Magnetic Spin Hall Effect in Collinear Antiferromagnets

Rafael González-Hernández,1,2 Libor Šmejkal,2,3,4 Karel Výborný,3 Yuta Yahagi,5 Jairo Sinova,2,3 and Jakub Železný3

1Grup de Investigació en Física Aplicada, Departamento de Física, Universidad del Norte, Barranquilla, Colombia
2Institut für Physik, Johannes Gutenberg Universität Mainz, D-55099 Mainz, Germany
3Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, 162 00 Praha 6 Czech Republic
4Faculty of Mathematics and Physics, Charles University in Prague, Ke Karlovu 3, 121 16 Prague 2, Czech Republic
5Department of Applied Physics, Tohoku University, Sendai, Japan

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The spin Hall effect as well as the recently discovered magnetic spin Hall effect are among the key spintronics phenomena as they allow for generating a spin current by a charge current. The mechanisms for this charge-spin conversion normally rely on either the relativistic spin-orbit coupling or non-collinear magnetic order, both of which break spin conservation. This limits the spin diffusion length and the charge-spin conversion efficiency connected to these mechanisms due to the internal competition between spin current generation and spin loss. In this work we show that the magnetic spin Hall effect can exist in collinear antiferromagnets and that in some antiferromagnets it exists even without spin-orbit coupling, thus allowing for a spin-charge conversion in a system which conserves spin. We find a very large spin current (∼ 8600 (ℏ/e)S/cm) and magnetic spin Hall angle (∼ 25%) in antiferromagnetic RuO2. In addition, we present a symmetry classification of the conventional and magnetic spin Hall effects and identify general symmetry requirements for their existence.

I. INTRODUCTION

One of the major recent breakthroughs in spintronics has been the discovery of powerful mechanisms for generating spin currents by charge currents or vice versa through the so-called spin Hall effect (SHE) and the inverse SHE [1]. These processes are commonly referred to as charge-spin or spin-charge conversion. The SHE occurs when an unpolarized charge current transverses a material with strong spin-orbit coupling (SOC) or non-collinear magnetic order [2], leading to a perpendicular spin current where up spins accumulate at one edge of the sample and down spins accumulate at the other edge [3] (see Fig.2a,b). Although the SHE was predicted theoretically in 1971 [4], it was only observed experimentally in GaAs in 2004 [5, 6]. SHE borrows directly from the physics and mechanism of the anomalous Hall effect (AHE) and correspondingly much of their description are parallel [2]. The SHE and the inverse SHE are widely used in spintronics. For example, the SHE is commonly used to electrically switch the magnetization in ferromagnetic films [8]. ISHE is a practical tool for the electrical detection of spin currents or, for example, for the generation of THz radiation from fs spin current pulses [9].

Recently a new type of a spin to charge conversion mechanism has been theoretically predicted [10] and consequently experimentally observed [11] in non-collinear antiferromagnetic systems. This so-called magnetic spin Hall effect (mSHE) differs from the conventional SHE in that it can only exist in magnetic materials. Specifically this means that whereas the SHE is even under reversal of the magnetic order, the mSHE is odd or equivalently that the SHE is even under time-reversal, whereas the mSHE is odd. This also means that the mSHE is necessarily a dissipative effect, whereas the SHE can be in principle non-dissipative. Microscopically, on the simplest level, the mSHE can be described by a Boltzmann equation and is proportional to the relaxation time, whereas the SHE is in the clean limit independent of the relaxation time and can be described by the intrinsic formula.

The SHE normally originates from the SOC, which is a relativistic interaction that couples spin to the orbital degree of freedom. In non-collinear systems, however, it can exist even in the absence of the SOC, as the non-collinear magnetic order plays a similar role to the SOC by breaking the spin rotation symmetry and coupling the spin to the lattice [2]. Similarly, the mSHE has been predicted to exist in the non-collinear antiferromagnets even in the absence of the SOC, whereas in simple collinear ferromagnets, the SOC is required [10]. Similar phenomenology is observed in other effects such as the AHE [2] [12] or the orbital magnetic moment [13]. These effects require SOC in collinear ferromagnets, but can also exist in the absence of SOC in non-collinear (or specifically non-coplanar) magnetic systems.

In this work we show that the mSHE can also exist in collinear antiferromagnets and that in some it can exist even in absence of the relativistic SOC. In this way it differs from the conventional SHE, which can only exist without SOC in non-collinear magnetic systems. This difference is crucial since in non-collinear magnetic systems no component of spin is a good quantum number and spin is thus not conserved, whereas in collinear magnetic systems without SOC, the component of spin along the magnetic order is a good quantum number and is thus conserved. Therefore, the mSHE in collinear antiferromagnets allows for charge-spin and spin-charge conversion in a system that conserves spin.

