\bar{3})$	4	B	1
$4/mm'm'$ $(4/m)$	4	P	1
$6'/m'$ $(\bar{3})$	4	B	2
$6'/m'm'm$ $(\bar{3}m)$	4	B	1
$6/mm'm'$ $(6/m)$	6	P	1
$m\bar{3}m'$ $(m\bar{3})$	6	B	1

(bcc Fe, hcp Co, and fcc Ni) and four binary antiferromagnetic compounds: FeO with a rock-salt structure [57], Mn_2Au with a body-centered tetragonal (bct) structure [58,59], RuO_2 with a rutile structure [60,61], and MnTe with a hexagonal structure [62]. The selected antiferromagnets are featured by simple magnetic structures, with one formula unit per magnetic unit cell for Mn_2Au [58,59], while two formula units form one magnetic unit cell in FeO [57], RuO_2 [60], and MnTe [62]; for all compounds, the positions of nonmagnetic atoms are taken into account. In the standard treatment, the resulting symmetry depends on the direction **n** of magnetic moments, whereas the results of the modified approach are insensitive to this direction. For ferromagnets listed in Table I, the standard magnetic point groups belong to category (c), while the modified ones belong to category (b), being identical with the crystallographic point groups of the underlying cubic (Fe, Ni) and hexagonal (Co) lattices. Different situations are found for antiferromagnets. For FeO, both groups are identical, belonging to category (a). For RuO_2 with magnetic moments along the (001) direction (the fourfold axis), both groups belong to category (c) and they represent two different versions of the group $4'/mm'm$ [the primed reflections are on the (110) and (100) planes in the standard and modified $\mathcal{P}_M$, respectively]. For all other systems, the modified groups belong to category (c) as well, but they differ explicitly from the standard ones. Moreover, no direct group-subgroup relation could be found in these cases between the modified and standard $\mathcal{P}_M$. Nevertheless, one can observe in Table I that the group order of the standard $\mathcal{P}_M$ divides that of the modified $\mathcal{P}_M$ in all studied cases; see the Supplemental Material [42] for more details.

The modification of the magnetic point groups naturally leads to a modification of the magnetic space groups. As an example, we mention the antiferromagnetic MnF_2 compound with a rutile structure and with Mn moments pointing along the tetragonal axis [14]; this system is equivalent to RuO_2 with Ru moments along the (001) direction. Its standard magnetic space group (for the system with spin-orbit interaction) is $P4'_2/mnm'$ and the modified group is $P4'_2/mn'm$ [14], in agreement with the two versions of the point group $4'/mm'm$ of RuO_2. A more detailed discussion of the space groups goes beyond the scope of the present study.

B. Classification of collinear nonrelativistic magnets

Inspection of the derived general formula for N even, given by Eq. (29), reveals that the superoperator $Q^{(N)}$ depends only on the Laue class of $\mathcal{P}_M$ (the magnetic Laue group is obtained by adding space inversion to all elements of the magnetic point group $\mathcal{P}_M$ [26]). This resembles the case of certain tensors, such as the conductivity tensor and the tensor of thermoelectric coefficients [25,26], and it simplifies the analysis of possible shapes of the tensors $T^{(N)}$ substantially. However, it should be noted that some of the magnetic point groups of category (c) belong to the Laue class of category (a); this happens if (and only if) the $\mathcal{P}_M$ contains the combination of space inversion and of the operation of antisymmetry. Further inspection of Eq. (29) proves that for a particular $\mathcal{P}_M$ (or its Laue class) of category (a), the superoperators $Q^{(N)}$ and the resulting tensors $T^{(N)}$ vanish identically for all N. The evaluation of Eqs. (29) and (30) thus has to be performed only for magnetic Laue groups of category (c); the total number of these nontrivial magnetic Laue groups amounts to 10.

Our results are summarized in Table II. For each magnetic Laue group, the lowest rank N of a nonvanishing tensor $T^{(N)}_{\mu_1\mu_2\ldots\mu_N}$ is given together with the number $q^{(N)}$ of its independent nonzero components. All these nonzero tensor components are listed explicitly in Appendix C; the symbols B (bulk) and P (planar) in Table II indicate which of the components k_x, k_y, and k_z of the **k** vector enter the leading term in the Taylor expansion (12) of $F(\mathbf{k})$. The symbol P refers to the cases where only two components in directions perpendicular to a prominent direction of the group are present, while the symbol B denotes all other cases. The most important observation is the fact that for each magnetic Laue group of category (c), a nonvanishing tensor $T^{(N)}$ exists, which in turn proves the presence of spin splitting in a neighborhood of the BZ center.

Let us briefly discuss the four antiferromagnets (FeO, Mn_2Au, RuO_2, MnTe) mentioned in Sec. III A; see, also, Table I. The modified $\mathcal{P}_M$ of FeO ($\bar{3}m1'$) belongs to category (a), incompatible with spin splitting. The modified $\mathcal{P}_M$ of RuO_2 ($4'/mm'm$) and that of MnTe ($6'/m'm'm$) are Laue

groups of category (c), compatible with spin splitting. The modified $\mathcal{P}_M$ of Mn_2Au ($4/m'mm$) is of category (c); however, its Laue class ($4/mmm1'$) is of category (a), which does not support spin splitting.

