

Symmetry-imposed shape of linear response tensors

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A scheme suggested in the literature to determine the symmetry-imposed shape of linear response tensors is revised and extended to allow for the treatment of more complex situations. The extended scheme is applied to discuss the shape of the spin conductivity tensor for all magnetic space groups. This allows in particular investigating the character of longitudinal as well as transverse spin transport for arbitrary crystal structure and magnetic order that give rise, e.g., to the spin Hall, Nernst, and the spin-dependent Seebeck effects.

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I. INTRODUCTION

The shape of a linear response tensor is of central importance as it decides whether a physical phenomenon may occur and what anisotropy may be expected for a solid with given crystal symmetry and magnetic order. A prominent and common example for this is the anomalous Hall effect in ferromagnetic solids, which is connected with the nonzero antisymmetric contributions to the electrical conductivity tensor. Accordingly, several schemes were suggested in the past to predict the shape of linear response tensors on the basis of group-theoretical arguments (for a corresponding review see for example Ref. [1]). Among the various schemes suggested, that of Kleiner [2–4] seems to be most convincing as it is starting from the expression for linear response tensors as given by Kubo’s linear response formalism and as it uses only the behavior of the involved operators under the appropriate space and time transformations of the relevant magnetic space group. A further appealing feature of Kleiner’s scheme is that it does not make use of Onsager’s relations but allows deriving them in a most general way.

Kleiner’s scheme was originally derived having response quantities in mind that are connected with the perturbation as well as the observable represented by the components of a single vector operator. A more general starting point is adopted in this contribution to allow the treatment of situations involving three operators. As a first simple application the tensors representing the charge and heat transport in response to an electric field and thermal gradient are considered. As a more complex transport quantity the corresponding spin conductivity is considered for all magnetic space groups. Among other things this allows the discussion of the transverse spin transport as occurring for the spin Hall [5,6] and spin Nernst [7,8] effects. In particular, it is demonstrated that these effects may be discussed without use of spin-projected conductivities [8,9].

II. SYMMETRY OF RESPONSE FUNCTIONS

Within Kubo’s linear response formalism, the change of the expectation value of an observable \hat{B}_i due to a time-dependent perturbation \hat{A}_j can be expressed by the corresponding

response function [10]

$$\begin{aligned} \tau_{\hat{B}_i \hat{A}_j}(\omega, \mathbf{H}) &= \int_0^\infty dt e^{-i\omega t} \int_0^\beta d\lambda \text{Tr}[\rho(\mathbf{H}) \hat{A}_j \hat{B}_i(t + i\hbar\lambda; \mathbf{H})]. \end{aligned} \quad (1)$$

Here $\rho(\mathbf{H}) = e^{-\beta\hat{H}(\mathbf{H})}/\text{Tr}(e^{-\beta\hat{H}(\mathbf{H})})$ is the density operator for the unperturbed system, the operators \hat{B}_i and \hat{A}_j in the Heisenberg picture are assumed to be the Cartesian components of a corresponding vector operator, and \mathbf{H} is an external magnetic field.

Equation (1) was used by Kleiner [2] as the starting point to investigate the symmetry of the tensors $\underline{\tau}$ that describe the charge and heat transport due to an electric field or thermal gradient. Kleiner’s scheme, however, is quite general and can be easily extended to deal with more complex situations. In the following, Kleiner’s scheme will be adopted to the case when the observable is represented by an operator product of the form $\hat{B}_i \hat{C}_j$, again with the operators \hat{C}_i , \hat{B}_j , and \hat{A}_k being the Cartesian components of a vector operator. In this case the corresponding response function is obviously given by

$$\begin{aligned} \tau_{(\hat{B}_i \hat{C}_j) \hat{A}_k}(\omega, \mathbf{H}) &= \int_0^\infty dt e^{-i\omega t} \int_0^\beta d\lambda \text{Tr} \\ &\times [\rho(\mathbf{H}) \hat{A}_k \hat{B}_i(t + i\hbar\lambda; \mathbf{H}) \hat{C}_j(t + i\hbar\lambda; \mathbf{H})], \end{aligned} \quad (2)$$

where by using the parentheses in the symbol $\tau_{(\hat{B}_i \hat{C}_j) \hat{A}_k}$ it is made clear that it is the observable and not the perturbation that consists of a product of two operators. The shape of the response tensor $\underline{\tau}$ in Eq. (2), i.e., the occurrence and degeneracy of nonzero elements, has to reflect the symmetry of the investigated solid. This shape can be found by considering the impact of a symmetry operation of the corresponding space group on Eq. (2), as this will lead to an equation connecting the elements of $\underline{\tau}$ or possibly of a complementary tensor $\underline{\tau}'$ (see below). Collecting the restrictions imposed by all symmetry operations the shape of $\underline{\tau}$ is obtained. In this context it is important to note that the magnetic structure of the system, if present, has to be considered. In this case, the set of symmetry operations contains unitary pure spatial (u), but also antiunitary symmetry operations (a).

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The general transformation properties of the operators $\hat{\mathbf{X}} \in \{\hat{\mathbf{A}}, \hat{\mathbf{B}}, \hat{\mathbf{C}}\}$ in Eq. (2) under unitary (u) and antiunitary symmetry operations (a) can be written as

$$u \hat{X}_i u^{-1} = \sum_j \hat{X}_j D^{(\hat{\mathbf{X}})}(u)_{ji}, \quad (3)$$

$$a \hat{X}_i a^{-1} = \sum_j \hat{X}_j D^{(\hat{\mathbf{X}})}(a)_{ji}, \quad (4)$$

where $\underline{\mathbf{D}}^{(\hat{\mathbf{X}})}(u)$ and $\underline{\mathbf{D}}^{(\hat{\mathbf{X}})}(a)$ are the representation matrices corresponding to the operator $\hat{\mathbf{X}}$ and operation u or a , respectively. The group properties are reflected by the following relations:

$$\underline{\mathbf{D}}(uu') = \underline{\mathbf{D}}(u) \underline{\mathbf{D}}(u'), \quad (5)$$

$$\underline{\mathbf{D}}(aa') = \underline{\mathbf{D}}(a) \underline{\mathbf{D}}(a')^*. \quad (6)$$