The intrinsic contribution to the conventional SHE can be understood as precession of the spin in spin-orbit field.
In non-collinear magnetic systems, the origin is similar, except the precession is not due to spin-orbit field, but due to non-collinear magnetic order. In a collinear system without SOC, the spin is conserved and this mechanism is thus not possible. In contrast, the mSHE originates from a redistribution of electrons, which does not rely on a change of the spin. The non-relativistic origin of mSHE in collinear antiferromagnet RuO$_2$ is illustrated in Fig. 1. When the relativistic SOC is neglected, the spin is a good quantum number and the wavefunctions of the system can be split up into spin-up and spin-down states. As illustrated in Fig. 1(a), the spin-up and spin-down Fermi surfaces are anisotropic and rotated with respect to each other. When electric field is applied along the $x$ or $y$ directions, the resulting spin-up and spin-down currents will flow at an angle with respect to the electric field (see Fig. 1(b)). As a consequence, the charge current flows in the direction of the electric field, whereas the spin current is perpendicular to it. The reason for the anisotropy of the Fermi surfaces is that the Ru sublattices have locally anisotropic crystalline environments, as illustrated on Figs. 1(c),(d). Because of this crystalline anisotropy, the electrons at the A and B Ru sublattices are flowing at an angle to the electric field and because of the antiferromagnetic order, this is also reflected in the spin-up and spin-down current directions.

The discussion in this work focuses mainly on spin currents that are transverse to the charge current (i.e. flowing in the transverse direction). This is the context in which the term spin-charge conversion is mainly used. However, both the time-reversal-even ($T$-even) spin currents (SHE) and the time-reversal-odd ($T$-odd) spin currents (mSHE) can also have a longitudinal component. The different types of spin currents are illustrated in Fig. 2, however, we note that the terminology of the various contributions is not very well established. In ferromagnets, the $T$-odd longitudinal component is usually referred to as the spin-polarized current and is primarily utilized for spin-transfer torque in magnetic junctions [14, 15]. In analogy with ferromagnets, the $T$-odd longitudinal current in non-collinear antiferromagnets has been referred to as a spin-polarized current [10]. The transverse component has been later referred to as the magnetic SHE and this is a terminology that we also use here. In a recent work, the term mSHE has been used only in relation to the antisymmetric component of the $T$-odd spin currents and it has been shown that this antisymmetric component is connected to spin current vorticity in the reciprocal space [16]. Here we use the term mSHE even for the symmetric component since the distinction between the symmetric and antisymmetric component is not as fundamental as in the case of charge conductivity. No special name has been used for the longitudinal component of the $T$-even currents [17]. We simply refer to it as the longitudinal SHE here, although it could be argued that this is not a good term since a longitudinal spin current is not really a “Hall effect”. It is not clear whether it is meaningful to use a different terminology for the longitudinal and transverse components since they can have the same origin, however, from practical point of view, the two are very different, since they are used for different purposes.

We demonstrate the existence of the mSHE and the spin-polarized current in two antiferromagnetic systems: MnTe and RuO$_2$ by utilizing symmetry arguments and ab-initio linear response calculations. We find that whereas in MnTe these $T$-odd spin currents exist only when the relativistic SOC is included, in RuO$_2$ they are present even in the non-relativistic limit. To understand the general symmetry requirements for the existence of the $T$-odd spin currents, we have performed a general classification of the $T$-odd and $T$-even spin currents. We find that the $T$-odd spin currents are allowed in all magnetic systems with broken $T\tau$ (time-reversal combined with translation) or $\mathcal{PT}$ (time-reversal combined with inversion) symmetries, or equivalently in all systems with broken time-reversal symmetry in the Laue group. Our result means that the $T$-odd spin currents can also exist in truly antiferromagnetic systems, i.e. in systems where no net magnetic moment is allowed.

![FIG. 1. Origin of the non-relativistic spin current in RuO$_2$. a) Simplified non-relativistic spin-up and spin-down Fermi surfaces of RuO$_2$ and the spin-up and spin-down currents originating from redistribution of electrons due to applied electric field. The dotted lines illustrate the redistribution of electrons. b) Schematic of the spin-up and spin-down currents caused by electric field applied along the [010] direction. c) Top-down view of the crystal structure of RuO$_2$ with charge density isosurface, illustrating the anisotropy of the Ru A and B sublattices. d) Same as in c) but with isosurfaces of spin-up and spin-down densities shown in red and blue respectively.](image-url)
Even
Odd
Longitudinal Spin Current
Transversal Spin Current

FIG. 2. Sketch showing the longitudinal and transversal spin-current generated by the \( T \)-even and \( T \)-odd components of the spin conductivity tensor. Note that the spin-polarization of spin currents shown here is just an illustration, other directions of spin-polarization can also occur depending on the symmetry of the material. a) Longitudinal SHE - \( T \)-even current that flows in the same direction as the charge current. b) SHE - \( T \)-even current that flows in a transverse direction to the charge current. c) Spin-polarized current - \( T \)-odd current flowing in the same direction as the charge current. d) mSHE - odd current flowing in the transverse direction to the charge current.

II. SPIN CURRENTS IN RUO\(_2\) AND MNTe

In order to study the mSHE in collinear AFMs, we carried out \textit{ab-initio} calculations within the density-functional theory (DFT) framework as implemented in the Vienna \textit{ab-initio} simulation package (VASP) \cite{18}. We have studied collinear antiferromagnets RuO\(_2\) and MnTe using the GGA+U method, as used in recent reports \cite{19,20}. We have performed both non-relativistic calculations and calculations with the relativistic spin-orbit coupling self-consistently included. Electron wave functions were expanded in plane waves up to a cut-off energy of 500 eV and a grid of 12x12x16 k-point has been used to sample the irreducible Brillouin zone. The calculated band-structures of RuO\(_2\) and MnTe are shown in Fig. 3 a),b).