The present identification of a broad pool of 10 nontrivial magnetic Laue groups, yielding the spin splitting of energy bands in antiferromagnets, is in full agreement with the ample occurrence of this phenomenon [8–12,15,17]. Moreover, a closer look at the results in Table II reveals a remarkable similarity with a classification scheme of altermagnets obtained by Šmejkal *et al.* [17]. The approach developed by the authors of Ref. [17] is based on spin point groups, on eigenvalues of model $\mathbf{k}\cdot\mathbf{p}$ Hamiltonians, and on an orbital-harmonic representation [63]. The 10 different altermagnetic cases, summarized in Table 1 of Ref. [17], are featured by the spin Laue group, a spin winding number W ($W = 2, 4, 6$), and the B/P symbol. An explicit one-to-one mapping between the 10 cases of Šmejkal *et al.* and those in Table II can be found after identification of N with the spin winding number W and by comparing the B/P symbols, the parent crystallographic point groups, and the subgroups of index two attached to the magnetic/spin Laue groups. This mapping is further corroborated by the resulting $\mathbf{k}$-dependent functions: $F(\mathbf{k})$, given by Eq. (12), and its eigenvalue-based counterpart [17]; see Appendix C.

The similarity of the results of both classification schemes deserves a brief comment. In the approach using the spin point groups, the reversal of local magnetic moments in antiferromagnets is achieved by the π rotation in the spin space around an axis perpendicular to the moment direction [17]. In the pseudoscalar-spin approach, the local moment reversal is owing to the operation of antisymmetry (spin-channel interchange) present in the modified magnetic groups. The latter approach then leads to a very simple classification of nonrelativistic collinear magnets: the ferro- and ferrimagnets (including the compensated ones) with different spin-up and spin-down band structures are characterized by the magnetic point group of category (b), the usual antiferromagnets without spin-split electronic structure possess the magnetic Laue group of category (a), and the antiferromagnets with spin splitting (altermagnets) are featured by the magnetic Laue group of category (c). These three categories of magnetic point and Laue groups proved very useful for understanding the transport phenomena in magnetic materials since the 1960's; one might expect that they will also be helpful in the field of antiferromagnets with momentum-dependent spin splitting.

As an example, let us consider the spin conductivity introduced in Sec. II D. The shape of the spin-conductivity tensor $\tilde{\sigma}_{\mu_1\mu_2}$ coincides with that of the tensor $T^{(2)}_{\mu_1\mu_2}$. According to Table II, this tensor is nonzero only for four magnetic Laue classes, namely, for $m'm'm$, $2'/m'$, $4'/m$, and $4'/mm'm$. This result explains different sources of the calculated spin conductivities of hexagonal MnTe and tetragonal RuO_2 systems [16]: in MnTe (modified $\mathcal{P}_M$ $6'/m'm'm$), it is caused solely by spin-orbit interaction, whereas in RuO_2 (modified $\mathcal{P}_M$ $4'/mm'm$), it is induced primarily by the anisotropic spin-split bands. The anisotropy of RuO_2 can easily be understood by inspecting the subgroup $\mathcal{S}$ of all elements without the operation of antisymmetry, which is the orthorhombic group mmm with mirror planes (001), (110), and $(1\bar{1}0)$. Consequently, the conductivities in each spin channel are different along the (110) and $(1\bar{1}0)$ directions, which (together with the spin-channel interchange accompanying the rotation by $\pi/2$ around the z axis present in $\mathcal{P}_M$) leads to the resulting nonzero spin conductivity [9,16].

The obtained classification scheme is also compatible with the recently formulated criteria for spin splitting in antiferromagnets, based on magnetic space groups [14,15]. All magnetic space groups $\mathcal{G}_M$ can be divided into four types [21], which correspond to the three categories of the magnetic point groups $\mathcal{P}_M$ derived from the $\mathcal{G}_M$ as follows. A group $\mathcal{G}_M$ of type I does not involve the operation of antisymmetry at all (neither as a separate element nor in a combination with a spatial operation); its $\mathcal{P}_M$ belongs to category (b). A group $\mathcal{G}_M$ of type II contains the pure operation of antisymmetry as a group element; its $\mathcal{P}_M$ belongs to category (a). A group $\mathcal{G}_M$ of type III contains the operation of antisymmetry only in a combination with a nontrivial rotation (combined optionally with a translation); its $\mathcal{P}_M$ belongs to category (c). For this type, further partitioning can be done which is equivalent to the two categories [(a) or (c)] relevant for the Laue class of the $\mathcal{P}_M$ of category (c). A group $\mathcal{G}_M$ of type IV contains the operation of antisymmetry in a combination with a nonprimitive translation; its $\mathcal{P}_M$ belongs to category (a). However, in application of both approaches to a particular system, the different nature of electron spin (vector or pseudoscalar) should also be taken into account. As an illustrating example, we consider the antiferromagnetic NiO system with a perturbed rock-salt structure in which each oxygen (111) plane is displaced slightly along the (111) direction towards the nearest nickel (111) plane with positive magnetic moments [49]. For Ni moments oriented along the $(11\bar{2})$ direction, the standard $\mathcal{G}_M$ is $C2'/m'$, which is of type III and which leads to the spin splitting of eigenvalues essentially throughout the whole BZ. Within the pseudoscalar-spin approach, the modified $\mathcal{P}_M$ is $\bar{3}m$ which belongs to category (b), leading thus to the same kind of spin splitting. This can easily be understood in terms of ferrimagnetism: nickel atoms with opposite signs of local moments behave (from a viewpoint of symmetry) as two chemically different species due to the adopted displacements of oxygen atoms. The system can thus be treated as a nearly compensated ferrimagnet with different band structures in spin-up and spin-down channels, which explains the resulting spin splitting. A more detailed comparison of the approach based on $\mathcal{G}_M$ [14,15] and the current one employing $\mathcal{P}_M$ goes beyond the scope of this work.