For all unitary operations u the expression under the trace in Eq. (2) can be reformulated by cyclic permutation and by inserting the factor $u^{-1}u = 1$:

$$\begin{aligned} \text{Tr}[e^{-\beta \hat{H}(\mathbf{H})} \hat{A}_k \hat{B}_i(t + i\hbar\lambda; \mathbf{H}) \hat{C}_j(t + i\hbar\lambda; \mathbf{H})] &= \text{Tr}[u^{-1} u e^{-\beta \hat{H}(\mathbf{H})} u^{-1} u \hat{A}_k u^{-1} u \hat{B}_j(t + i\hbar\lambda, \mathbf{H}) u^{-1} u C_i(t + i\hbar\lambda; \mathbf{H})] \\ &= \text{Tr}[(u e^{-\beta \hat{H}(\mathbf{H})} u^{-1})(u \hat{A}_k u^{-1})(u \hat{B}_i(t + i\hbar\lambda, \mathbf{H}) u^{-1})(u \hat{C}_j(t + i\hbar\lambda, \mathbf{H}) u^{-1})]. \end{aligned} \quad (7)$$

The four expressions grouped in parentheses can now be dealt with separately. The term containing \hat{A}_k can be rewritten using Eq. (3). For the term containing \hat{B}_j one has accordingly

$$u \hat{B}_i(t + i\hbar\lambda, \mathbf{H}) u^{-1} = \sum_m \hat{B}_m(t + i\hbar\lambda, \mathbf{H}_u) D^{(\hat{\mathbf{B}})}(u)_{mi}, \quad (8)$$

with \mathbf{H}_u the transformed field

$$u \hat{H}(\mathbf{H}) u^{-1} = \hat{H}(\mathbf{H}_u) \quad (9)$$

connected with the operation u . For the term containing $C_j(t + i\hbar\lambda, \mathbf{H})$ an analogous expression is obtained. Inserting these relations into Eq. (7) one obtains

$$\begin{aligned} \text{Tr}[e^{-\beta \hat{H}(\mathbf{H})} \hat{A}_k \hat{B}_i(t + i\hbar\lambda, \mathbf{H}) \hat{C}_j(t + i\hbar\lambda, \mathbf{H})] \\ = \sum_{lmn} \text{Tr}[e^{-\beta \hat{H}(\mathbf{H}_u)} \hat{A}_l \hat{B}_m(t + i\hbar\lambda, \mathbf{H}_u) \hat{C}_n(t + i\hbar\lambda, \mathbf{H}_u) D^{(\hat{\mathbf{A}})}(u)_{lk} D^{(\hat{\mathbf{B}})}(u)_{mi} D^{(\hat{\mathbf{C}})}(u)_{nj}]. \end{aligned} \quad (10)$$

This equation must hold for any operators \hat{A}_k , \hat{B}_j , and \hat{C}_i , i.e., also in the special case $\hat{A}_k = \hat{B}_j = \hat{C}_i = \mathbb{1}$, leading to

$$\text{Tr}(e^{-\beta \hat{H}(\mathbf{H})}) = \text{Tr}(e^{-\beta \hat{H}(\mathbf{H}_u)}). \quad (11)$$

Inserting the two last equations into Eq. (2) for the general transport coefficients, one obtains the transformation behavior of $\underline{\tau}$ under a unitary symmetry operation u :

$$\tau_{(\hat{B}_i \hat{C}_j) \hat{A}_k}(\omega, \mathbf{H}) = \sum_{lmn} \tau_{(\hat{B}_m \hat{C}_n) \hat{A}_l}(\omega, \mathbf{H}_u) D^{(\hat{\mathbf{A}})}(u)_{lk} D^{(\hat{\mathbf{B}})}(u)_{mi} D^{(\hat{\mathbf{C}})}(u)_{nj}. \quad (12)$$

A similar procedure can be applied for antiunitary operators a that contain the time-reversal T , i.e., that can be decomposed as $a = vT$ with v a unitary operator describing a pure spatial operation. For antiunitary operators cyclic permutation under the trace does not hold, but one may use the relation

$$\text{Tr}(aa') = [\text{Tr}(a'a)]^*. \quad (13)$$

This expression can be used to transform Eq. (2) in a similar way as done for Eq. (7) leading to

$$\begin{aligned} \text{Tr}[e^{-\beta \hat{H}(\mathbf{H})} \hat{A}_k \hat{B}_i(t + i\hbar\lambda, \mathbf{H}) \hat{C}_j(t + i\hbar\lambda, \mathbf{H})] &= \text{Tr}[a^{-1} a e^{-\beta \hat{H}(\mathbf{H})} a^{-1} a \hat{A}_k a^{-1} a \hat{B}_i(t + i\hbar\lambda, \mathbf{H}) a^{-1} a \hat{C}_j(t + i\hbar\lambda, \mathbf{H})] \\ &= \{ \text{Tr}[(a e^{-\beta \hat{H}(\mathbf{H})} a^{-1})(a \hat{A}_k a^{-1})(a \hat{B}_i(t + i\hbar\lambda, \mathbf{H}) a^{-1})(a \hat{C}_j(t + i\hbar\lambda, \mathbf{H}) a^{-1})] \}^*. \end{aligned} \quad (14)$$

Of the four expressions in parentheses, the second one is directly given by Eq. (4), while the first one can be rewritten by introducing \mathbf{H}_a via the definition

$$a \hat{H}(\mathbf{H}) a^{-1} = \hat{H}(\mathbf{H}_a). \quad (15)$$

Expressing the last two terms according to

$$a \hat{B}_i(t + i\hbar\lambda, \mathbf{H}) a^{-1} = \sum_m \hat{B}_m(-t + i\hbar\lambda, \mathbf{H}) D^{(\hat{\mathbf{B}})}(a)_{mi}, \quad (16)$$

which follows directly from the fact that a contains the time-reversal operation, and inserting these expressions into Eq. (14) one arrives at

$$\begin{aligned} \text{Tr} [e^{-\beta\hat{H}(\mathbf{H})} \hat{A}_k \hat{B}_i(t + i\hbar\lambda, \mathbf{H}) \hat{C}_j(t + i\hbar\lambda, \mathbf{H})] &= \sum_{lmn} \text{Tr} [e^{-\beta\hat{H}(\mathbf{H}_a)} \hat{A}_l \hat{B}_m(-t + i\hbar\lambda, \mathbf{H}_a) \hat{C}_n(-t + i\hbar\lambda, \mathbf{H}_a)]^* D^{(\hat{A})}(a)_{lk}^* \\ &\times D^{(\hat{B})}(a)_{mi}^* D^{(\hat{C})}(a)_{nj}^*. \end{aligned} \quad (17)$$

