Spin-orbit torques due to extrinsic spin-orbit scattering of
topological insulator surface states: out-of-plane magnetization

Mohsen Farokhnezhad 1, Reza Asgari 2,3 ,∗ and Dimitrie Culcer 1

1 School of Nanoscience, Institute for Research in Fundamental Sciences, IPM, Tehran 19395-5531, Iran
2 School of Physics, Institute for Research in Fundamental Sciences, IPM, Tehran 19395-5531, Iran
3 School of Physics, University of New South Wales, Kensington, NSW 2052, Australia

Abstract

The origins of the spin-orbit torque (SOT) at ferromagnet/topological insulator interfaces are incompletely understood. The theory has overwhelmingly focussed on the Edelstein effect due to the surface states in the presence of a scalar scattering potential. We investigate here the contribution to the SOT due to extrinsic spin-orbit (SO) scattering of the surface states, focusing on the case of an out-of-plane magnetization. We show that SO scattering brings about a sizable renormalization of the field-like SOT, which exceeds 20% at larger strengths of the extrinsic SO parameter. The resulting SOT exhibits a maximum as a function of the Fermi energy, magnetization, and extrinsic SO strength. The field-like SOT decreases with increasing disorder strength, while the damping-like SOT is independent of the impurity density. With experimental observation in mind we also determine the role of extrinsic SO scattering on the anomalous Hall effect. Our results suggest extrinsic SO scattering is a significant contributor to the surface SOT stemming from the Edelstein effect when the magnetization is out of the plane.

1. Introduction

The discovery of spin-orbit torques (SOTs) [1–13] has attracted enormous interest from the perspectives of both basic science and industrial applications, as it represents a very promising way to electrically and locally manipulate a magnetic devices at the nanoscale. For high-performance magnetic memory, logic, and oscillators, strong SOTs can enable ultrafast, energy-efficient modulation of magnetization. The strong spin-orbit (SO) interaction [14, 15], which relates electron orbital and spin degrees of freedom, and the exchange interaction, which couples electron spin and a magnetic moment in a ferromagnet, combine to produce a powerful mechanism for manipulating magnetic spin textures [16–19]. The general form of the non-equilibrium spin polarization $s(r,t)$ can be deduced by considering moving electrons in the presence of both an inhomogeneous non-equilibrium magnetization $M(r,t)$ and a electric field $E(t)$. The gradient expansion of $s(r,t)$ can be written in terms of $M$ and $E$ by assuming that the fields are slow and smooth on the spatial and temporal scales set by the electron scattering time and the mean free path. Thus we have

$$s_i = K_{ij}E_j + R_{ij}E_j \nabla_i M_k + \ldots$$

where the tensor $K$ leads to the SOT via e.g. Rashba or Dresselhaus SO interactions [20]. Note that without SO interactions, simple symmetry considerations lead to zero $K$. The tensor $R$ represents spin-transfer torques that occur when a spin-polarized current flows from a paramagnet through a perfect interface into a ferromagnet and the direction of the spin-transfer torque depends on the polarity of the current flow [21, 22]. Positive current, electrons flowing from the free layer to the fixed layer, favours anti-parallel alignment between the two ferromagnetic layers, while negative current, electrons flowing from the fixed layer to the free layer, favours parallel alignment. Notice that the fixed and free layers refer to magnetic layers with stationary and non-stationary magnetic dynamics against spin torque originating from spin-polarized current. In practice the fixed layer is considerably thicker than the free layer. The origin of the spin transfer torque is a transfer of spin angular momentum from the conduction electrons.
Considerable controversy continues to surround the origins of the SOT in TIs. The relative contributions of surface and bulk states have been under scrutiny [38], including a recent study by some of us [39]. Our focus in the present work is on the surface states. It is known that these contribute to the spin torque via the Rashba-Edelstein effect [40–42] and via the spin transfer torque caused by the inhomogeneity in the magnetization [43, 44]. With the exception of the brief discussion in [38], the role of extrinsic SO scattering in the surface state contribution has not been addressed systematically, a fact that we seek to remedy here. Our study is motivated by the knowledge that, in materials with strong band structure SO interactions such as TIs, extrinsic spin–orbit coupling in the impurity scattering potential is necessarily large. Therefore, it is normal to expect a large extrinsic contribution in TIs [45, 46] because SO dominates the surface state spectrum of TI. Extrinsic SO scattering results in the deflection of electrons via two extensively studied mechanisms. The first is skew scattering [47–49]. The skew scattering mechanism consists of asymmetric scattering of up and down spins. For a scalar band structure it arises in the second Born approximation, though for TIs and systems with strong band structure SO interactions in general skew scattering is already present in the first Born approximation. The second mechanism is side jump scattering [50], which describes the lateral displacement of the electron centre of mass during scattering events, again having opposite signs for up and down spins. The surface contribution to the SOT in a realistic ferromagnet/TI structure is determined by the chiral spin textures as well as by scalar and SO scattering, and their individual roles need to be elucidated.