C. Spin splitting in a model antiferromagnet

In this section, we briefly discuss the physical mechanisms behind the spin splitting of eigenvalues in collinear antiferromagnets. Since the only known monatomic collinear antiferromagnet is chromium on a bcc lattice, which however forms a spin-density wave with a wavelength incommensurate with the bcc lattice parameter [64], one can conclude that nonmagnetic atoms play an important role for collinear antiferromagnets with perfect translation invariance. The effect of the nonmagnetic atoms is manifold. First, they are responsible for stabilization of the geometric structure of the systems.

Second, they often lead to the formation of the local magnetic moments and to their antiferromagnetic exchange coupling. Finally, the nonmagnetic atoms create local electric crystal fields around the magnetic atoms, which in combination with spin-group symmetries of the one-electron Hamiltonian give rise to the spin splitting [17]. The important role of nonmagnetic atoms has also been proved in a recent study of NiO with a rock-salt structure, in which small displacements of oxygen atoms were introduced, which generated a pronounced spin splitting [49].

Let us assess the relative importance of the nonmagnetic atoms and of the group symmetry using an example of the antiferromagnetic KRu_4O_8 compound with a bct structure, which exhibits the spin splitting [17]. The potassium atoms occupy the Wyckoff 2(b) positions of the space group (space group $I4/m$, No. 87), while the ruthenium atoms as well as both kinds of oxygen atoms occupy the Wyckoff 8(h) positions [65]. The three fundamental vectors of the Bravais bct lattice are $\mathbf{a}_1 = (a, 0, 0)$, $\mathbf{a}_2 = (0, a, 0)$, and $\mathbf{a}_3 = (a/2, a/2, c/2)$, where a and c are the bct lattice parameters. The basis vectors of Ru atoms are $\mathbf{B}_1 = (ua, va, 0)$, $\mathbf{B}_2 = (-va, ua, 0)$, $\mathbf{B}_3 = -\mathbf{B}_1$, and $\mathbf{B}_4 = -\mathbf{B}_2$, where u and v are dimensionless atomic coordinates. The local magnetic moments of Ru atoms at $\mathbf{B}_1$ and $\mathbf{B}_3$ are identical, being opposite to those of Ru atoms at $\mathbf{B}_2$ and $\mathbf{B}_4$. The magnetic point group (with pseudoscalar spin) of the whole system is $4'/m$, which is compatible with the existence of the spin splitting according to Table II. However, the same magnetic point group is also obtained for a hypothetical four-site bct system derived from KRu_4O_8 by removing all nonmagnetic atoms (K, O), thus keeping only the magnetic Ru atoms with their antiferromagnetic structure. This indicates that the spin splitting might be obtained even without any nonmagnetic atoms in this case.

In order to verify this idea on a very simple model, we performed band-structure calculations for this four-site bct model using the linear muffin-tin orbital (LMTO) method in the atomic sphere approximation [66], in which the angular-momentum cutoff was set to $\ell_{\max} = 0$, thus corresponding to a single orbital per atom. The LMTO potential parameter Δ, which controls the bandwidth, was set to $\Delta = 1.8w^{-2}$, where w denotes the Wigner-Seitz radius of the lattice, and the dimensionless LMTO potential parameter was taken as $\gamma = 0.4$, which is a typical value for s orbitals of transition metals. The LMTO potential parameter C, which controls the position of the bands on the energy scale, was set to zero for a nonmagnetic system, whereas exchange-split values of $C = \pm\Delta$ were used to simulate the antiferromagnetic order. The geometric structure of the model is defined by $u = 0.27$, $v = 0.08$, and $c/a = 0.4$ (these values were chosen in order to achieve good space filling by the atomic spheres).

The resulting band structures are displayed in Fig. 1 along the $Y - \Gamma - X$ path in the bct BZ, i.e., for $k_z = 0$, $k_y = |k_x|$, and $-\pi \leqslant ak_x \leqslant \pi$. One can clearly observe the spin splitting in the antiferromagnetic state, in qualitative agreement with that found in the realistic band structure of the KRu_4O_8 compound [17]. A similar result has recently been obtained for a single-orbital four-site antiferromagnetic model without nonmagnetic atoms, derived from a pyrochlore structure [11] and characterized by the magnetic point group $4'/mm'm$. These results prove that the nontrivial magnetic Laue group of the system is the most important prerequisite for the appearance of spin splitting; other features present in real materials, such as the local electric fields and magnetic exchange interactions due to the nonmagnetic atoms, or the true orbital structure of the magnetic transition-metal atoms, are less essential in this respect (despite their primary importance for the realistic band structure and the splitting strength).