We evaluate the charge and spin conductivities within the linear response theory using the Kubo formula with the constant scattering-rate \( \Gamma \) approximation \cite{10} as implemented in the Wannier-linear-response code \cite{21}. Within the linear response the charge conductivity is described by the conductivity tensor: \( j_i = \sigma_{ij}E_j \), where \( j \) is the current, \( E \) is the electric field and \( \sigma_{ij} \) is the conductivity tensor. Similarly, the spin-conductivity is described by a spin-conductivity tensor \( \sigma_{ij}^{\text{sp}} \), where \( i \) corresponds to the spin-polarization of the spin current, \( k \) to the direction of spin current flow and \( j \) to the direction of electric field. The Kubo formula within the constant \( \Gamma \) approximation can be split in two contributions given by

\[
\chi^I = -\frac{e\hbar}{\pi} \text{Re} \sum_{k,m,n} \frac{\left\langle u_n(k)\hat{A}u_m(k)\hat{v}_j u_n(k)\right\rangle \Gamma^2}{(E_F - E_n(k))^2 + \Gamma^2} (E_F - E_m(k))^2 + \Gamma^2)
\]

\[
\chi^{II} = -2e\hbar \text{Im} \sum_{k,m\neq n} \frac{\left\langle u_m(k)\hat{A}u_m(k)\hat{v}_j u_n(k)\right\rangle (E_n(k) - E_m(k))^2}{E_n(k) - E_m(k)^2}
\]

Here \( \chi \) is either \( \sigma_{ij} \) or \( \sigma_{ij}^{\text{sp}} \). \( u_n(k) \) are the Bloch functions of a single band \( n \), \( k \) is the Bloch wave vector, \( \varepsilon_n(k) \) is the band energy, \( E_F \) is the Fermi energy, \( \hat{v}_j \) is the velocity operator, \( \hat{A} \) is the current density operator \( \hat{A} = -e\vec{v}_j/V \) in the case of charge conductivity and the spin-current operator \( \hat{A} = \frac{1}{2}\{\hat{s}_i, \hat{v}_j\} \) in the case of the spin-conductivity. In order to evaluate the Kubo formula, we have used an effective tight-binding Hamiltonian constructed in the maximally localized Wannier basis \cite{22} as a post-processing step of the DFT calculations. For the integration, a dense 32x32x3 k-mesh was used.

For small \( \Gamma \), the Eq. (1) scales as \( 1/\Gamma \) and corresponds to the Boltzmann formula with a constant relaxation time. Eq. (2) is the so-called intrinsic contribution, which is \( \Gamma \) independent. As discussed in Ref. \cite{10}, for charge conductivity, Eq. (1) is even under time-reversal and Eq. (2) is odd, whereas for the spin conductivity the situation is reversed. For charge conductivity, Eq. (1) corresponds to the ordinary conductivity and Eq. (2) corresponds to the AHE. For spin conductivity, Eq. (1) corresponds to the spin-polarized current and the mSHE and Eq. (2) corresponds to the SHE. In this work we mainly focus on the \( T \)-odd spin conductivity. However, for comparison we also calculate the SHE and the AHE and in order to evaluate the spin-charge conversion efficiency, we also calculate the ordinary charge conductivity.

RuO\(_2\) is a conductive transition metal oxide with orthorhombic rutile-type structure \cite{19}. The primitive unit cell contains two Ru atoms surrounded by six O atoms that form a distorted octahedron. Recently, it was found that the Ru atoms can exhibit a collinear antiferromagnetic order and it was predicted that the AHE exists in the material \cite{23}. Because the AHE is in this case caused by a combination of symmetry breaking by the antiferromagnetic order and by the crystal, this effect was referred to as the crystal Hall effect in Ref. \cite{23}. The origin of antiferromagnetism in RuO\(_2\) was recently studied in Ref. \cite{24}. MnTe is a collinear antiferromagnet that crystallizes in the hexagonal NiAs-type structure. It has recently been used to demonstrate anisotropic magnetoresistance in an antiferromagnet \cite{25}. It is a semiconductor, with a 1.46 eV indirect bandgap, however, the thin films used for the anisotropic magnetoresistance experiments exhibit an unintentional p-doping \cite{25}. We model this by shifting the Fermi level, however, since the experimentally observed doping corresponds to only a very small
shift, for which it is very difficult to accurately evaluate the response, we instead consider a larger shift of 0.25 eV in most calculations.

We now focus on the $T$-odd spin currents. For RuO$_2$ calculations we use $\Gamma \approx 6.6 \, \text{meV}$, which is obtained by comparing the calculated conductivity (see Fig. ??) with the average experimental conductivity at 300K ($\sim 28400 \, \text{S/cm}$) [29]. For MnTe we have estimated the $\Gamma$ value to be close to 45 $\text{meV}$ by comparing the relaxation time ($\tau = h/2\Gamma$) with the experimental value ($\tau = m^*_e\mu/e$) of the electron mobility measures [27]. We give the general form of the spin-conductivity tensors in RuO$_2$ and MnTe in Table I We find that with SOC the $T$-odd spin currents are allowed by symmetry in both materials. This is confirmed by calculations shown in Figs. 3b and 3d for RuO$_2$ and MnTe, respectively. Here, we rotate the Néel vector in-plane for both RuO$_2$ and MnTe. We note that unlike the AHE, the $T$-odd spin currents do not vanish in RuO$_2$ when the Néel vector is oriented along the $z$ direction, however, in analogy with Ref. [23] we nevertheless consider the in-plane rotation of the Néel vector. When the SOC is turned off we find that in MnTe no $T$-odd spin currents exist. In RuO$_2$ we find that some components of the $T$-odd spin currents remain even in the non-relativistic calculation. This is confirmed by symmetry analysis, using the so-called spin groups which describe symmetry of magnetic systems in absence of SOC. The symmetry of the $T$-odd spin conductivity tensors in absence of SOC is summarized in Table. II in Appendix A.