Using the relation [11]

$$\text{Tr}[e^{-\beta\hat{H}} \hat{\mathbf{A}}\hat{\mathbf{B}}(\tau)\hat{\mathbf{C}}(\tau)] = \text{Tr}[e^{-\beta\hat{H}} \hat{\mathbf{A}}(-\tau)\hat{\mathbf{B}}\hat{\mathbf{C}}] \quad (18)$$

one arrives at an expression that is completely analogous to Eq. (10):

$$\text{Tr} [e^{-\beta\hat{H}(\mathbf{H})} \hat{A}_k \hat{B}_i(t + i\hbar\lambda, \mathbf{H}) \hat{C}_j(t + i\hbar\lambda, \mathbf{H})] = \sum_{lmn} \text{Tr} [e^{-\beta\hat{H}(\mathbf{H}_a)} \hat{C}_n^\dagger \hat{B}_m^\dagger \hat{A}_l^\dagger(t + i\hbar\lambda, \mathbf{H}_a) D^{(\hat{A})}(a)_{lk}^* D^{(\hat{B})}(a)_{mi}^* D^{(\hat{C})}(a)_{nj}^*], \quad (19)$$

where

$$(\text{Tr } L)^* = \text{Tr}(L^\dagger), \quad (20)$$

with L being a linear operator was used. Again, this equation must also hold for the special case $\hat{\mathbf{A}} = \hat{\mathbf{B}} = \hat{\mathbf{C}} = \mathbb{1}$, thus

$$\text{Tr}(e^{-\beta\hat{H}(\mathbf{H})}) = \text{Tr}(e^{-\beta\hat{H}(\mathbf{H}_a)}). \quad (21)$$

Finally, inserting all these relations one obtains the transformation behavior for $\underline{\tau}$ as

$$\tau_{(\hat{B}_i \hat{C}_j) \hat{A}_k}(\omega, \mathbf{H}) = \sum_{lmn} \tau_{\hat{A}_l^\dagger (\hat{C}_n^\dagger \hat{B}_m^\dagger)}(\omega, \mathbf{H}_a) D^{(\hat{A})}(a)_{lk}^* D^{(\hat{B})}(a)_{mi}^* D^{(\hat{C})}(a)_{nj}^*, \quad (22)$$

which is the counter part of Eq. (12), but for antiunitary operators a .

It is important to note that in general the tensors $\tau_{(\hat{B}_i \hat{C}_j) \hat{A}_k}$ and $\tau_{\hat{A}_k^\dagger (\hat{B}_i^\dagger \hat{C}_j^\dagger)}$ are different objects representing different response functions which are only interrelated by Eq. (22). Accordingly, the symbols $\underline{\tau}$ and $\underline{\tau}'$ will be used below to distinguish them. Obviously the two tensors $\underline{\tau}$ and $\underline{\tau}'$ coincide only if all operators and their adjointed ones are the same, i.e., $\hat{A}_i = \hat{B}_i$ and so on.

Equations (12) and (22) relate the elements of the tensor $\underline{\tau}$ with all the elements of $\underline{\tau}$ and $\underline{\tau}'$, respectively. As mentioned above, these relations impose for each symmetry operation restrictions on the shape of $\underline{\tau}$ that determine which elements have to be zero and which are degenerate. However, to find the final shape of $\underline{\tau}$ it is not necessary to derive restrictions for all symmetry operations of the relevant space group. Instead, it is sufficient to use only a generating set of symmetry operations [2]. Finally, as was stressed by Kleiner [2], for the application of Eqs. (12) and (22) it is not necessary to know the explicit form of the operators \hat{A}_i , \hat{B}_j , and \hat{C}_k , but only their behavior under a symmetry operation expressed by Eqs. (3) and (4).

III. APPLICATIONS

A. Symmetry operations and magnetic Laue groups

For a periodic solid, the corresponding unitary symmetry operations u can be represented by the Seitz symbol [12]

$$u = \{R | t\}, \quad (23)$$

where R describes a (proper or improper) rotation and t describes a translation. The application of this symmetry operation on a three-dimensional vector \mathbf{v} is defined as

$$u \mathbf{v} = \underline{\mathbf{D}}(R) \mathbf{v} + \mathbf{t}, \quad (24)$$

where $\underline{\mathbf{D}}(R)$ is the three-dimensional matrix representation of the rotation R and \mathbf{t} is a three-dimensional translation vector. For an antiunitary symmetry operation a , the time-reversal operation T has to be considered in addition to the spatial symmetry operations. It can be included in the Seitz symbol according to

$$a = \{R | t\} T. \quad (25)$$

The transformation properties of a vector \mathbf{v} under a depend now on its behavior under space inversion and time reversal. A vector that reverses its orientation under space inversion is called a spatial vector (or polar vector), if it stays unaltered it is called a pseudovector or axial vector.

Generally, the transformation of a vector field $\mathbf{v}(\mathbf{r})$ under an arbitrary symmetry operation s is given accordingly by

$$s \mathbf{v}(\mathbf{r}) = \pm \underline{\mathbf{D}}(R) \mathbf{v}(s^{-1} \mathbf{r}), \quad (26)$$

where the sign is determined by the behavior of $\mathbf{v}(\mathbf{r})$ under time-reversal T that may be part of s . On the other hand, a pseudovector field $\mathbf{v}(\mathbf{r})$ transforms as

$$s \mathbf{v}(\mathbf{r}) = \pm \det(\underline{\mathbf{D}}(R)) \underline{\mathbf{D}}(R) \mathbf{v}(s^{-1} \mathbf{r}). \quad (27)$$

An example for this is the magnetic field \mathbf{H} . As \mathbf{H} changes sign under time reversal, the minus sign in Eq. (27) applies. In particular one has

$$I \mathbf{H} = +\mathbf{H}, \quad (28)$$

$$T \mathbf{H} = -\mathbf{H}, \quad (29)$$

for the application of space inversion I and time reversal T . In the following we will use in parallel the symbols \bar{I} and \bar{T} for I and T , respectively.

TABLE I. Magnetic point groups of category (a) and their corresponding magnetic Laue group. In parentheses the magnetic Laue group according to its old definition used by Kleiner [2] is given (see text). Because equivalent magnetic point group and Laue group symbols have not been removed (see text) there are 62 and 12 instead of 53 and 11, respectively, entries.