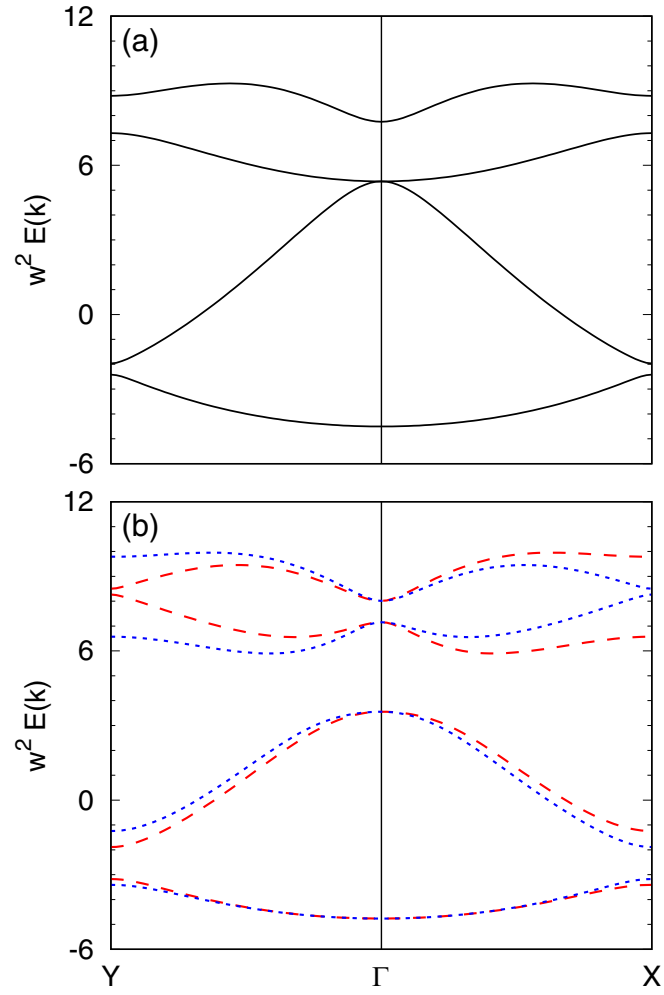

FIG. 1. The band structure of the four-site model on a bct lattice: (a) in the nonmagnetic state, (b) in the antiferromagnetic state. In (b), the dotted and dashed curves correspond to the two spin channels $s = 1$ and $s = -1$, respectively.

IV. CONCLUSIONS

We have introduced the concept of a pseudoscalar electron spin appropriate for a theoretical treatment of the electronic structure of nonrelativistic collinear magnets. The substitution of the original vector spin by the pseudoscalar spin brings about a modification of magnetic groups of crystalline systems. We have defined an infinite-dimensional representation of the modified magnetic point groups, which enabled us to avoid any approximations in solving the Hamiltonian eigenvalue problem. This representation is single valued and unitary, which might be beneficial in future extensions of the formalism.

The developed theory was used for an analysis of spin splitting of electron states in antiferromagnets near the center of the Brillouin zone. Our results provide an alternative view on the recently introduced altermagnetic systems [17]; their different classes were identified unambiguously with the nontrivial magnetic Laue classes that are relevant for shape restrictions of various transport tensor quantities. As a consequence, the spin conductivity induced by spin-split bands in certain antiferromagnets has been ascribed to four specific magnetic Laue classes. A brief discussion of a model antiferromagnet without nonmagnetic atoms revealed that the point-group symmetry of the system represents the key factor for the existence of the spin splitting, while the nonmagnetic atoms only influence the splitting magnitude.

The present work was confined to magnetic point groups; it can be, together with recent studies based on magnetic space groups [14,15,49] and on spin point groups [17], considered as one of the starting points towards a complete symmetry analysis of transport properties and electron states in collinear nonrelativistic magnets, which should inevitably include spin space groups [37]. This topic has to be left for the future.

APPENDIX A: HAMILTONIAN AND TRANSFORMATION OF OPERATORS

The Hamiltonian (1) is represented in the basis of orthonormal vectors $|\mathbf{G}s\rangle = |\mathbf{G}\rangle \otimes |s\rangle$, where the spatial part for a given $\mathbf{k}$ point is defined by

$$\langle \mathbf{r}|\mathbf{G}\rangle = \Omega^{-1/2} \exp[i(\mathbf{k}-\mathbf{G})\cdot\mathbf{r}], \tag{A1}$$

where Ω denotes the volume of the primitive cell in the real space. The full Hamiltonian matrix in this basis is

$$\langle \mathbf{G}s|\tilde{H}(\mathbf{k})|\mathbf{G}'s'\rangle = [(\mathbf{k}-\mathbf{G})^2\delta_{\mathbf{G}\mathbf{G}'} + \tilde{V}_s(\mathbf{G}-\mathbf{G}')]\delta_{ss'}, \tag{A2}$$

where we introduced Fourier coefficients $\tilde{V}_s(\mathbf{G})$ of the potentials $V_s(\mathbf{r})$, so that

$$V_s(\mathbf{r}) = \sum_{\mathbf{G}} \tilde{V}_s(\mathbf{G}) \exp(-i\mathbf{G}\cdot\mathbf{r}). \tag{A3}$$

Consequently, matrix elements of the operators h, J_μ, and $L_{\mu_1\mu_2}$, which define the full $\mathbf{k}$ dependence of $\tilde{H}(\mathbf{k})$, given by Eq. (6), are equal to

$$\begin{aligned}
\langle \mathbf{G}s|h|\mathbf{G}'s'\rangle &= [\mathbf{G}^2\delta_{\mathbf{G}\mathbf{G}'} + \tilde{V}_s(\mathbf{G}-\mathbf{G}')]\delta_{ss'},\\
\langle \mathbf{G}s|J_\mu|\mathbf{G}'s'\rangle &= -2G_\mu\delta_{\mathbf{G}\mathbf{G}'}\delta_{ss'},\\
\langle \mathbf{G}s|L_{\mu_1\mu_2}|\mathbf{G}'s'\rangle &= \delta_{\mu_1\mu_2}\delta_{\mathbf{G}\mathbf{G}'}\delta_{ss'}.
\end{aligned} \tag{A4}$$

The last relation implies that $L_{\mu_1\mu_2} = I\delta_{\mu_1\mu_2}$, where I is the unit operator. We also mention the matrix elements of the spin operator σ, which reduce to

$$\langle \mathbf{G}s|\sigma|\mathbf{G}'s'\rangle = s\delta_{\mathbf{G}\mathbf{G}'}\delta_{ss'}. \tag{A5}$$

Note that Eq. (A2) represents a starting point for accurate eigenvalues of the Hamiltonian (1), provided that the basis set $\{|\mathbf{G}s\rangle\}$ is not truncated.