The origin of non-relativistic spin current in RuO$_2$ is illustrated in Fig. 1 Since RuO$_2$ is a collinear magnetic material, in absence of SOC, the component of spin along the magnetic order direction is a good quantum number, i.e. it is a conserved quantity. As a consequence the eigenstates of the Hamiltonian can be separated into spin-up and spin-down states and the electrical current can be separated into spin-up and spin-down currents. Since spin-flip scattering is usually much smaller than spin conserving scattering, the two currents can be approximately treated as independent. This is known as the two current model and it is commonly used to describe the spin-polarized current in ferromagnets. In the case of ferromagnets, the two currents typically flow in the same direction, but are different in magnitude, thus they result in a longitudinal spin current (i.e. the spin-polarized current) and no transverse spin current.

In RuO$_2$ when electric field is applied along the [100] or [010] direction, it creates a spin-up and spin-down currents flowing at an angle with respect to the electric field. This results into an unpolarized longitudinal charge current and pure transverse spin current. A similar result is found for electric field along the [010] direction, however, interestingly we find that for the [110] and [-110] direction, the spin current is flowing in the same direction as the charge current and the charge current is thus spin-polarized. This is fully in agreement with the symmetry analysis shown in Appendix A.

The magnitude of SHE is often given in terms of the spin Hall angle (SHA), which is defined as $(e/\hbar)\sigma_{jk}/\sigma_{kk}$, where $\sigma_{kk}$ is the longitudinal electrical conductivity. The
SHA can be used the same way for the magnetic SHE or any other spin current. We find that in RuO$_2$ the magnetic SHA angle for the largest component is very large, $\approx 25^\circ$. This component corresponds to a configuration such that the electric field and the spin current are both in the $xy$ plane and the spin-polarization is given by the Néel vector direction. In comparison the SHA in MnTe is much smaller. The likely explanation of this is that in MnTe the origin of the effect is the SOC, which is relatively small effect even in materials containing heavy elements. In contrast, in RuO$_2$, the origin is the exchange interaction only, which is much stronger. In absolute values the spin conductivity in RuO$_2$ is very large $\approx 8600 (\hbar/e)$S/cm for the largest component. For comparison, in the widely used Pt, the intrinsic spin Hall conductivity is only 2180 $(\hbar/e)$S/cm and the spin Hall angle is only several percent (though a large variation between experimental results exists). Furthermore, as shown in Fig. 4, the SHC can reach even larger values when the Fermi level is shifted. For a shift of -0.6 eV, the spin conductivity becomes 25000 $(\hbar/e)$S/cm. This is in contrast to Pt, where the Fermi level is exactly at the maximum of the Fermi level conductivity [28]. Furthermore, we note that our calculations utilize $\Gamma$ corresponding to room temperature resistivity. In RuO$_2$ the resistance at low temperatures was found to be 100 to 4000 times lower than the room temperature resistivity. Since for small $\Gamma$ the conductivity and $T$-odd spin conductivity depend on $\Gamma$ as $1/\Gamma$, this will correspond to an equivalent increase in the spin-conductivity and the $T$-odd spin conductivity will thus be much higher at low temperatures.

### III. SYMMETRY CLASSIFICATION

The $T$-odd spin currents have been studied in ferromagnets (primarily in the context of the spin-polarized current), in non-collinear antiferromagnets of the Mn$_3$X type [10, 11] and in the collinear antiferromagnets discussed in this work. All of these systems are systems in which the AHE exists. Conversely in simple antiferromagnets no $T$-odd spin currents are allowed by symmetry and neither is the AHE. This thus begs the question of whether the symmetry of the $T$-odd spin currents is somehow related to the symmetry of the AHE and what are the general requirements for the existence of the $T$-odd spin currents. For AHE, the symmetry requirements can be easily formulated. AHE can exist only in systems in which a net magnetic moment is allowed [29]. This is because AHE can be expressed as a $T$-odd pseudovector and thus it transforms the same as a magnetic moment. We note, however, that in some AHE systems such as the ones discussed here, the net magnetic moment itself is very small and not directly related to AHE.

In general, the shape of linear response tensor for a particular material in an external electric field is determined by the crystal symmetry and magnetic order, which is, in the presence of SOC, described by the magnetic space group. Since the spin conductivity is invariant under translation and inversion, it is sufficient to consider the magnetic Laue groups. These are groups obtained from the magnetic space groups by removing translations and adding inversion to every group (alternatively the inversion could instead be removed). The symmetry of the full spin conductivity tensors was already given in Ref. [30] for all magnetic Laue groups. In that work no separation of the $T$-even and $T$-odd currents was done and thus no information about the requirements for the existence of $T$-odd spin currents can be obtained. Here we study the symmetry of the $T$-even and $T$-odd spin conductivity tensors separately using a method described in Ref. [31] and the Symmetr code. We use here the conventional labeling of Laue groups also used in Seemann et al. [30], where also the corresponding point groups to each Laue group are given.