In this paper, we investigate the SOT in a hybrid system comprising spin–momentum locked massless Dirac fermions in TIs [51–56] interacting with a ferromagnetic layer [57], taking into account both intrinsic and extrinsic SO interactions. The magnetization is taken to be out of the plane, as in figure 1, while the in-plane case will be considered in a future publication. Although the strength of the extrinsic spin–orbit coupling is not known for TI, its form is straightforwardly deduced by symmetry considerations, and estimates are based on the regime of applicability of the theory. We determine the SOT in the presence of a homogeneous magnetization, building on the formalism introduced in [58] by considering extrinsic impurity scattering in the broader context of ferromagnetic materials. The microscopic SOT is decomposed into two parts: a damping-like SOT and a field-like SOT around momenta at the interface. Our calculations show that the field-like and damping-like SOTs are dependent on the Fermi energy, the external magnetization strength and the extrinsic impurity scattering and in addition, SOT is strongly nonlinear in terms of the extrinsic SO scattering for not small Fermi energy, given by equation (22). At a low extrinsic SO scattering strength, \( \lambda = \lambda_0 k_F^2 \), as well as \( M/\varepsilon_F \), the field-like SOT behaves like \( \tau_{DL} \sim \varepsilon_F M (1 + \lambda)/\varepsilon_F \) and the damping-like torque is given by \( \tau_{DL} \sim M^2 (1 + \lambda)/\varepsilon_F \) where \( \tau \) is the electron relaxation time. Moreover, they can be tuned to their maximum value by adjusting the \( M, \varepsilon_F \) and \( \lambda \). The field-like SOT component decreases in a disordered system, despite the fact that the strength of damping-like SOT component is independent of the impurity density.

Since in a realistic sample individual contributions to the SOT are difficult to disentangle, we also consider the fingerprints of extrinsic SO scattering in the anomalous Hall effect (AHE) [59–64]. We show...
that the anomalous Hall resistivity is influenced by extrinsic SOT scattering, and its parameter dependence may offer clues as to the importance of extrinsic processes in a particular sample. Whereas the anomalous Hall conductivity is independent on the impurity in a case of short-range impurity scattering, it depends on a highly nonlinear on impurity parameter in the case of the extrinsic SO scattering.

This paper is organized as follows. In section 2, we present the model Hamiltonian in the presence of extrinsic SO scattering. The quantum kinetic theory is discussed in section 3, including the electric field correction to the scattering term and corrections to the density matrix up to the sub-leading term in the impurity density. The SOT and AHE in the presence of short-range and extrinsic SO scatterings are presented in sections 4 and 5, respectively. Finally, we summarize our main results in the concluding part of the manuscript.

2. Model Hamiltonian and theory

TIs exhibit strong SO coupling both in the band structure and in the impurity potentials. We consider the surface state of a 3D TI in the presence of magnetization $M$ where its direction is perpendicular to the plane: a ferromagnet with magnetization perpendicular to the 2D plane is placed on a TI in figure 1, and thus the magnetization opens a gap in the surface state spectrum of the TI [65–67]. The exchange coupling between the magnetic moments and the conduction electron spins is represented by the term $M\sigma_z$ where $\sigma$ is the vector of Pauli matrices representing the spin operators of conduction electrons. The band Hamiltonian that describes low-energy excitations in the surface of 3D TIs is given by [68, 69]

$$
H_0 = \hbar v_F (k_x \sigma_y - k_y \sigma_x) + M\sigma_z,
$$

(1)

where $v_F$ is the effective Fermi velocity and $k$ is the momentum vector of electrons. We neglected the higher order warping factors and solely concentrated on the impact of extrinsic SO scattering since we are addressing low-Fermi energy, where the impact of warping terms would be minimal. The warping terms could result in some novel SOT equations at higher Fermi energies [70]. The eigenvalues of $H_0$ are $\varepsilon_k = \pm \sqrt{(\hbar v_F k)^2 + M^2}$, where $\pm$ labels conduction/valence band and the eigenstates are $|\psi_k\rangle = \frac{1}{\sqrt{2}}(e^{i\theta_k} \sqrt{1 + \frac{\lambda_0}{\xi_k}}, -e^{i\theta_k} \sqrt{1 - \frac{\lambda_0}{\xi_k}})$ where $\xi_k = M/\lambda_0$ with $\lambda_0 = \sqrt{(\hbar v_F k)^2 + M^2}$, $s = \pm 1$, and $\theta_k = \arctan(k_y/k_x)$.