Let us now prove the basic property (14) of the representation $\mathcal{D}(\alpha,\eta)$ of the magnetic point group $\mathcal{P}_\mathrm{M}$, defined by Eq. (13). If we denote $(\alpha_1,\eta_1)(\alpha_2,\eta_2) = (\alpha_1\alpha_2, \eta_1\eta_2) \equiv (\alpha_3,\eta_3)$, then the corresponding translations $\mathbf{t}_j$, $j\in\{1,2,3\}$, entering Eq. (5), satisfy $\mathbf{t}_3 = \alpha_1\mathbf{t}_2 + \mathbf{t}_1$. We get, for an arbitrary basis vector $|\mathbf{G}s\rangle$,

$$\begin{aligned}
&\mathcal{D}(\alpha_1,\eta_1)\mathcal{D}(\alpha_2,\eta_2)|\mathbf{G}s\rangle\\
&\quad= \mathcal{D}(\alpha_1,\eta_1)|\alpha_2\mathbf{G},\eta_2 s\rangle \exp(i\alpha_2\mathbf{G}\cdot\mathbf{t}_2)\\
&\quad= |\alpha_1\alpha_2\mathbf{G},\eta_1\eta_2 s\rangle \exp(i\alpha_1\alpha_2\mathbf{G}\cdot\mathbf{t}_1)\exp(i\alpha_2\mathbf{G}\cdot\mathbf{t}_2)\\
&\quad= |\alpha_1\alpha_2\mathbf{G},\eta_1\eta_2 s\rangle \exp[i\alpha_1\alpha_2\mathbf{G}\cdot(\mathbf{t}_1+\alpha_1\mathbf{t}_2)]\\
&\quad= |\alpha_3\mathbf{G},\eta_3 s\rangle \exp(i\alpha_3\mathbf{G}\cdot\mathbf{t}_3) = \mathcal{D}(\alpha_3,\eta_3)|\mathbf{G}s\rangle.
\end{aligned} \tag{A6}$$

This completes the proof of Eq. (14).

Let us now turn to the transformation of relevant operators, as summarized in Eq. (15). We start with the reference Hamiltonian h. We evaluate $\mathcal{D}(\alpha,\eta)h$ and $h\mathcal{D}(\alpha,\eta)$ for $(\alpha,\eta)\in\mathcal{P}_\mathrm{M}$ and compare the results. We get, for an arbitrary basis vector $|\mathbf{G}'s\rangle$,

$$\begin{aligned}
\mathcal{D}(\alpha,\eta)h|\mathbf{G}'s\rangle &= \mathcal{D}(\alpha,\eta)\sum_{\mathbf{G}''}|\mathbf{G}''s\rangle\langle\mathbf{G}''s|h|\mathbf{G}'s\rangle = \sum_{\mathbf{G}''}|\alpha\mathbf{G}'',\eta s\rangle\exp(i\alpha\mathbf{G}''\cdot\mathbf{t})[(\mathbf{G}')^2\delta_{\mathbf{G}''\mathbf{G}'} + \tilde{V}_s(\mathbf{G}''-\mathbf{G}')]\\
&= \sum_{\mathbf{G}}|\mathbf{G},\eta s\rangle\exp(i\mathbf{G}\cdot\mathbf{t})[(\mathbf{G}')^2\delta_{\mathbf{G},\alpha\mathbf{G}'} + \tilde{V}_s(\alpha^{-1}\mathbf{G}-\mathbf{G}')],
\end{aligned} \tag{A7}$$

where we replaced the summation lattice vector $\mathbf{G}''$ by $\mathbf{G} = \alpha\mathbf{G}''$. Similarly, we get

$$\begin{aligned}
h\mathcal{D}(\alpha,\eta)|\mathbf{G}'s\rangle &= h|\alpha\mathbf{G}',\eta s\rangle\exp(i\alpha\mathbf{G}'\cdot\mathbf{t}) = \sum_{\mathbf{G}}|\mathbf{G},\eta s\rangle\langle\mathbf{G},\eta s|h|\alpha\mathbf{G}',\eta s\rangle\exp(i\alpha\mathbf{G}'\cdot\mathbf{t})\\
&= \sum_{\mathbf{G}}|\mathbf{G},\eta s\rangle\exp(i\alpha\mathbf{G}'\cdot\mathbf{t})[\mathbf{G}^2\delta_{\mathbf{G},\alpha\mathbf{G}'} + \tilde{V}_{\eta s}(\mathbf{G}-\alpha\mathbf{G}')].
\end{aligned} \tag{A8}$$

The difference of both results yields

$$[\mathcal{D}(\alpha,\eta)h - h\mathcal{D}(\alpha,\eta)]|\mathbf{G}'s\rangle = \sum_{\mathbf{G}}|\mathbf{G},\eta s\rangle[\exp(i\mathbf{G}\cdot\mathbf{t})\tilde{V}_s(\alpha^{-1}\mathbf{G}-\mathbf{G}') - \exp(i\alpha\mathbf{G}'\cdot\mathbf{t})\tilde{V}_{\eta s}(\mathbf{G}-\alpha\mathbf{G}')]. \tag{A9}$$