The Laue groups can be split into three categories. The groups of category (a) are groups which contain time-reversal as a separate element. These are groups which correspond either to a nonmagnetic crystal or to an antiferromagnet invariant under $T\tau$ or $PT$ symmetries. The groups of category (b) are groups in which no symmetry operation contains time-reversal. The groups of category (c) are groups in which some symmetry operations contain time-reversal, but time-reversal is not present separately. All groups of category (b) and (c) correspond to magnetic systems.

The SHE is allowed by symmetry in any material when...
SOC is present. We give the general form of the $T$-even spin-conductivity tensors for Laue groups of categories (a), (b) and (c) in Tables III, IV, V respectively. Since both the AHE and the $T$-odd spin currents are odd under time-reversal, they have to vanish in Laue groups of category (a). We give the general shape of the $T$-odd spin conductivity tensors for groups (b) and (c) in Tables VI, VII respectively. To compare with AHE, we also give the allowed magnetic moment for each Laue group. From this the AHE can be determined, since it holds for the AHE current that $j = g \times E$, where $g$ has the same symmetry as $M$. Interestingly, we find that, unlike for the AHE, the symmetry of the $T$-odd spin currents is unrelated to the magnetization and is much less restrictive. Whereas the AHE is present in only 10 of the 21 Laue groups of category (b) and (c), the $T$-odd spin-conductivity is present in all 21 groups. This also means that the $T$-odd spin currents can exist in truly antiferromagnetic systems in which no net magnetic moment is allowed by symmetry. There results are also evidenced by our calculations. As shown in Fig. 3, for example, the AHE vanishes in every high-symmetry direction, whereas the $T$-odd spin currents remain. We also find that in all of the 21 Laue groups, apart from the group m-3m, both transverse and longitudinal components are allowed for some directions of electric field. In the group m-3m, the $T$-odd spin currents are transverse for any direction of electric field and thus no spin-polarized current can exist in materials with this symmetry.

The symmetry requirements for the existence of $T$-odd spin currents can be thus formulated in a simple way. These spin currents will be present in every system in which the $T$, $T\tau$ and $PT$ symmetries are broken. They are therefore different than the AHE, which has much more stricter symmetry requirements for its existence. It can be said, however, that in every system in which the $T$-odd spin currents exist, the AHE will also exist if the magnetic order is rotated out of high symmetry direction. This is because rotating the magnetic order out of high symmetry direction breaks all rotation symmetries.

Similar classification for existence of spin conserving pure transverse spin currents is significantly more involved and is left to future work. Nevertheless, some rules can be formulated. Since the ordinary SHE can only exist without SOC in a non-collinear magnetic system it cannot exist in a system that conserves spin. Thus only the mSHE can be considered for the transverse spin currents and the above rules, therefore, also apply. This means that a collinear magnetic system with broken $T\tau$ and $PT$ is needed. Although a non-relativistic transverse spin current could also exist in a low symmetry ferromagnet, for spin-charge conversion a pure spin current is utilized, which would be hard to achieve in a ferromagnet. Therefore, we can generally say that to achieve a spin conserving spin-charge conversion, we need a collinear antiferromagnet that breaks the $T\tau$ and $PT$ symmetries and that has asymmetric crystalline environment at each sublattice that allows for existence of a transverse current at each sublattice.

V. DISCUSSION

The limitations of spin-charge conversion mechanisms based on SOC or non-collinear magnetism are quite fundamental. Since these mechanisms do not conserve spin it is simply not possible to have an efficient spin charge conversion based on these mechanisms in system that approximately conserves spin. This has important consequences. First, it limits the possible functionalities of devices since it means that the spin diffusion length is very short and the spin to charge conversion thus always happens very close to the interface and no long term spin transport through the spin to charge conversion material is possible. Second, theoretical description and experimental study of such spin currents is problematic in absence of spin conservation. This is part of the reason why the origin of the spin-orbit torque in bilayer systems is still not fully understood despite years of intensive research [8]. In contrast the spin-transfer torque, which can be described with the two-current model, is much better understood [14, 15]. Third, the short spin diffusion length significantly reduces the efficiency of the spin-charge conversion. Although the spin current itself does not depend on the spin relaxation length, for practical purposes only the spin accumulation or spin torque due to the spin current are utilized and these strongly depend on the spin relaxation length [32].

With the presently proposed mechanism, no such limitations exist. Although no system conserves spin perfectly, the advantage of the mechanism proposed in this work is that the spin to charge conversion efficiency can be tuned independently of the spin conservation and the mechanism could thus in principle exist in systems in which the SOC is small and the spin approximately conserved, which might result in larger efficiency of a current induced spin accumulation or spin torque.

A spin current with a similar origin to the nonrelativistic mSHE in RuO$_2$ has been recently theoretically studied in an organic antiferromagnet [33]. Organic materials have very small SOC, which could result in much longer spin relaxation lengths than in RuO$_2$, but on the other hand the studied organic antiferromagnet has very low Néel temperature. We also note than in contrast to what is claimed in Ref. [33], the conventional SHE does not require broken inversion symmetry; is not necessarily represented by antisymmetric tensor and does not always originate from SOC. Instead, the core difference between the non-relativistic mSHE in collinear AFMs and the conventional SHE is the transformation under time-reversal.