The total Hamiltonian describing the conduction electrons is

$$
H = H_0 + V(\mathbf{r}) + U(\mathbf{r}),
$$

(2)

where $V(\mathbf{r})$ represents the electrostatic potential which has the form $V(\mathbf{r}) = e\mathbf{E} \cdot \mathbf{r}$, implying a uniform electric field $\mathbf{E}$, which corresponds to the overwhelming majority of experimental setups. Also, $U = U(\mathbf{r})$ represents the disorder scattering potential for the conduction electrons. In order to capture general behaviour of SOT in the system, we consider short-range scattering together with extrinsic SO scattering. For short-range scalar scattering, we consider $U_0(\mathbf{r}) = \sum_i u_0 \delta(\mathbf{r} - \mathbf{R}_i)$, where $\mathbf{R}_i$ denote random locations of the impurities and $u_0$ is a parameter that measures the strength of the disorder potential [58]. The average over impurity configurations $\langle U_0(\mathbf{r}) \rangle = 0$. Extrinsic SO scattering [71] is contained in the following term

$$
U_{\text{so}}(\mathbf{r}) = \lambda_0 \sigma \cdot \nabla U_0 (\mathbf{r}) \times \mathbf{p},
$$

(3)

where $\mathbf{p}$ is the momentum operator and $\lambda_0$ is the effective extrinsic SO impurity scattering strength. The matrix elements of the impurity potentials in reciprocal space are $U_0^{\mathbf{k}\mathbf{k'}} = \langle s, \mathbf{k}| U_0 (\mathbf{r}) |s', \mathbf{k'} \rangle$. The extrinsic SO scattering term can be assumed as a random effective magnetic field, which depends on an electron’s incident and scattered wave vectors. $\lambda_0$ can have either sign. Moreover, it is assumed that $\lambda_0 \ll 1$, and this term is typically treated in perturbation theory. Finally, the disorder potential including scalar and SO impurities reads as

$$
U_0^{\mathbf{k}\mathbf{k'}} = u_0 \sum_i \mathbf{e}^\mathbf{q} \mathbf{R}_i \langle u_0^i \rangle \left[ \sigma_0 + i\lambda_0 \sigma \cdot (\mathbf{k} - \mathbf{k'}) \right] |u_0^i\rangle |u_0^{i'}\rangle,
$$

(4)

where $\sigma_0$ is the $2 \times 2$ in spin space and $\mathbf{q} = \mathbf{k'} - \mathbf{k}$. If $|\mathbf{k}| = |\mathbf{k'}| = k_F$ and assuming that there are no spatial correlations in the disorder potential, the scattering matrix elements will be

$$
U_0^{\mathbf{k}\mathbf{k'}} = u_0 (\mathbf{e}^\mathbf{q}) \left[ \sigma_0 + i\lambda \sigma_2 \sin \gamma \right] |u_0^i\rangle |u_0^{i'}\rangle,
$$

(5)

where $\lambda = \lambda_0 k_F^2$ and $\gamma = \theta_{k'} - \theta_k$. Averaging over impurity configurations, the first-order term in the potential vanishes due to the randomness of the impurity locations as usual, while the second-order term

3
where \( m' \) and \( m''' \) are spin indices and \( n_i \) indicating the impurity concentration.

3. Quantum kinetic theory

The density matrix \( \rho = f_k + g_0 \) characterizes the system considered in equation (2), where \( f_k \) is averaged over disorder configurations and has matrix elements connecting different bands, and \( g_0 \) is the fluctuating part. For the disorder-averaged component in equilibrium, the density matrix obeys the quantum kinetic equation [72]

\[
\frac{\partial f_k}{\partial t} + \frac{i}{\hbar}[H_{0k}, f_k] + I_0(f_k) = \frac{eE_{ext}}{\hbar} \frac{Df_k}{Dk} - J_E(f_k),
\]

where the covariant derivative is as follows:

\[
\frac{D}{\partial k} = \frac{\partial}{\partial k} - i[R_k, f_k]
\]

where \( R_k \) is the Berry connection. In order to solve equation (7), the density matrix is divided into band-diagonal and off-diagonal parts, namely \( f_k = n_k + S_k \) [72, 73]. The band diagonal term \( n_k \) represents the fraction of carriers in a given band and is essentially the solution to the ordinary Boltzmann equation, while \( S_k \) contains the effect of interband coherence. \( I_0(f_k) \) is the collision integral due to the impurity potential, and \( J_E(f_k) \) is a correction of the collision integral due to the external electric field, see appendix.

We expand the density matrix \( f_k \) to linear order in the electric field as \( f_k^{mn} = f_0(\epsilon^m_k)\delta_{mn} + n_\epsilon(\epsilon^m_k) + S_k^{mn} \). The diagonal subleading distribution function \( n_\epsilon^{(0)} \) can be calculated as \( f(n_\epsilon^{(0)}) = f_0(S_\epsilon^{(0)}) - J_E(f_0(E)) \) where the right hand side plays as the driving term. By solving this equation, we get two different contributions to the subleading diagonal density matrix as \( n_\epsilon^{(0)} = n_\epsilon^{(0)} + n_\epsilon^{(ak)} \) and one can write \( f(n_\epsilon^{(0)}) = f(n_\epsilon^{(0)}) - J_E(f_0(E)) \), and \( f(n_\epsilon^{(ak)}) = f_0(S_\epsilon^{(0)}) \) with \( n_\epsilon^{(0)} \) and \( n_\epsilon^{(ak)} \) are due to the side jump and skew scattering contributions, respectively. We can also decompose the off-diagonal density matrix into \( S_k^{mn} = S_k^{mn} + S_k^{mnt} \). Having calculated the scattering terms and after straightforward but lengthy calculations, we find