After application of an auxiliary identity (valid for all reciprocal lattice vectors $\mathbf{G}$),

$$\tilde{V}_s(\mathbf{G}) = \exp(-i\alpha\mathbf{G}\cdot\mathbf{t})\tilde{V}_{\eta s}(\alpha\mathbf{G}), \tag{A10}$$

with $\mathbf{G}$ replaced by $(\alpha^{-1}\mathbf{G}-\mathbf{G}')$, we get, finally,

$$\mathcal{D}(\alpha,\eta)h - h\mathcal{D}(\alpha,\eta) = 0, \tag{A11}$$

which proves the invariance of the Hamiltonian h, given by Eq. (15). The auxiliary identity (A10) follows from Eq. (5) combined with the Fourier expansion (A3),

$$\begin{aligned}\sum_{\mathbf{G}} \tilde{V}_s(\mathbf{G})\exp(-i\mathbf{G}\cdot\mathbf{r}) &= \sum_{\mathbf{G}'} \tilde{V}_{\eta s}(\mathbf{G}')\exp[-i\mathbf{G}'\cdot(\alpha\mathbf{r}+\mathbf{t})] = \sum_{\mathbf{G}} \tilde{V}_{\eta s}(\alpha\mathbf{G})\exp[-i\alpha\mathbf{G}\cdot(\alpha\mathbf{r}+\mathbf{t})] \\ &= \sum_{\mathbf{G}} \tilde{V}_{\eta s}(\alpha\mathbf{G})\exp(-i\alpha\mathbf{G}\cdot\mathbf{t})\exp(-i\mathbf{G}\cdot\mathbf{r}).\end{aligned} \tag{A12}$$

The comparison of coefficients at $\exp(-i\mathbf{G}\cdot\mathbf{r})$ on both sides of this relation yields the identity (A10).

The transformation of the other operators can be obtained in a similar way. As an example, let us consider the velocities J_μ. We get, for an arbitrary basis vector $|\mathbf{G}s\rangle$,

$$\begin{aligned}\mathcal{D}(\alpha,\eta)J_\mu|\mathbf{G}s\rangle &= \mathcal{D}(\alpha,\eta)(-2G_\mu)|\mathbf{G}s\rangle \\ &= -2G_\mu|\alpha\mathbf{G},\eta s\rangle\exp(i\alpha\mathbf{G}\cdot\mathbf{t})\end{aligned} \tag{A13}$$

and

$$\begin{aligned}J_\mu\mathcal{D}(\alpha,\eta)|\mathbf{G}s\rangle &= J_\mu|\alpha\mathbf{G},\eta s\rangle\exp(i\alpha\mathbf{G}\cdot\mathbf{t}) \\ &= -2(\alpha\mathbf{G})_\mu|\alpha\mathbf{G},\eta s\rangle\exp(i\alpha\mathbf{G}\cdot\mathbf{t}) \\ &= -2\sum_\nu \alpha_{\mu\nu}G_\nu|\alpha\mathbf{G},\eta s\rangle\exp(i\alpha\mathbf{G}\cdot\mathbf{t}).\end{aligned} \tag{A14}$$

This means that

$$J_\mu\mathcal{D}(\alpha,\eta) = \sum_\nu \alpha_{\mu\nu}\mathcal{D}(\alpha,\eta)J_\nu = \mathcal{D}(\alpha,\eta)\sum_\nu \alpha_{\mu\nu}J_\nu, \tag{A15}$$

from which the transformation of J_μ, given by Eq. (15), immediately follows.

APPENDIX B: SPIN CONDUCTIVITY

The spin-conductivity tensor $\sigma^\lambda_{\mu_1\mu_2}$ of a nonrelativistic collinear magnet can be written according to a general formula for the static linear response of noninteracting electron systems [67,68] at zero temperature as

$$\begin{aligned}\sigma^\lambda_{\mu_1\mu_2} = -2c\int_{-\infty}^{E_\mathrm{F}} dE\,\overline{\mathrm{Tr}}\big\{&\sigma^\lambda p_{\mu_1}Z'(E_+)p_{\mu_2}[Z(E_+)-Z(E_-)] \\ &-\sigma^\lambda p_{\mu_1}[Z(E_+)-Z(E_-)]p_{\mu_2}Z'(E_-)\big\}.\end{aligned} \tag{B1}$$

Here the prefactor c is inversely proportional to the size of the system (a big finite crystal with periodic boundary conditions), the integration is carried out over the occupied part of the valence spectrum (for energies E up to the Fermi energy E_F), and the trace $\overline{\mathrm{Tr}}$ refers to the Hilbert space of the entire system. The quantities σ^λ denote the Pauli spin matrices, $(\sigma^x,\sigma^y,\sigma^z)=\boldsymbol{\sigma}$, the quantities p_μ refer to the momentum operator, $(p_x,p_y,p_z)=\mathbf{p}$, the symbol $Z(E_\pm) = Z(E\pm i0)$ denotes the retarded and advanced one-electron propagator (resolvent), and the prime at $Z(E_\pm)$ denotes the energy derivative. Note that evaluation of Eq. (B1) involves implicitly averaging over all $\mathbf{k}$ vectors in the whole BZ. The direction of all magnetic moments (and exchange fields) of the collinear system is specified by a unit vector $\mathbf{n}=(n_x,n_y,n_z)$. The momentum operator p_μ is spin independent; the spin dependence of the propagators $Z(E_\pm)$ can be written as a sum over the spin-channel index s ($s=\pm1$) as

$$Z(E_\pm) = \sum_s Z_s(E_\pm)\otimes\Pi_s(\mathbf{n}), \quad \Pi_s(\mathbf{n}) = \frac{1+s\mathbf{n}\cdot\boldsymbol{\sigma}}{2}, \tag{B2}$$