From a general point of view, utilizing magnetic materials for spin-charge conversion could have some advantages over the common approach based on the SHE in nonmagnetic materials. The symmetry of the conventional SHE in nonmagnetic systems is quite restricted. In most commonly used materials, the SHE has a sym-
metry such that the direction of electric field, direction of the spin current flow and the spin-polarization of the spin current are all perpendicular. This limits its possible applications. For example, in bilayer systems the spin current flows in the out-of-plane direction, which means that the spin-polarization for the conventional SHE is in-plane. The magnetization of the ferromagnetic layer is typically out-of-plane, however, and then for the most efficient switching based on the antidamping torque, out-of-plane polarization of the spin current is required. In contrast, the symmetry of the ordinary and mSHE in magnetic systems is less restricted. Even more importantly, the spin currents generated in magnetic systems can be controlled by manipulating the magnetic order. This is especially true for the mSHE as illustrated in Fig. 3, but also applies for the ordinary SHE, as shown in Appendix C. This could allow for completely new functionalities. We note that in the case of the non-relativistic mSHE in RuO$_2$ the only dependence on the Néel vector direction is in that the spin-polarization of the spin current is given by the Néel vector direction. Although this is quite simple dependence, it could also be useful since it allows, for example, for reversing the sign of the spin current by reversing the magnetic order.

The $\mathcal{T}$-odd spin currents and the AHE share some common symmetry requirements and because of that they often occur in similar materials. The two effects are not otherwise related, however. As discussed in Ref. [10], they have a different microscopic origin and as shown in this work, the general symmetry requirements for their existence are different. The only similarity is that both effects require breaking of the $\mathcal{T}$, $\mathcal{T}\tau$ and $\mathcal{PT}$ symmetries. Whereas the $\mathcal{T}$ symmetry is broken by any magnetic order, the later two are often present in antiferromagnetic systems. In the case of the non-collinear AFMs the $\mathcal{T}\tau$ and $\mathcal{PT}$ are broken by the non-collinear magnetic order, whereas in the case of RuO$_2$ and MnTe they are broken by the collinear magnetic order together with the non-magnetic atoms, as discussed in detail in [23].

The direct mSHE discussed in this work allows for converting a charge current into a spin current. As with the SHE, the existence of the direct mSHE effect directly implies the existence of the inverse effect, which allows for converting a spin current into a current charge current. We focus only on the direct effect here since its theoretical description is simpler, however, the inverse effect can be directly obtained from the direct effect through the Onsager relations [30]. Crucially, the existence of a large direct effect also implies existence of a large inverse effect.

We have mostly discussed the transverse spin currents here (i.e., the mSHE), however, our calculations show that the longitudinal spin currents are also present in the studied systems and are in fact intimately connected to the transverse currents. As mentioned previously, the longitudinal current can be understood as a spin-polarized current. The spin-polarized currents are also very relevant for spintronics since they are utilized for the most widely used spintronics devices: the ferromagnetic spin-valves and tunneling junctions. As discussed in Ref. [10] the antiferromagnetic spin-polarized currents could likely be used for the same purpose.

V. CONCLUSIONS

Based on symmetry analysis and ab-initio calculations we find that $\mathcal{T}$-odd spin currents that were recently found in non-collinear antiferromagnets can also exist in collinear antiferromagnetic systems. We identify two antiferromagnetic materials in which they are exist: MnTe and RuO$_2$. Both the longitudinal component, corresponding to the spin-polarized current, and transverse component, corresponding to the mSHE are present, similarly to the non-collinear antiferromagnets. Our results show that in RuO$_2$ the $\mathcal{T}$-odd spin currents survive even when no relativistic SOC is included. In such a case, since RuO$_2$ is a collinear magnetic system, the net spin is conserved. This thus allows for a spin-charge conversion in a spin-conserving system, which could improve efficiency of spin-charge conversion devices or even allow for new spintronics functionalities. We predict a large $\approx 25\%$ magnetic spin Hall angle in RuO$_2$, which together with the non-relativistic origin of the $\mathcal{T}$-odd spin currents, makes this a very interesting spin-charge conversion material. We identify a general symmetry requirements for the existence of the $\mathcal{T}$-odd spin currents. We find that they are allowed in all magnetic materials with broken $\mathcal{T}\tau$ or $\mathcal{PT}$ symmetries, or equivalently in all materials that have broken time-reversal symmetry in the Laue group.

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Appendix A: Symmetry of spin-conductivity tensors in RuO$_2$ and MnTe

Here we list the general form of spin-conductivity tensors in RuO$_2$ and MnTe, obtained using the Symmetry code [34]. The method is described in Ref. [31] for symmetry with SOC and Ref. [2] for the symmetry without SOC. All the results are given in cartesian coordinate systems. In RuO$_2$ this is simply a coordinate system oriented along the principal axes of the crystal. In MnTe, this is a coordinate system such that $x$ is oriented along the [1000] direction and $z$ along the [0001] direction.