Magnetic point group	Magnetic Laue group
$11', \bar{1}', \bar{1}1'$	$\bar{1}1' (1')$
$21', m1', 2/m1', 2'/m, 2/m'$	$2/m1' (21')$
$2221', mm21', m'mm,$ $mmm1', m'm'm'$	$mmm1' (2221')$
$41', \bar{4}1', 4/m', 4/m1', 4'/m'$	$4/m1' (41')$
$4221', 4mm1', \bar{4}2m1',$ $\bar{4}m21', 4/m'mm, 4'/m'm'm,$ $4/mmm1', 4'/m'mm', 4/m'm'm'$	$4/mmm1' (42221')$
$31', \bar{3}', \bar{3}1'$	$\bar{3}1' (3')$
$3121', 31m1', \bar{3}'1m, \bar{3}'1m', \bar{3}1m1'$	$\bar{3}1m1' (3'2)$
$3211', 3m11', \bar{3}'m1, \bar{3}'m'1, \bar{3}m11'$	$\bar{3}m11' (3'2)$
$61', \bar{6}1', 6'/m, 6/m', 6/m1'$	$6/m1' (61')$
$6221', 6mm1', \bar{6}m21',$ $\bar{6}2m1', 6/m'mm, 6'/mm'm,$ $6'/mmm', 6/mmm1', 6/m'm'm'$	$6/mmm1' (6221')$
$231', m'\bar{3}', m\bar{3}1'$	$m\bar{3}1' (23')$
$4321', \bar{4}3m1', m'\bar{3}'m, m'\bar{3}'m', m\bar{3}m1'$	$m\bar{3}m1' (43'2)$

Taking into account the time-reversal operation, the full symmetry of a periodic solid is represented by its magnetic space group \mathcal{G} that combines all symmetry operations of the type given in Eqs. (23) and (25). Altogether there are 1651 magnetic space groups that fall into three categories [13]:

- (a) \mathcal{G} contains the time-reversal operation T as an element,
- (b) \mathcal{G} does not contain T at all, neither as a separate element nor in a combination,
- (c) \mathcal{G} contains T only in combination with another symmetry element.

Only nonmagnetic solids possess one of the 230 space groups of category (a), while magnetically ordered solids belong either to category (b) or (c). Category (b) consists of 230 space groups, isomorphic to the nonmagnetic space groups, and category (c) combines the remaining 1191 space groups.

Since the operators $\hat{\mathbf{X}}$ appearing in Eqs. (12) and (22) are translational invariant, it is sufficient to consider only the corresponding magnetic point group operations instead of all elements of the magnetic space group. If the operators representing perturbation and response behave identically under space inversion, as it is, e.g., the case for the electrical conductivity (see below), it is possible to restrict the consideration further to the corresponding magnetic Laue group of a solid that is generated by adding the inversion operation I to the crystallographic magnetic point group. This conventional definition [14] deviates from the older one used by Kleiner [2] that derives the Laue group from the corresponding crystallographic point group by removing from each improper rotation $R = P_R I$ its improper part I . For this reason we list in Tables I–III all magnetic point groups of the three categories together with their corresponding magnetic

TABLE II. Magnetic point groups of category (b) and their corresponding magnetic Laue group. In parentheses the magnetic Laue group according to its old definition used by Kleiner [2] is given (see text). Because equivalent magnetic point group and Laue group symbols have not been removed (see text) there are 37 and 12 instead of 32 and 11, respectively, entries.

Magnetic point group	Magnetic Laue group
$1, \bar{1}$	$\bar{1} (1)$
$2, m, 2/m$	$2/m (2)$
$222, mm2, mmm$	$mmm (222)$
$4, \bar{4}, 4/m$	$4/m (4)$
$422, 4mm, \bar{4}2m, \bar{4}m2, 4/mmm$	$4/mmm (422)$
$3, \bar{3}$	$\bar{3} (3)$
$312, 31m, \bar{3}1m$	$\bar{3}1m (32)$
$321, 3m1, \bar{3}m1$	$\bar{3}m1 (32)$
$6, \bar{6}, 6/m$	$6/m (6)$
$622, 6mm, \bar{6}m2, \bar{6}2m, 6/mmm$	$6/mmm (622)$
$23, m\bar{3}$	$m\bar{3} (23)$
$432, \bar{4}3m, m\bar{3}m$	$m\bar{3}m (432)$

Laue group. The symbol in parentheses gives in addition the magnetic Laue group as used by Kleiner [2].

Deriving the symbols for the magnetic point and Laue groups from those for the magnetic space groups, one may be led in some cases to two symbols that differ only concerning the sequence of the second and third generators (one of these might be a dummy 1). As this depends on the chosen coordinate system and because the shape of the response tensor may depend on this choice, both symbols are listed although being

TABLE III. Magnetic point groups of category (c) and their corresponding magnetic Laue group. In parentheses the magnetic Laue group according to its old definition used by Kleiner [2] is given (see text). Because equivalent magnetic point group and Laue group symbols have not been removed (see text) there are 52 and 13 instead of 37 and 10, respectively, entries.

Magnetic point group	Magnetic Laue group
$2', m', 2'/m'$	$2'/m' (2')$
$2'2'2', m'm2', m'm'2, m'm'm$	$m'm'm (2'2'2)$
$4', \bar{4}', 4'/m$	$4'/m (4')$
$4'2'2', 4'm'm, \bar{4}'2'm,$ $\bar{4}'m'2, 4'/mm'm$	$4'/mm'm (4'22')$
$4'22', 4'mm', \bar{4}'2m',$ $\bar{4}'m2', 4'/mmm'$	$4'/mmm' (4'22')$
$42'2', 4m'm', \bar{4}2'm',$ $\bar{4}m'2', 4/mm'm'$	$4/mm'm' (42'2')$
$312', 31m', \bar{3}1m'$	$\bar{3}1m' (32')$
$32'1, 3m'1, \bar{3}m'1$	$\bar{3}m'1 (32')$
$6', \bar{6}', 6'/m'$	$6'/m' (6')$
$6'2'2', 6'm'm, \bar{6}'m'2,$ $\bar{6}'2'm, 6'/m'm'm$	$6'/m'm'm (6'22')$
$6'22', 6'mm', \bar{6}'m2',$ $\bar{6}'2m', 6'/m'mm'$	$6'/m'mm' (6'22')$
$62'2', 6m'm', \bar{6}m'2',$ $\bar{6}2'm', 6/mm'm'$	$6/mm'm' (62'2')$
$4'32', \bar{4}'3m', m\bar{3}m'$	$m\bar{3}m' (4'32')$

completely equivalent. This applies to $\bar{3}1m1'$ and $\bar{3}m11'$ of category (a), $\bar{3}1m$ and $\bar{3}m1$ of category (b), and $4'/mm'm$ and $4'/mmm'$, $\bar{3}1m'$ and $\bar{3}m'1$, as well as $6'/m'm'm$ and $6'/m'mm'$ of category (c). Furthermore, it should be noted that for the magnetic Laue groups $2/m1'$ of category (a), $2/m$ of category (b), and $2'/m'$ of category (c), the coordinate system has been chosen according to *cell choice 1* of space group $2/m$ as documented in the *International Tables for Crystallography* [15].