and similarly for the derivatives $Z'(E_\pm)$. Here the symbol $a\otimes b$ means an operator involving an operator a acting only in the orbital space and an operator b acting only in the two-dimensional spin space. The quantities $Z_s(E_\pm)$ in Eq. (B2) thus refer to the propagators in the spin channel s ($s=\pm1$), while the $\Pi_s(\mathbf{n})$ denotes a projection operator in the spin space (projecting on the spin channel s with respect to the spin quantization axis $\mathbf{n}$). Evaluation of the trace follows the rule $\overline{\mathrm{Tr}}(a\otimes b) = \underline{\mathrm{Tr}}(a)\mathrm{tr}(b)$, where the traces $\underline{\mathrm{Tr}}$ and tr refer to the orbital and spin space, respectively. Using Eq. (B2) in the starting formula (B1) together with the relation

$$\mathrm{tr}[\sigma^\lambda\Pi_s(\mathbf{n})\Pi_{s'}(\mathbf{n})] = n_\lambda s\delta_{ss'} \tag{B3}$$

leads to the final expression for the spin-conductivity tensor $\sigma^\lambda_{\mu_1\mu_2}$ as

$$\begin{aligned}&\sigma^\lambda_{\mu_1\mu_2} = n_\lambda\tilde{\sigma}_{\mu_1\mu_2}, \quad \tilde{\sigma}_{\mu_1\mu_2} = \sum_s s\sigma^{(s)}_{\mu_1\mu_2}, \\ &\sigma^{(s)}_{\mu_1\mu_2} = -2c\int_{-\infty}^{E_\mathrm{F}} dE\,\underline{\mathrm{Tr}}\{p_{\mu_1}Z'_s(E_+)p_{\mu_2}[Z_s(E_+)-Z_s(E_-)] \\ &\qquad - p_{\mu_1}[Z_s(E_+)-Z_s(E_-)]p_{\mu_2}Z'_s(E_-)\}.\end{aligned} \tag{B4}$$

This result proves the reduction of the tensor $\sigma^\lambda_{\mu_1\mu_2}$ of rank three to a tensor $\tilde{\sigma}_{\mu_1\mu_2}$ of rank two; the latter equals the difference of tensors $\sigma^{(s)}_{\mu_1\mu_2}$ for the majority (spin-up, $s=1$) and minority (spin-down, $s=-1$) channels. The tensor $\sigma^{(s)}_{\mu_1\mu_2}$ coincides with the electrical conductivity tensor in channel s, which can be expressed by the Kubo-Greenwood formula [69] in terms of the spin-resolved propagators only at the Fermi energy. This yields

$$\sigma^{(s)}_{\mu_1\mu_2} = c\underline{\mathrm{Tr}}\big[p_{\mu_1}\Gamma_s p_{\mu_2}\Gamma_s\big], \quad \Gamma_s = i[Z_s(E_{\mathrm{F},+}) - Z_s(E_{\mathrm{F},-})]. \tag{B5}$$

Using the pseudoscalar spin operator σ, the notation of Sec. II A, and an operator Γ, diagonal in the spin-channel index and defined by its spin-resolved blocks Γ_s, the reduced spin-conductivity tensor $\tilde{\sigma}_{\mu_1\mu_2}$ can be rewritten as

$$\tilde{\sigma}_{\mu_1\mu_2} = c\overline{\mathrm{Tr}}\big(\sigma\, p_{\mu_1}\Gamma p_{\mu_2}\Gamma\big). \tag{B6}$$

The group invariance of the system means that the Hamiltonian commutes with a unitary operator D representing the combination of a rotation α, translation $\mathbf{t}$, and spin-channel interchange η; see Eq. (5). The latter operator is defined by its action on all basic kets as $D|\mathbf{r}s\rangle = |\mathbf{r}'s'\rangle$, where $\mathbf{r}' = \alpha\mathbf{r} + \mathbf{t}$ and $s' = \eta s$. As a consequence, one can derive transformations of the operators in Eq. (B6) as

$$D^{-1}\sigma D = \eta\sigma, \quad D^{-1}\Gamma D = \Gamma, \quad D^{-1}p_\mu D = \sum_\nu \alpha_{\mu\nu}p_\nu, \tag{B7}$$

in complete analogy with Eq. (15). This leads to a condition for the tensor $\tilde{\sigma}_{\mu_1\mu_2}$:

$$\begin{aligned}\tilde{\sigma}_{\mu_1\mu_2} &= c\overline{\mathrm{Tr}}\big(D\eta\sigma D^{-1}p_{\mu_1}D\Gamma D^{-1}p_{\mu_2}D\Gamma D^{-1}\big)\\ &= \eta\sum_{\nu_1\nu_2}\alpha_{\mu_1\nu_1}\alpha_{\mu_2\nu_2}c\overline{\mathrm{Tr}}\big(\sigma p_{\nu_1}\Gamma p_{\nu_2}\Gamma\big)\\ &= \eta\sum_{\nu_1\nu_2}\alpha_{\mu_1\nu_1}\alpha_{\mu_2\nu_2}\tilde{\sigma}_{\nu_1\nu_2},\end{aligned} \tag{B8}$$

which has the same form as Eq. (21) for the tensor $T^{(2)}_{\mu_1\mu_2}$. The derived condition (B8) does not explicitly contain the translation vector $\mathbf{t}$, so that it holds for all elements (α, η) of the magnetic point group $\mathcal{P}_\mathrm{M}$. This proves that the shapes of both symmetric tensors $\tilde{\sigma}_{\mu_1\mu_2}$ and $T^{(2)}_{\mu_1\mu_2}$ are identical.