|     | $\sigma^x$ | $\sigma^y$ | $\sigma^z$ |
|-----|------------|------------|------------|
| RuO$_2$ $\mathbf{n}[001]$ | (0 0 0 0)  | (0 0 $\sigma_{yx}$ 0) | (0 $\sigma_{yx}$ 0 0) |
|     | (0 $\sigma_{yx}$ 0 0) | (0 0 0 0) | (0 $\sigma_{yx}$ 0 0) |
|     | (0 0 0 0)  | (0 $\sigma_{yx}$ 0 0) | (0 0 0 0) |

| RuO$_2$ $\mathbf{n}[100]$ | (0 $\sigma_{yx}$ 0 0) | (0 0 0 0) | (0 $\sigma_{yx}$ 0 0) |
|     | (0 0 0 0)  | (0 $\sigma_{yx}$ 0 0) | (0 0 0 0) |
|     | (0 0 0 0)  | (0 $\sigma_{yx}$ 0 0) | (0 0 0 0) |
| MnTe $\mathbf{n}[0001]$ | (0 0 0 0)  | (0 $\sigma_{yx}$ 0 0) | (0 $\sigma_{yx}$ 0 0) |
|     | (0 0 0 0)  | (0 $\sigma_{yx}$ 0 0) | (0 0 0 0) |
|     | (0 0 0 0)  | (0 $\sigma_{yx}$ 0 0) | (0 0 0 0) |

| MnTe $\mathbf{n}[100]$ | (0 0 0 0)  | (0 $\sigma_{yx}$ 0 0) | (0 $\sigma_{yx}$ 0 0) |
|     | (0 0 0 0)  | (0 $\sigma_{yx}$ 0 0) | (0 0 0 0) |
|     | (0 0 0 0)  | (0 $\sigma_{yx}$ 0 0) | (0 0 0 0) |

TABLE I: Symmetry of spin-conductivity tensors in RuO$_2$ and MnTe in the presence of SOC.

|     | $\sigma^x$ | $\sigma^y$ | $\sigma^z$ |
|-----|------------|------------|------------|
| RuO$_2$ $\mathbf{n}[001]$ | (0 0 0 0)  | (0 0 0 0) | (0 $\sigma_{yx}$ 0 0) |
|     | (0 0 0 0)  | (0 0 0 0) | (0 $\sigma_{yx}$ 0 0) |
|     | (0 0 0 0)  | (0 0 0 0) | (0 0 0 0) |
| MnTe $\mathbf{n}[0001]$ | (0 0 0 0)  | (0 0 0 0) | (0 $\sigma_{yx}$ 0 0) |
|     | (0 0 0 0)  | (0 0 0 0) | (0 0 0 0) |
|     | (0 0 0 0)  | (0 0 0 0) | (0 0 0 0) |

TABLE II: Symmetry of spin-conductivity tensors in RuO$_2$ and MnTe without SOC. The direction of $\mathbf{n}$ for MnTe is arbitrary.

Appendix B: Symmetry tables

All tensors are given in cartesian coordinate systems. These are defined the same way as in Ref. [31]. The cartesian systems are defined in terms of the conventional basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ (see the International Tables for Crystallography [33]). The choice of the cartesian system is straightforward for the orthorhombic, tetragonal and cubic groups. The tensors for the triclinic group 1 have a completely general form and the choice of the coordinate system is thus irrelevant for this group. For hexagonal and trigonal groups, we choose the right-handed coordinate system that satisfies $\mathbf{x} = \mathbf{a}/|\mathbf{a}|$, $\mathbf{z} = \mathbf{c}/|\mathbf{c}|$. For the monoclinic groups we use the unique axis $b$ setting $\mathbf{b} = \mathbf{b}/|\mathbf{b}|$ and choose the right-handed coordinate system that satisfies $\mathbf{x} = \mathbf{a}/|\mathbf{a}|$, $\mathbf{y} = \mathbf{b}/|\mathbf{b}|$.

| Laue group | $\sigma^x$ | $\sigma^y$ | $\sigma^z$ |
|------------|------------|------------|------------|
| -11'       | (0 $\sigma_{yx}$ $\sigma_{xz}$ $\sigma_{yy}$) | (0 $\sigma_{yx}$ $\sigma_{yz}$ $\sigma_{zz}$) | (0 $\sigma_{yx}$ $\sigma_{yz}$ $\sigma_{zz}$) |
| 2/m1'      | (0 $\sigma_{yx}$ 0 $\sigma_{yz}$) | (0 $\sigma_{yx}$ 0 $\sigma_{yz}$) | (0 $\sigma_{yx}$ 0 $\sigma_{yz}$) |
| Laue group | $\sigma^x$ | $\sigma^y$ | $\sigma^z$ |
|------------|-----------|-----------|-----------|
| -11'       | $\sigma_{xx}$ $\sigma_{xy}$ $\sigma_{xz}$ | $\sigma_{yz}$ $\sigma_{yy}$ $\sigma_{yz}$ | $\sigma_{zz}$ $\sigma_{zy}$ $\sigma_{zz}$ |
|            | $\sigma_{xy}$ $\sigma_{yx}$ $\sigma_{xy}$ | $\sigma_{yz}$ $\sigma_{yy}$ $\sigma_{yz}$ | $\sigma_{zz}$ $\sigma_{zy}$ $\sigma_{zz}$ |
| 2/m1'      | $\sigma_{xx}$ $\sigma_{xy}$ $\sigma_{xz}$ | $\sigma_{yz}$ $\sigma_{yy}$ $\sigma_{yz}$ | $\sigma_{zz}$ $\sigma_{zy}$ $\sigma_{zz}$ |
|            | $\sigma_{yz}$ $\sigma_{yx}$ $\sigma_{zz}$ | $\sigma_{yz}$ $\sigma_{yy}$ $\sigma_{zz}$ | $\sigma_{zz}$ $\sigma_{zy}$ $\sigma_{zz}$ |
| m-31'      | $\sigma_{xx}$ $\sigma_{xy}$ $\sigma_{xz}$ | $\sigma_{yz}$ $\sigma_{yy}$ $\sigma_{yz}$ | $\sigma_{zz}$ $\sigma_{zy}$ $\sigma_{zz}$ |
| m-31'      | $\sigma_{xx}$ $\sigma_{xy}$ $\sigma_{xz}$ | $\sigma_{yz}$ $\sigma_{yy}$ $\sigma_{yz}$ | $\sigma_{zz}$ $\sigma_{zy}$ $\sigma_{zz}$ |