B. Thermoelectric coefficients

Within linear response theory, the induced electric current density \mathbf{j} and the heat current density \mathbf{q} are given by [2]

$$\begin{pmatrix} \mathbf{j} \\ \mathbf{q} \end{pmatrix} = \begin{pmatrix} |e|\underline{\mathbf{L}}_{11} & |e|\underline{\mathbf{L}}_{12} \\ -\underline{\mathbf{L}}_{21} & -\underline{\mathbf{L}}_{22} \end{pmatrix} \begin{pmatrix} \nabla\mu \\ \frac{1}{T}\nabla T \end{pmatrix}, \quad (30)$$

with $e = |e|$ the elementary charge and the electrochemical potential μ which is related to the chemical potential μ_c and the electric potential φ via

$$\mu = \mu_c - |e|\varphi. \quad (31)$$

As explicitly demonstrated by Kleiner [2] as well as below, the coefficients $\underline{\mathbf{L}}_{ij}$ satisfy Onsager relations of the form

$$\underline{\mathbf{L}}_{11}(\mathbf{H}) = \underline{\mathbf{L}}_{11}(-\mathbf{H}), \quad (32)$$

$$\underline{\mathbf{L}}_{22}(\mathbf{H}) = \underline{\mathbf{L}}_{22}(-\mathbf{H}), \quad (33)$$

$$\underline{\mathbf{L}}_{12}(\mathbf{H}) = \underline{\mathbf{L}}_{21}^T(-\mathbf{H}). \quad (34)$$

Identifying the operators \hat{A}_i and \hat{B}_i with one of the components of the electric current density operator $\hat{\mathbf{j}}$ and the heat current density operator $\hat{\mathbf{q}}$ and setting $\hat{C}_i = 1$, Eqs. (12) and (22) reduce to the expressions given by Kleiner to investigate the symmetry properties of the thermoelectric coefficients $\underline{\mathbf{L}}_{ij}$. His derivation will be repeated here in a modified way as we use the conventional definition for the Laue group and as the results will be used later on.

Expressing the electric current density operator $\hat{\mathbf{j}} = -|e|\hat{\mathbf{v}}$ as a product of the electronic charge $-|e|$ and the velocity operator $\hat{\mathbf{v}}$ one can see that $\hat{\mathbf{j}}$ transforms as a vector that changes sign under time-reversal T and space inversion I :

$$I \hat{j}_i = -\hat{j}_i, \quad (35)$$

$$T \hat{j}_i = -\hat{j}_i. \quad (36)$$

The same relations apply for the heat current density operator $\hat{\mathbf{q}}$ [2,16]. The corresponding 3×3 matrix representation for a unitary operator $u = \{R|t\}$ and an antiunitary operator $a = \{R|t\}T$ to be used in Eqs. (12) and (22) is

$$\underline{\mathbf{D}}^{\hat{\mathbf{q}}}(u) = \underline{\mathbf{D}}^{\hat{\mathbf{q}}}(a) = \underline{\mathbf{D}}(R), \quad (37)$$

$$\underline{\mathbf{D}}^{\hat{\mathbf{j}}}(a) = \underline{\mathbf{D}}^{\hat{\mathbf{j}}}(u) = -\underline{\mathbf{D}}(R). \quad (38)$$

Equations (12) and (22) (with $\hat{C}_i = 1$) can be brought into a more convenient form by replacing every $\underline{\mathbf{D}}(R)$ by $\underline{\mathbf{D}}(R^{-1})$ and \mathbf{H} by $\mathbf{H}_{u^{-1}}$ or $\mathbf{H}_{a^{-1}}$, respectively. Thus, Eq. (12) for unitary

operators u simplifies to

$$\tau_{\hat{B}_i, \hat{A}_j}(\omega, \mathbf{H}(R)) = \sum_{kl} \tau_{\hat{B}_k, \hat{A}_l}(\omega, \mathbf{H}) D(R)_{ki} D(R)_{lj} \quad (39)$$

and Eq. (22) for antiunitary operators a to

$$\tau_{\hat{B}_i, \hat{A}_j}(\omega, -\mathbf{H}(R)) = \sum_{kl} \tau_{\hat{A}_l, \hat{B}_k}(\omega, \mathbf{H}) D(R)_{ki} D(R)_{lj}, \quad (40)$$

where

$$\mathbf{H}(R)_i = \sum_j D(P_R)_{ij} H_j. \quad (41)$$

Here we used the fact that the matrices $\underline{\mathbf{D}}(R)$ are real and that \mathbf{H} is a pseudovector. A further simplification can be achieved by splitting R in a proper rotation P_R and the space inversion I , if it is contained in R . Explicitly, this means that $R = P_R$ if R is a proper rotation and $R = P_R I$ if R is an improper rotation. For proper rotations one has $\det(\underline{\mathbf{D}}(R)) = +1$ while for improper rotations $\det(\underline{\mathbf{D}}(R)) = -1$ holds. Because the space inversion amounts to a simple multiplication with $-\mathbb{1}_3$, this splitting can be expressed by

$$\underline{\mathbf{D}}(R) = \det(\underline{\mathbf{D}}(R)) \underline{\mathbf{D}}(P_R). \quad (42)$$

Since the matrix $\underline{\mathbf{D}}(R)$ appears twice in Eqs. (39) and (40), the two factors $\det(\underline{\mathbf{D}}(R))$ compensate each other, regardless whether R is a proper or an improper rotation. Thus, the final equation for the unitary operators is

$$\tau_{\hat{B}_i, \hat{A}_j}(\omega, \mathbf{H}) = \sum_{kl} \tau_{\hat{B}_k, \hat{A}_l}(\omega, \mathbf{H}) D(P_R)_{ki} D(P_R)_{lj}, \quad (43)$$

and for antiunitary operators

$$\tau_{\hat{B}_i, \hat{A}_j}(\omega, -\mathbf{H}) = \sum_{kl} \tau_{\hat{A}_l, \hat{B}_k}(\omega, \mathbf{H}) D(P_R)_{ki} D(P_R)_{lj}. \quad (44)$$

This splitting of R enables one to consider the symmetry property of the thermogalvanic coefficients of a solid on the basis of its magnetic Laue group instead of its magnetic point group. This applies whether the conventional definition of the Laue group (see Sec. III A) is applied or that used by Kleiner [2]. In the latter case the removal of the ineffective inversion I happens already when constructing the Laue group. In the former case, one may add improper rotations $R = P_R I$, where again I is ineffective and P_R is an element of both groups. Working only with the magnetic Laue group has the obvious advantage that less cases have to be considered (see Tables I–III) as there are only 32 magnetic Laue groups, while there are 122 different crystallographic magnetic point groups.