\[
n_\epsilon^{(ak)}(\epsilon^m_k) = eZ_k^2(1 - \xi_k^2)E \cdot \hat{\sigma}_z,
\]

and,

\[
n_\epsilon^{(q)}(\epsilon^m_k) = Z_k \left[ 1 + 0.5\lambda(1 + \xi_k^2)(1 - \xi_k^2)^{-1} \right] E \cdot \hat{k}
\]

where

\[
Z_k^2 = \frac{8\hbar v_F}{\lambda_k^2} \frac{\xi_k(1 - \xi_k^2)^2 \delta(\epsilon_F - \epsilon^+_k)}{\chi^\alpha(\lambda)},
\]

here \( \chi(\lambda) = 4(1 + 3\xi_k^2) + \lambda^2(5 + 3\xi_k^2) + 8\lambda(1 - \xi_k^2) \). Furthermore, the extrinsic and intrinsic contributions of the off diagonal term is given by

\[
S_{ext} = \frac{\hbar}{2\lambda_k} \frac{e\tau_F}{4\tau} v_F(1 - \xi_k^2)(3 - 2\lambda + \frac{3}{4}\lambda^2)\xi_k E \cdot \hat{\sigma}_x - (1 - \frac{3}{4}\lambda^2)E \cdot \hat{k}\sigma_x,
\]

and

\[
S_{int} = \frac{e\hbar v_F}{2\lambda_k} \left[ f_0(\epsilon_F) - f_0(\epsilon^+_k) \right] \times \left( E \cdot \hat{k}\sigma_x - \xi_k E \cdot \hat{\sigma}_x \right),
\]

where \( \tau_F = \tau / \chi(\lambda) \) with \( 1 / \tau = n_F v_F^2 \rho(\epsilon_F) / \hbar \), and \( \rho(\epsilon_F) = \epsilon_F / 2\pi\hbar^2v_F^2 \) is the density of states. Here, \( \hat{k} = \hat{x}\cos\theta + \hat{y}\sin\theta \) and \( \hat{\sigma}_x = -\hat{x}\sin\theta + \hat{y}\cos\theta \).

It is clear that the extrinsic SO scattering renormalizes physical quantities given by equations (8)–(12) through the parameter \( \lambda \).

4. Spin density and spin orbit torque

The spin density and SOTs in TIs with out-of-plane magnetization are determined in this section. The spin density has five contributions: a leading contribution at the Fermi surface analogous to the Drude conductivity, an intrinsic contribution that takes into account the Fermi sea, an extrinsic contribution due to the Fermi surface that is formally zeroth order in the impurity potential strength, a side-jump contribution at
where we have multiplied by a factor of 

\[ \eta \]

In order to find the spin density related to the subleading of side jump, we determine each of these in turn below.

Let us calculate the leading order contribution to the spin density. It is

\[ \langle s_x \rangle = \sum_{m,k} \delta_{m,k} n(e_k^m). \tag{13} \]

With the leading order density matrix \( n(e_k^m) = -e_{\sigma F} E \cdot v^m \delta(e_k^m - e_F) \), we find the spin density as

\[ \langle s_x \rangle^{\text{leading}} = \frac{1}{2} (1 - \xi_k^z) e_{\sigma F} v_F \rho(e_F). \tag{14} \]

Note that the contributions including \( v_s \) due to \( \int_0^{2\pi} d\theta_k \sin \theta_k \cos \theta_k = 0 \) is zero. In a similar manner we find

\[ \langle s_y \rangle^{\text{leading}} = -\frac{4 e_{\sigma F} v_F \rho(e_F) (1 - \xi_k^z)}{\chi(\lambda)}. \tag{15} \]

Let us now consider the off-diagonal intrinsic density matrix contribution. First, the off-diagonal spin expectation value is

\[ \sum_k 2 \text{Re}[s_{x}^{\pm -} + s_{z}^{\pm \pm}] = \frac{e_{\sigma F} \hbar v_F M}{2} \rho(e_F). \tag{16} \]

Furthermore, we consider the off-diagonal extrinsic density matrix contribution as

\[ \sum_k \text{Re}[s_{x}^{\pm -} + s_{z}^{\pm \pm}] = e_{\sigma F} \frac{M}{\rho(e_F)} (1 - \xi_k^z) (2 - \lambda) \frac{1}{\chi(\lambda)} \].