*TABLE III: T-even part of the spin-conductivity tensor, Laue groups of category (a)*
| Laue group | $\sigma^x$ | $\sigma^y$ | $\sigma^z$ |
|-----------|-----------|-----------|-----------|
| $2'/m'$   | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ |
| $m'm'm$   | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ |
| $4'/m$    | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ |
| $4'/mm'm$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ |
| $4'/mm'm$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ |
| $-31m'$   | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ |
| $6'/m'$   | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ |
| $6'/mm'm$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ |
| $m-3m'$   | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ |

TABLE IV: $T$-even part of the spin-conductivity tensor, Laue groups of category (b)

| Laue group | $\sigma^x$ | $\sigma^y$ | $\sigma^z$ | $M$ |
|-----------|-----------|-----------|-----------|-----|
| -1        | $\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$ | $\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$ | $\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$ | $(M_x \ M_y \ M_z)$ |
| $2/m$     | $\begin{pmatrix} 0 & \sigma_{xz} & 0 \\ \sigma_{yz} & 0 & \sigma_{zy} \\ 0 & \sigma_{zy} & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & \sigma_{xz} & 0 \\ \sigma_{yz} & 0 & \sigma_{zy} \\ 0 & \sigma_{zy} & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & \sigma_{xz} & 0 \\ \sigma_{yz} & 0 & \sigma_{zy} \\ 0 & \sigma_{zy} & 0 \end{pmatrix}$ | $(0 \ M_y \ 0)$ |
| mmm       | $\begin{pmatrix} 0 & 0 & \sigma_{yz} \\ 0 & 0 & \sigma_{zy} \\ \sigma_{zy} & \sigma_{zy} & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & \sigma_{yz} \\ 0 & 0 & \sigma_{zy} \\ \sigma_{zy} & \sigma_{zy} & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & \sigma_{yz} \\ 0 & 0 & \sigma_{zy} \\ \sigma_{zy} & \sigma_{zy} & 0 \end{pmatrix}$ | $(0 \ 0 \ 0)$ |
| $4/m$     | $\begin{pmatrix} 0 & 0 & \sigma_{zz} \\ 0 & 0 & \sigma_{zz} \\ \sigma_{zz} & \sigma_{zz} & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & \sigma_{zz} \\ 0 & 0 & \sigma_{zz} \\ \sigma_{zz} & \sigma_{zz} & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & \sigma_{zz} \\ 0 & 0 & \sigma_{zz} \\ \sigma_{zz} & \sigma_{zz} & 0 \end{pmatrix}$ | $(0 \ 0 \ M_z)$ |
| 4/mmm     | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \sigma_{zz} \\ \sigma_{zz} & \sigma_{zz} & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \sigma_{zz} \\ \sigma_{zz} & \sigma_{zz} & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \sigma_{zz} \\ \sigma_{zz} & \sigma_{zz} & 0 \end{pmatrix}$ | $(0 \ 0 \ 0)$ |

TABLE V: $T$-even part of the spin-conductivity tensor, Laue groups of category (c)
### TABLE VI: T-odd part of the spin-conductivity tensor, Laue groups of category (b)

| Laue group | $\sigma^t$ | $\sigma^u$ | $\sigma^z$ | M        |
|------------|-------------|-------------|-------------|----------|
| 2'/m'      | (σ_{xxx} 0 0) | (σ_{yyz} 0 0) | (σ_{zzz} 0) | (M_x M_z) |
| m'm'm      | (0 0 0) | (0 0 0) | (0 0 0) | (0 0 M_z) |
| 4'/m       | (0 0 0) | (0 0 0) | (0 0 0) | (0 0 M_z) |
| 4'/mm'm    | (0 0 0) | (0 0 0) | (0 0 0) | (0 0 M_z) |
| 4/mm'm'    | (0 0 0) | (0 0 0) | (0 0 0) | (0 0 M_z) |
| -3m        | (σ_{xxx} 0 0) | (σ_{yyz} 0 0) | (σ_{zzz} 0) | (0 0 M_z) |
| 6'/m'      | (σ_{xxx} 0 0) | (σ_{yyz} 0 0) | (σ_{zzz} 0) | (0 0 M_z) |
| 6'/m'm'm   | (0 0 0) | (0 0 0) | (0 0 0) | (0 0 M_z) |

### TABLE VII: T-odd part of the spin-conductivity tensor, Laue groups of category (c)

Appendix C: Angular dependence of SHE
FIG. 5. Angular dependence of SHE components ($\sigma^x$, $\sigma^y$ and $\sigma^z$) for a) RuO$_2$ and b) MnTe AFMs, when the Néel vector $\mathbf{n}$ is rotated in the $xy$-plane. $\Phi$ denotes the in-plane angle from the $x$-axis. Only the largest components are shown and the energy was set to 0.25 eV below the valence band maximum for the case of MnTe.

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