On the basis of Eqs. (43) and (44) it is now rather straightforward to give explicit forms for the response tensors $\underline{\mathbf{L}}_{ij}$ in Eq. (30). For this purpose the abbreviations $\tau_{ij} = \tau_{\hat{A}_i, \hat{B}_j}$, $\tau'_{ij} = \tau_{\hat{B}_i, \hat{A}_j}$, and $\sigma_{ij} = \tau_{\hat{A}_i, \hat{A}_j}$ will be used, where $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ can stand for $\hat{\mathbf{j}}$ or $\hat{\mathbf{q}}$. Accordingly, $\underline{\boldsymbol{\tau}}$ and $\underline{\boldsymbol{\tau}'}$ represent either $\underline{\mathbf{L}}_{12}$ or $\underline{\mathbf{L}}_{21}$ or the other way around, and $\underline{\boldsymbol{\sigma}}$ represents $\underline{\mathbf{L}}_{11}$ or $\underline{\mathbf{L}}_{22}$, respectively, which obviously have to have the same structure. It is interesting to note that Eq. (44) can lead to restrictions on the tensor elements in addition to those imposed by Eq. (43). These hold even for the tensors of type $\underline{\boldsymbol{\tau}'}$.

In the case of a magnetically ordered solid having a magnetic space group of category (b) the restrictions to the

TABLE IV. Tensor forms for magnetic Laue groups of category (a).

Magnetic Laue group	$\underline{\tau}'$	$\underline{\sigma}$
$\bar{1}1'$	$\begin{pmatrix} \tau_{xx} & \tau_{yx} & \tau_{zx} \\ \tau_{xy} & \tau_{yy} & \tau_{zy} \\ \tau_{xz} & \tau_{yz} & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{pmatrix}$
$2/m1'$	$\begin{pmatrix} \tau_{xx} & 0 & \tau_{zx} \\ 0 & \tau_{yy} & 0 \\ \tau_{xz} & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & \sigma_{xz} \\ 0 & \sigma_{yy} & 0 \\ \sigma_{xz} & 0 & \sigma_{zz} \end{pmatrix}$
$mmm1'$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{yy} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$\bar{3}1', 4/m1', 6/m1'$	$\begin{pmatrix} \tau_{xx} & -\tau_{xy} & 0 \\ \tau_{xy} & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$\bar{3}1m1', \bar{3}m11', 4/mmm1', 6/mmm1'$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$m\bar{3}1', m\bar{3}m1'$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{xx} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{xx} \end{pmatrix}$

shape of the thermogalvanic tensors result only from the application of Eq. (43) as there are no antiunitary operations. As a consequence, all tensors $\underline{\sigma}$, $\underline{\tau}$, and $\underline{\tau}'$ have the same shape. Accordingly, only the shape of $\underline{\tau}$ is given in Table V, that is in full agreement with Kleiner's Table IV [2].

For magnetic space groups belonging to category (a) or category (c) Eq. (44) has to be applied in addition to Eq. (43). In general, this leads to different symmetry restrictions for the tensors of type $\underline{\tau}'$ and $\underline{\sigma}$. The resulting shape of the tensors for category (a) is given in Table IV. These results agree with those given by Kleiner's Table V [2], apart from those for the Laue groups $\bar{3}1'$, $4/m1'$, and $6/m1'$. Since the magnetic Laue groups in category (a) differ from those in (b) only by the time-reversal $1'$ as an element of its own, the tensor shapes in Table IV

TABLE V. Tensor forms for magnetic Laue groups of category (b).

Magnetic Laue group	$\underline{\tau}$
$\bar{1}$	$\begin{pmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{pmatrix}$
$2/m$	$\begin{pmatrix} \tau_{xx} & 0 & \tau_{xz} \\ 0 & \tau_{yy} & 0 \\ \tau_{zx} & 0 & \tau_{zz} \end{pmatrix}$
mmm	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{yy} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$
$\bar{3}, 4/m, 6/m$	$\begin{pmatrix} \tau_{xx} & \tau_{xy} & 0 \\ -\tau_{xy} & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$
$\bar{3}1m, \bar{3}m1, 4/mmm, 6/mmm$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$
$m\bar{3}, m\bar{3}m$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{xx} \end{pmatrix}$

TABLE VI. Tensor forms for magnetic Laue groups of category (c). The tensor forms for the groups $4'/mm'm$ and $4'/mmm'$ are related to each other by a rotation of the coordinate system around the principal (z) axis by $\pi/4$.

Magnetic Laue group	$\underline{\tau}'$	$\underline{\sigma}$
$2'/m'$	$\begin{pmatrix} \tau_{xx} & -\tau_{yx} & \tau_{zx} \\ -\tau_{xy} & \tau_{yy} & -\tau_{zy} \\ \tau_{xz} & -\tau_{yz} & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ -\sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & -\sigma_{yz} & \sigma_{zz} \end{pmatrix}$
$m'm'm'$	$\begin{pmatrix} \tau_{xx} & -\tau_{yx} & 0 \\ -\tau_{xy} & \tau_{yy} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$4'/m$	$\begin{pmatrix} \tau_{yy} & -\tau_{xy} & 0 \\ -\tau_{yx} & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$4'/mm'm'$	$\begin{pmatrix} \tau_{xx} & -\tau_{xy} & 0 \\ -\tau_{xy} & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$4'/mmm'$	$\begin{pmatrix} \tau_{yy} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$\bar{3}1m', \bar{3}m'1, 4'/mm'm', 6'/mm'm'$	$\begin{pmatrix} \tau_{xx} & \tau_{xy} & 0 \\ -\tau_{xy} & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$6'/m'$	$\begin{pmatrix} \tau_{xx} & -\tau_{xy} & 0 \\ \tau_{xy} & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$6'/m'm'm', 6'/m'mm'$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$m\bar{3}m'$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{xx} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{xx} \end{pmatrix}$

alternatively can be deduced from those in Table V simply by considering in addition the effect of $1'$. In case of $\underline{\sigma}$ this can lead to additional restrictions (degeneracies and zero elements) since in this case the antiunitary time reversal connects $\underline{\sigma}$ with itself according to its definition given above. For the thermoelectric tensor on the other hand, this just states the usual Onsager relations as expressed by $\tau'_{ij}(\mathbf{H}) = \tau_{ji}(-\mathbf{H})$ [see Eq. (34)]. Table VI gives the results for category (c) that are in full agreement with those given by Kleiner's Table VI [2]. Obviously the results presented in Tables IV–VI fulfill the Onsager relations given by Eqs. (32) to (34) that are not postulated *a priori*.