Moreover, the diagonal subleading density function of skew scattering will be as

\[ \langle s_x \rangle^{(0)} = 8 e_{\sigma F} \frac{M}{\rho(e_F)} (1 - \xi_k^z)^2 \frac{1}{\chi^2}. \tag{18} \]

In order to find the spin density related to the subleading of side jump,

\[ \langle s \rangle = e_{\sigma F} \rho(e_F) \frac{M}{\rho(e_F)} \left[ \frac{4 (1 - \xi_k^z)}{\chi(\lambda)} + 2 \lambda (1 + \xi_k^z) \right] \cdot \mathbf{E}. \tag{19} \]

The \( z \)-component of spin expectation, on the other hand, are found as \( s_{k}^{\pm \pm} = \langle u_k^s \vert \sigma_z \vert u_k^s \rangle = \pm \) and \( s_{k}^{\pm \mp} = \langle u_k^s \vert \sigma_z \vert u_k^\mp \rangle = (1 - \xi_k^z)^{1/2} \) which are angle independent and therefore, the \( z \)-component spin density vanishes:

\[ \langle s_z \rangle^{\text{leading}} = \sum_k s_{k,z}^{+ +} n(e_k^+) + \sum_k s_{k,z}^{+ -} n(e_k^-) = -2 \sum_k e_{\sigma F} v_F \xi_k (1 - \xi_k^z)^{1/2} \left( E_x \sin \theta_k + E_y \cos \theta_k \right) \left[ \delta(e_k^- - e_F) + \delta(e_k^+ - e_F) \right] = 0. \tag{20} \]

Now we add all these contributions and get

\[ \langle s \rangle = \text{Tr} \{ \mathbf{s} \} = -4 e_{\sigma F} v_F \rho(e_F) \frac{(1 - \xi_k^z)}{\chi(\lambda)} \cdot \mathbf{z} \times \mathbf{E} + e_{\sigma F} \rho(e_F) \frac{M}{\rho(e_F)} \frac{\eta(\lambda)}{2 \chi^2} \cdot \mathbf{E}, \tag{21} \]

where \( \eta(\lambda) = \chi^2 + 8 \lambda \xi_k^z \chi + 16(1 - \xi_k^z)(1 + \chi - \xi_k^z) \). It is worthwhile mentioning that the effect of the SO impurity scattering is explicitly appeared in the results through parameter \( \lambda \).

The spin orbit torque is defined as \( \frac{d\mathbf{m}}{dt} = (2M/\hbar) \mathbf{m} \times \langle s \rangle \) where \( \mathbf{m} \) is a unit vector along the \( \mathbf{z} \) direction. With the spin density we already calculated we get

\[ \frac{d\mathbf{m}}{dt} = -4M e_{\sigma F} v_F \rho(e_F) \frac{(1 - \xi_k^z)}{\chi(\lambda)} \mathbf{m} \times (\mathbf{z} \times \mathbf{E}) + e_{\sigma F} \rho(e_F) M^2 \frac{\eta(\lambda)}{2 \chi^2} \mathbf{m} \times \mathbf{E}, \tag{22} \]

where we have multiplied by a factor of \( \hbar/2 \) the spin density since we traced only the Pauli matrix.
The effective Dirac SOT is defined as \( \frac{dm}{dt} = \tau_{FL} m \times (\hat{z} \times eE) + \tau_{DL} m \times eE \), where the first term which is proportional to \( m \times (\hat{z} \times eE) \) is odd upon magnetization reversal, proportional to the \( \tau \) and acts like a field-like torque, while the second term, \( m \times eE \), is even in magnetization reversal acts like a damping torque. The damping-like SOT is located in the \((m, E)\) plane, is often associated with the longitudinal component, and functions effectively as a magnetic damping. However, the field-like SOT, also known as the perpendicular component, sits normal to the \((m, E)\) plane and behaves as an actual magnetic field. The Rashba-Edelstein effects due to spin-momentum locking on the surface of the TI are responsible for the field-like contribution \([74]\), while the electromagnetic coupling is responsible for the damping-like contribution \([67]\). According to equation \((22)\), we expect \( \tau_{FL} \gg \tau_{DL} \) because the calculations is performed in the regime \( \epsilon_F \tau/\hbar \gg 1 \).