APPENDIX C: DETAILED RESULTS OF SYMMETRY ANALYSIS

In this part, we list more details of the resulting nonvanishing tensors $T^{(N)}_{\mu_1\mu_2\ldots\mu_N}$, briefly sketched in Table II for all 10 nontrivial magnetic Laue groups. For groups possessing only one rotation axis of the maximal order, this axis coincides with the z axis; further information on the orientation of the symmetry elements with respect to the coordinate system is given below for each particular group. In listing the independent nonzero tensor components, relations reflecting the full symmetry of $T^{(N)}_{\mu_1\mu_2\ldots\mu_N}$, such as $T^{(2)}_{xy} = T^{(2)}_{yx}$, are not explicitly mentioned. We also give the leading term of the Taylor expansion of the function $F(\mathbf{k})$, given by Eq. (12); the symbols c_1 and c_2 below denote two arbitrary constants.

For the group $m'm'm$, we chose the unprimed reflection on the $x-y$ plane and the primed reflections on the $x-z$ and $y-z$ planes. We get $N = 2$ and a single component $T^{(2)}_{xy}$. This yields

$$F(\mathbf{k}) \sim k_x k_y. \tag{C1}$$

For the group $2'/m'$, we get $N = 2$ and two components, $T^{(2)}_{xz}$ and $T^{(2)}_{yz}$. This yields

$$F(\mathbf{k}) = c_1 k_x k_z + c_2 k_y k_z. \tag{C2}$$

For the group $4'/m$, we get $N = 2$ and two components, $T^{(2)}_{xx} = -T^{(2)}_{yy}$ and $T^{(2)}_{xy}$. This yields

$$F(\mathbf{k}) = c_1\big(k_x^2 - k_y^2\big) + c_2 k_x k_y. \tag{C3}$$

For the group $4'/mm'm$, the primed reflection was on the (110) plane. We get $N = 2$ and a single component $T^{(2)}_{xx} = -T^{(2)}_{yy}$. This yields

$$F(\mathbf{k}) \sim k_x^2 - k_y^2. \tag{C4}$$

For the group $\bar{3}m'$, the primed reflection was on the $y-z$ plane. We get $N = 4$ and a single component $T^{(4)}_{xxxz} = -T^{(4)}_{xyyz}$. This yields

$$F(\mathbf{k}) \sim k_x k_z\big(k_x^2 - 3k_y^2\big). \tag{C5}$$

For the group $4/mm'm'$, one of the primed reflections was on the $y-z$ plane. We get $N = 4$ and a single component $T^{(4)}_{xxxy} = -T^{(4)}_{xyyy}$. This yields

$$F(\mathbf{k}) \sim k_x k_y\big(k_x^2 - k_y^2\big). \tag{C6}$$

For the group $6'/m'$, we get $N = 4$ and two components, $T^{(4)}_{xxxz} = -T^{(4)}_{xyyz}$ and $T^{(4)}_{xxyz} = -T^{(4)}_{yyyz}$. This yields

$$F(\mathbf{k}) = c_1 k_x k_z\big(k_x^2 - 3k_y^2\big) + c_2 k_y k_z\big(k_y^2 - 3k_x^2\big). \tag{C7}$$

For the group $6'/m'm'm$, the unprimed reflection was on the $y-z$ plane. We get $N = 4$ and a single component $T^{(4)}_{xxyz} = -T^{(4)}_{yyyz}$. This yields

$$F(\mathbf{k}) \sim k_y k_z\big(3k_x^2 - k_y^2\big). \tag{C8}$$

For the group $6/mm'm'$, the primed reflections were on the $x-z$ and $y-z$ planes. We get $N = 6$ and a single component $T^{(6)}_{xxxxxy} = -T^{(6)}_{xxxyyy} = T^{(6)}_{xyyyyy}$. This yields

$$F(\mathbf{k}) \sim k_x k_y\big(3k_x^2 - k_y^2\big)\big(3k_y^2 - k_x^2\big). \tag{C9}$$

For the group $m\bar{3}m'$, the threefold rotation axes were chosen along the (111), (11$\bar{1}$), (1$\bar{1}$1), and (1$\bar{1}\bar{1}$) directions. We get $N = 6$ and a single component $T^{(6)}_{xxxxyy} = -T^{(6)}_{xxxxzz} = -T^{(6)}_{xxyyyy} = T^{(6)}_{xxzzzz} = T^{(6)}_{yyyyzz} = -T^{(6)}_{yyzzzz}$. This yields

$$F(\mathbf{k}) \sim \big(k_x^2 - k_y^2\big)\big(k_y^2 - k_z^2\big)\big(k_z^2 - k_x^2\big). \tag{C10}$$

The obtained functions $F(\mathbf{k})$ for the individual magnetic point groups can be compared with their eigenvalue-based counterparts. These functions for the groups $m'm'm$ (C1), $\bar{3}m'$ (C5), $4/mm'm'$ (C6), $6/mm'm'$ (C9), and $m\bar{3}m'$ (C10) are identical to those of Ref. [17]. In two other cases, differences are encountered which, however, can easily be removed by rotations of the coordinate systems: for the group $4'/mm'm$ (C4), a rotation by $\pi/4$ around the z axis is needed, while for the group $6'/m'm'm$ (C8), a rotation by $\pi/2$ around the z axis is needed (these rotations correspond to an interchange of the secondary and tertiary symmetry directions for both groups). In the remaining three cases, i.e., for the groups $2'/m'$ (C2), $4'/m$ (C3), and $6'/m'$ (C7), the derived functions $F(\mathbf{k})$ contain two terms, whereby only one of them coincides with the corresponding single-term expression of Ref. [17]. This can be ascribed to the fact that all elements of these point groups are insensitive to the choice of a direction of the x (and y) axis, whereas this ambiguity is always missing in a model calculation using a particular lattice, which leads to a suppression of one of both terms.

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