Kleiner's scheme was applied here to derive the shape of the tensors representing homogeneous bulk systems. However, it may also be applied to investigate the symmetry restrictions on the so-called layer-resolved conductivity tensor $\underline{\sigma}^{IJ}$ with I and J labeling atomic layers of a two-dimensional periodic system [17]. This concept may be used for example in the context of electrical transport in layered GMR systems [18,19] or magneto-optical properties of surface systems [20,21]. Another extension of Kleiner's scheme is the discussion of nonlinear effects [17].

C. Shape of the spin conductivity tensor

Spin transport as reflected for example by the spin Hall effect is usually described by use of the spin conductivity σ_{ij}^k

that gives the current density along direction i for the spin polarization with respect to the k axis induced by an electrical field along the j axis. Within a single-particle description of the electronic structure the Kubo formalism leads for σ_{ij}^k to an expression analogous to the Kubo-Bastin equation [22] for the electrical conductivity [23,24]:

$$\sigma_{ij}^k = \frac{i\hbar}{V} \int_{-\infty}^{\infty} dE f(E) \text{Tr} \left\langle \hat{J}_i^k \frac{dG^+(E)}{dE} \hat{J}_j \delta(E - \hat{H}) - \hat{J}_i^k \delta(E - \hat{H}) \hat{J}_j \frac{dG^-(E)}{dE} \right\rangle. \quad (45)$$

Here \hat{H} is the Hamiltonian of the system, $G^+(E)$ and $G^-(E)$ are the corresponding retarded and advanced Green functions, and \hat{J}_j is the ordinary electrical current density operator. A straightforward definition for the spin current density operator $\hat{J}_i^k = \frac{1}{2}\{\hat{v}_i, \sigma_k\}$ consists in the anticommutator of the conventional velocity operator \hat{v}_i and the Pauli spin matrix σ_k [25]. As the spin conductivity is caused by spin-orbit coupling a coherent relativistic implementation of Eq. (45) seems to be more appropriate. This implies that the electrical current density operator $\hat{J}_j = -|e|c\alpha_j$ is expressed in terms of the 4×4 Dirac α matrices [26]. A corresponding expression for the spin current density operator $\hat{J}_i^k = \hat{T}_k \hat{J}_i$ was suggested by Vernes *et al.* [27] that involves the spatial part \hat{T}_k of the spin polarization operator introduced by Bargmann and Wigner [28]:

$$\hat{T}_k = \beta \Sigma_k - \frac{1}{mc} \gamma_5 \Pi_k. \quad (46)$$

Here β , γ_5 , Σ_k are again standard 4×4 Dirac matrices, m is the electron mass, and Π_k stands for the kinetic momentum [26]. In fact this approach was adopted by Lowitzer *et al.* [23,24] when dealing with the spin Hall effect of disordered alloys. However, as mentioned above, for an investigation of the shape of a response tensor the explicit expressions for the involved operators are not relevant but only their behavior under symmetry operations. Both definitions of \hat{J}_i^k given above consist of a combination of the current density operator \hat{J}_i with an operator that represents the spin polarization of an electron. In contrast to \hat{J}_i [see Eq. (38)], the latter one (e.g., \hat{T}_k) transforms as a pseudovector which changes sign under time reversal. Accordingly, one has for the transformation matrices

$$\underline{\mathbf{D}}^{(\hat{T}_k)}(u) = \det(R) \underline{\mathbf{D}}(R), \quad (47)$$

$$\underline{\mathbf{D}}^{(\hat{T}_k)}(a) = -\det(R) \underline{\mathbf{D}}(R), \quad (48)$$

corresponding to Eqs. (5) and (6).

Identifying now $\hat{A}_i = \hat{J}_i$, $\hat{B}_j = \hat{J}_j$, and $\hat{C}_k = \hat{T}_k$ in Eqs. (12) and (22) one finds the behavior of σ_{ij}^k under unitary transformations

$$\sigma_{ij}^k = \sum_{lmn} \det(R) D(R)_{li} D(R)_{mj} D(R)_{nk} \sigma_{lm}^n, \quad (49)$$

and under antiunitary transformations

$$\sigma_{ij}^k = - \sum_{lmn} \det(R) D(R)_{li} D(R)_{mj} D(R)_{nk} \sigma_{lm}^n, \quad (50)$$

respectively. In analogy to the treatment of thermoelectric coefficients presented above one may again split the rotation

R into its proper part P_R and, if present, improper part as given in Eq. (42). The resulting equation for unitary transformations is then

$$\sigma_{ij}^k = \sum_{lmn} D(P_R)_{li} D(P_R)_{mj} D(P_R)_{nk} \det(R)^4 \sigma_{lm}^n \quad (51)$$

$$= \sum_{lmn} D(P_R)_{li} D(P_R)_{mj} D(P_R)_{nk} \sigma_{lm}^n \quad (52)$$

and

$$\sigma_{ij}^k = - \sum_{lmn} D(P_R)_{li} D(P_R)_{mj} D(P_R)_{nk} \sigma_{lm}^n \quad (53)$$

for antiunitary transformations, respectively. As a consequence, as found for the thermoelectric coefficients by Kleiner [2] also for the spin conductivity tensor it is sufficient to consider the magnetic Laue group of the solid.

Using Eqs. (52) and (53) the shape of the inverse spin conductivity tensor was determined with the results given in the left column of Tables VII–IX for magnetic Laue group of categories (a)–(c).

It should be noted that these tables for the spin conductivity and its inverse effect can be seen as an equivalent to the generalized Onsager relations derived by Kleiner for the thermogalvanic transport tensors $\underline{\tau}$ and $\underline{\tau}'$. In particular, they give the shape of the tensors $\underline{\sigma}^k$ representing the Onsager reciprocal quantity, e.g., the inverse spin Hall effect (ISHE) as counterpart to the spin Hall effect (SHE), as discussed for instance by Shi *et al.* [25].

Because $\hat{\mathbf{j}}$ and $\hat{\mathbf{q}}$ have the same transformation properties and because the tensors $\tau_{(\hat{B}_i \hat{C}_j) \hat{A}_k}$ and $\tau_{\hat{A}_i (\hat{B}_m \hat{C}_n)}$ in Eq. (22) are different objects in both cases, the tensor shapes for tensors describing the connection between spin currents and heat currents have exactly the same shape as those tabulated in the left column of Tables VII, VIII, and IX.