Expanding the SOTs for \( \lambda \ll 1 \) and skipping terms including \( \xi_F^n \) for \( n > 2 \), we have

\[
\tau_{DL} \approx \frac{3M^2}{2\pi\hbar v_F \epsilon_F} \left[ \left( 1 + \lambda + \frac{41}{12} \lambda^2 \right) - \left( \frac{M}{\epsilon_F} \right)^2 \left( 4 + 11\lambda + 55\lambda^2 \right) \right]
\]

\[
\tau_{FL} \approx -\frac{M_0 \gamma}{2\pi \hbar^2 v_F} \left[ \left( 1 - 2\lambda + \frac{71}{4} \lambda^2 \right) - \left( \frac{M}{\epsilon_F} \right)^2 \left( 4 - 16\lambda + 190\lambda^2 \right) \right].
\]

(23)

We consider a TI (i.e. Bi\(_2\)Se\(_3\)) whose Fermi velocity of its massless Dirac fermions is \( v_F \simeq 5 \times 10^5 \) m s\(^{-1}\). For all figures the impurity density and the amplitude of the scattering potential are given as

Figure 2. Field-like SOT as a function of the Fermi energy for the various (a) positive (c) negative values of the extrinsic SO scattering strength. Damping-like SOT as a function of the Fermi energy for the various (b) positive (d) negative values of the extrinsic SO scattering strength. The exchange field due to magnetization is considered as \( M = 10 \) meV.
$n_i = 1 \times 10^{10}$ cm$^{-2}$ and $\nu_0 = 5$ eV nm$^2$ or otherwise specified. Figure 2 shows the field-like and damping-like SOTs in terms of Fermi energy for some positive and negative different values of extrinsic SO scattering strength. As seen, the field-like SOT in figures 2(a) and (c) is larger than the damping-like SOT shown in in figures 2(b) and (d). As the Fermi energy increases the extrinsic mechanisms including skew and side-jump scatterings become stronger and lead to an increase in the field-like SOT. The extrinsic SO scattering strength plays a crucial role in renormalizing the SOTs so that for positive (negative) $\lambda_0$ will have a decrease (an increase) in the SOTs. In principle, the field-like SOT depends on the density of impurities through the relaxation time.

It should be noticed that the strength of the impurity-induced spin–orbit coupling $\lambda_0$ can be significantly enhanced when the system is placed near materials with strong SOI by the proximity effect [75]. Likewise, interface engineering can provide an efficient way to tune the SOI strength in TI/FM heterostructures [76, 77].

As seen in figure 3(a), with increasing impurity density, the relaxation time $\tau$ decreases, causing a decrease in the field-like SOT. Notice that the damping-like SOT is independent of impurity density. Moreover, we plotted the damping-like and field-like SOTs as a function of extrinsic SO scattering strength for the distinctive values of Fermi energy in figure 3(b). It is seen that at larger negative values of $\lambda_0$ and of the Fermi energy the field-like SOT reaches a maximum value. However, the damping-like SOT shows a peculiar behaviour as a function of the Fermi energy, decreasing at larger values of $\epsilon_F$. For $\epsilon_F = M = 10$ meV (i.e. $\xi_k = 1$) only the intrinsic mechanism contributes to SOTs. When the extrinsic SO scattering strength ($\lambda_0 < 0$) increases other mechanisms such as skew and side-jump scattering contribute to SOTs and lead to an increase in SOTs.

According to figure 3(b), field-like SOT changes from 0.49.6 to 0.64 nm$^{-1}$ when $\lambda_0$ changes from 0 to $-0.5$ for a constant value of the Fermi energy $\epsilon_F = 200$ meV and the magnetization strength $M = 10$ meV. Thus, $\frac{\Delta |\tau_{FL}|}{|\tau_{FL}(\lambda_0=0.5)|} \times 100 = \frac{0.64 - 0.49}{0.64} = 22.5\%$. For damping-like, we have $\frac{\Delta |\tau_{DL}|}{|\tau_{DL}(\lambda_0=0.5)|} \times 100 = \frac{0.80 - 0.64}{0.80} = 20\%$.

The simultaneous effect of the exchange field strength or Fermi energy and the extrinsic SO scattering strength on the damping-like and field-like SOTs are investigated in the density plots of figure 4. The value of the SOT depends strongly on the Fermi energy and magnetization. The field-like SOT increases by with increasing $\epsilon_F$ or $M$, while the damping-like SOT decreases with increasing Fermi energy. Moreover, as shown in figure 4(a), the field-like SOT behaves nonlinearly in terms of $\lambda_0 \leq 0$ for $\epsilon_F \leq 100$ meV at $M = 10$ meV, while the damping-like SOT is highly nonlinear for $\lambda_0 \geq 0$ as shown in figure 4(c). Therefore, the SOT behaves highly nonlinearly for large Fermi energy in terms of $\lambda_0$. In addition, the SOT increases with increasing exchange field strength, as shown in figures 4(b) and (d).

Notice that the ultimate aim of experiments is to increase the SOT efficiency in order to accomplish a quick and energy-efficient magnetization change. High-performance SOT devices must achieve a maximum value of SOT in order to achieve this. In this context the fact that extrinsic SO scattering seems to place a cap on the fastest switching that can be achieved is a factor that will influence device design.

Figure 3. Field-like SOT as a function of the extrinsic SO scattering strength, $\lambda_0$ (a) for some distinctive values of impurity density and (b) for different values of the Fermi energy. Here, the damping-like SOT is independent of impurity density. The inset of (b) shows the corresponding damping like SOT. The exchange field due to magnetization is considered as $M = 10$ meV.
5. AHE in the presence of extrinsic SO scattering

Since the SO interaction together with the interband mixing result in an anomalous velocity in the direction transverse to the electric field, extrinsic processes, such as side jump and skew scatterings, contribute to the anomalous Hall conductivity when the Fermi energy crosses into the conduction or valence band. The extrinsic spin–orbit coupling is effectively a random Rashba SO field that scatters spin-up and spin-down electrons asymmetrically. In the presence of a magnetization the numbers of spin up and down electrons are not equal, so the asymmetric scattering leads to a Hall current.

The effect is essentially the same when the Fermi energy resides in the conduction or valence bands, and for simplicity we focus on the conduction band. We note that, when the Fermi energy resides in the gap, the intrinsic mechanism, which is brought on by the chiral edge states, is what primarily controls the anomalous Hall conductivity. We do not focus on this case here.

The anomalous Hall conductivity contains four contributions: an intrinsic contribution from the Fermi sea, a contribution due to the extrinsic velocity at the Fermi surface which is nominally of zeroth order in the disorder strength, a side-jump contribution at the Fermi energy including the electric field correction to the collision integral and a contribution due to skew scattering. First we have to determine the expected velocity value as an operator trace $\text{Tr}(\dot{r}f)$, where $\dot{r} = (i/\hbar)[H, r]$ represents the Matrix elements of the velocity operator. The Hamiltonian of the system, $V(r)$ commutes with the position operator while we ignore the contribution of the extrinsic SO scattering, which $U(r)$ contributes to the velocity operator.

The extrinsic velocity in the conduction band is obtained as

$$\beta_k^+ = \frac{1}{\tau} \xi_k (1 - \xi_k^2)^{1/2} \frac{\hbar v_F}{\lambda_k} (1 - \lambda) \sigma_0 \hat{\theta},$$

where $\hat{\theta} = (-\sin \theta, \cos \theta)$. Note that the extrinsic velocity is proportional to the impurity density and in contrast to the group velocity, which is a velocity between collisions, the extrinsic velocity includes the effect of disorder on carrier dynamics, and can be read as an effective velocity of the electron after numerous collisions.
Figure 5. (a) The anomalous Hall conductivity in term of $\lambda_0$ for different values of the Fermi energy. The inset of (a) shows longitudinal conductivity of a TI. (b) Different contributions to the Hall conductivity for a fixed value of the Fermi energy $\varepsilon_F = 200$ meV. Notice that the exchange field due to magnetization is $M = 10$ meV.

The contribution to the anomalous Hall conductivity related to the skew scattering and side jump corrections is

$$\sigma_{yx} = \sigma^0_{yx} \left[ \eta(\lambda) + 4\lambda(1 - \xi^2_{k_F})\chi(\lambda) \right],$$  \hspace{1cm} (25)

where $\sigma^0_{yx} = 2e^2/\pi\hbar$. While the Hall conductivity is independent on the impurity in a case of short-range impurity scattering, it depends a highly nonlinear on $\lambda$ in the case of the extrinsic SO scattering. The Hall conductivity can be expand for $\lambda \ll 1$ up to $\lambda^2$ and $\xi_{k_F} < 1$ (i.e. $\varepsilon_F > M$), and we thus obtain

$$\sigma_{yx} \approx \frac{\sigma^0_{yx}}{4} \left[ 6 \frac{1}{1 + 6\xi^2_{k_F}} - \frac{11}{1 + 9\xi^2_{k_F}} \lambda - \frac{1.5\xi_{k_F} + 4}{1 + 12\xi^2_{k_F}} \lambda^2 \right].$$  \hspace{1cm} (26)

It can be found from above equation, the Hall conductivity decreases (increases) for $\lambda_0 > 0$ ($\lambda_0 < 0$) as $\sigma_{yx} \sim \varepsilon_M(\varepsilon_F^2 - M^2)\lambda_0$. The longitudinal conductivity

$$\sigma_{xx} = \frac{2e^2\varepsilon_F}{\pi\hbar^2} \frac{1 - \xi^2_{k_F}}{\chi(\lambda)}.$$  \hspace{1cm} (27)

Note that our calculations were performed in the $\varepsilon_FT/\hbar \gg 1$ regime, i.e. as expected from the $\sigma_{xx} \gg \sigma_{xy}$ equations above. The result for the longitudinal conductivity agrees with the literature $\sigma_{xx} \sim (e^2/\hbar)(v_{F\tau})/2$ (see equation (12) in [78]) obtained from the Keldysh-Green's function.