For convenience, it is possible to alter the notation of these symmetry-restricted matrices in such a way that the symmetry of the spin conductivity tensor is easier to recognize at first sight. This is achieved by removing the time-reversal operator $1'$ from every antiunitary operation (or by omitting it if it appears on its own). However, this reduction leads to the loss of the specific meaning, i.e., the generalized Onsager relations, contained in the tensors $\underline{\sigma}^k$. The reduced tensors are tabulated for categories (a), (b), and (c) in the right column of Tables VII, VIII, and IX, respectively.

As discussed in the context of the charge and heat current in response to an electric field the corresponding operators \hat{J}_i and \hat{q}_i have the same symmetry properties. As a consequence the tensors $\underline{\mathbf{L}}_{11}$ and $\underline{\mathbf{L}}_{22}$ in Eq. (30) have the same shape given by $\underline{\sigma}$ in Tables IV–VI. For the same reason the tensor representing the spin current induced by a thermal gradient has the same shape as that connected with an electric field with both given by the right column of Tables VII–IX.

One of the major benefits of Tables VII–IX is obviously the prediction of all possible linear response spin transport phenomena induced by an electric field or a thermal gradient for any solid based on its magnetic space group. The occurrence of antisymmetric off-diagonal elements in the tensor $\underline{\sigma}^k$ ($k = x, y, z$) in Table VII implies that the transverse spin Hall effect is, in principle, allowed by symmetry in any paramagnetic

solid. However, one has to stress that in case of the magnetic Laue groups $\bar{1}$, $2/m$, and $mmm1'$ the shape of the tensor is not purely antisymmetric. The same is true for a ferromagnetic solid according to Tables VIII and IX, i.e., the spin Hall and Nernst effects are symmetry allowed in any magnetic solid as well (again not all cases show purely antisymmetric elements). Considering as an example a ferromagnetic cubic solid with the magnetic Laue group $4/m\bar{m}'m'$ (e.g., bcc-Fe or fcc-Ni with the magnetization along the z direction) its spin conductivity tensor is very different from the form of its nonmagnetic counterpart with $m\bar{3}m1'$. For the nonmagnetic case only the elements σ_{ij}^k with $i \neq j \neq k \neq i$ are nonzero. In addition, these are the same for a cyclic permutation of (i, j, k) and change the sign for an anticyclic one. For the ferromagnetic case additional off-diagonal elements may appear, with the degeneracies depending on the spin projection component k , and the tensors are no longer purely antisymmetric. In particular one notes that there are diagonal elements that imply the occurrence of a longitudinal spin current induced by an electric field that in general will depend on whether the electric field is along (σ_{zz}^z) or perpendicular ($\sigma_{xx}^z = \sigma_{yy}^z$) the magnetization. These tensor elements are obviously responsible for the occurrence of the spin-dependent Seebeck effect [29]. Interestingly, for a nonmagnetic solid there are several magnetic space groups that also imply a nonvanishing diagonal tensor element σ_{ii}^k , i.e., a longitudinal current along the direction of the applied electric field or thermal gradient. This was demonstrated recently by corresponding numerical work on nonmagnetic $(\text{Au}_{1-x}\text{Pt}_x)_4\text{Sc}$ showing that the longitudinal spin conductivity can be comparable in magnitude to the transverse spin Hall conductivity [30].

D. Implementation

The symmetry restrictions imposed on the thermogalvanic tensors by Eqs. (43) and (44) as well as on the spin conductivity tensor by Eqs. (52) and (53), respectively, were determined by means of a Python script that is based on the *Computational Crystallography Toolbox*, *cctbx* [31]. Although this library provides support only for the nonmagnetic crystallographic operations, it is also of great value when dealing with magnetic solids. To determine the magnetic space group of a solid all possible magnetic space groups are simply scanned through and checked which fits to the system under investigation. The corresponding symmetry operations are taken from the magnetic space group data file `magnetic_data.txt` [13,32]. Once the magnetic point group has been found, the u and a operators needed for an application of Eqs. (43) and (44) or Eqs. (52) and (53), respectively, are fixed. Going through all elements of the magnetic point group leads to a set of

connecting equations between the tensor elements which can then be solved to get the shape of the tensor. For these symbolic calculations the *SymPy* library [33] is used. Although in principle the generators of a magnetic point group are sufficient to obtain all symmetry restrictions, it turned out to be more convenient to apply all symmetry operations since the *cctbx* library and the magnetic space group tables do not provide a set of generators.

Finally, it should be mentioned that the results for the spin conductivity tensor $\underline{\sigma}^z$ for the spin polarization along the z axis have been checked against the output of the SPRKKR program package [34] that allows calculating this tensor on the basis of the relativistic Kubo formalism [35]. For all investigated magnetic Laue groups of categories (a) ($\bar{1}'$, $mm1'$, $2/m1'$, $4/m1'$, $4/m\bar{m}m1'$, $6/m\bar{m}m1'$, $m\bar{3}m1'$), (b) ($4/m$), and (c) ($2'/m'$, $m'm'm$, $4/m\bar{m}'m'$, $\bar{3}m'1$, $6/m\bar{m}'m'$) the numerical results for $\underline{\sigma}^z$ were found to be completely in line with the analytical predictions given in Tables VII–IX.

IV. SUMMARY

Kleiner's scheme to determine the shape of a linear response tensor has been extended to deal with more complex situations. The resulting set of equations has been used to revise the shape of the electric charge and heat conductivity tensors for all magnetic space groups. It was demonstrated that for this only the magnetic Laue group of a solid is relevant. This also holds for the spin conductivity tensor that is used among other to discuss the longitudinal spin-dependent Seebeck effect as well as the transverse spin Hall and Nernst effects. Results for all magnetic space groups are presented in an easily accessible way, by giving in addition to the tensors $\underline{\sigma}^k$ containing the generalized Onsager relations also the reduced tensor forms $\underline{\sigma}^k$. Furthermore, the axis conventions of the space groups are preserved when constructing the magnetic Laue groups and therefore, although redundant, the tensor forms are given in both coordinate systems whenever there is an ambiguity. Interestingly, several magnetic Laue groups for nonmagnetic solids were identified that should show a new longitudinal spin transport phenomenon [30]. Finally, it should be stressed that the scheme presented here can be applied straightforwardly to any other response function. Examples relevant for spintronics and related fields are the response tensors representing spin-orbit torque, Gilbert damping, or the Edelstein effect [36].

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