The anomalous Hall conductivity as a function of the extrinsic SO scattering strength $\lambda_0$ (which is defined in $\lambda = \lambda_0 k_F^2$) for the different values of the Fermi energy is shown in figure 5. The anomalous Hall conductivity is independent of the extrinsic SO scattering strength at $\varepsilon_F = M = 10$ meV (i.e. $\xi_{k_F} = 1$) since it is only determined by the intrinsic contribution (i.e. $\sigma_{yx} = \sigma^0_{yx}$). In this case, the Berry curvature arises from electrons below the Fermi surface as a result of the topological properties induced by the SO coupling in Bloch bands and consequently, the longitudinal conductance is zero. When the Fermi energy crosses the conduction band $\varepsilon_F > M$, extrinsic SO mechanisms including side-jump and skew scattering contribute to the anomalous Hall conductivity. For $\lambda_0 < 0$ ($\lambda_0 > 0$), an increase in the extrinsic SO scattering strength leads to an increase (decrease) in the transport time and an increase (decrease) in the anomalous Hall and longitudinal conductivity values. As can be observed from figure 5(a), increasing the Fermi energy for a fixed magnetization (i.e. $M = 10$ meV), the anomalous Hall conductivity decreases. In this case, the longitudinal conductance increases because $\sigma_{xx} \sim \varepsilon_F$ as shown in the inset of figure 5(a). We plot the various contributions to the anomalous Hall conductivity for a fixed value of Fermi energy $\varepsilon_F = 200$ meV as seen in figure 5(b). In this figure, the extrinsic-scattering contribution dominates at larger values of the SO scattering strength.
6. Conclusion

We have investigated the SOT and electronic AHE due to massless Dirac fermions in a 2D TI with spin-momentum locking in the presence of a magnetization perpendicular to the TI plane. We found that both scalar and extrinsic SO scattering play important roles in determining the magnitude of the SOT.

The Fermi energy, external magnetization strength, and intrinsic impurity scattering all affect the field-like and damping-like SOTs. The SOTs reach a maximum value by modifying the $M$, $F$, and $\lambda$. Despite the fact that the strength of the damping-like SOT component is independent of the impurity density, the field-like SOT component decreases in a disordered system. The anomalous Hall conductivity, on the other hand, is independent of the impurity strength in the case of short-range impurity scattering, but highly nonlinear in the extrinsic SO scattering strength.

The physics for an in-plane magnetization is highly non-trivial and wholly different from that discussed here. It will be addressed in a future publication.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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Appendix

$J_0(f_k)$ is the collision integral due to the impurity potential, which is defined as $J_0(f_k) = \frac{1}{i\hbar} \langle [U, g_0] \rangle$, where $g_0$ in terms of Green's functions can be expressed as

$$ g_0 = \frac{1}{2\pi i} \int_0^\infty d\epsilon [G_0^R(\epsilon) U G_0^A(\epsilon), f_k]. \tag{28} $$

Also, $G_0^R(\epsilon)$ is a free retarded Green function obtained as

$$ G_0^R(\epsilon) = -\frac{i}{\hbar} \int_0^\infty dt e^{-i\epsilon t/\hbar} e^{i\epsilon t/\hbar} e^{-\eta t}, \tag{29} $$

where we introduce the factor $e^{-\eta t}$ to ensure convergence and the advanced Green function is defined as $G_0^A(\epsilon) = G_0^R(\epsilon)$.

Now we want to include the effect of the driving electrostatic potential up to linear order [58]. Adding an electric field to the Hamiltonian implies a correction of the function $g$. Moreover, $J_0(f_k)$ is a correction of the collision integral due to the external electric field and is given by $J_0(f_k) = \frac{1}{i\hbar} \langle [U, g_E] \rangle$, where the $g_E$, which reflects it is the electric field correction and off diagonal in the momentum and in the band index, defined as

$$ g_E = \frac{1}{2\pi i} \int_0^\infty d\epsilon [G_0^R(\epsilon) [V, g_0]] G_0^A(\epsilon). \tag{30} $$

To perform a linear response, one can use equation (28) as a function of the equilibrium distribution function $f_0(\epsilon)$.

The kinetic equation (i.e. equation (7)) for the diagonal part of the density matrix is written as

$$ [J_0(n_E)]_{kk}^{mm} = \frac{eE}{\hbar} \frac{\partial f_0(\epsilon_k^m)}{\partial \epsilon_k}. \tag{31} $$

Notice that the kinetic equation is considered to linear order of the electrical field and basically $n_E$ begins at order $-1$ in terms of small parameter $\hbar/\epsilon_F T$ [72] where $\tau$ is the momentum relaxation time. If the band dispersion is isotropic (e.g. band dispersion for TIs), one can assume $[J_0(n_E)]_{kk}^{mm} = n_E(\epsilon_k^m)/\tau(\epsilon_k)$, so the equation above becomes as

$$ n_E(\epsilon_k^m) = \frac{\tau(\epsilon_k)}{\hbar} \frac{eE}{\hbar} \frac{\partial \epsilon_k^m}{\partial \epsilon_k} \frac{\partial f_0(\epsilon_k^m)}{\partial \epsilon_k}. \tag{32} $$
Using the expression of \( J_0(f_k) \), the diagonal part of the Born approximation collision integral can also be written as

\[
[J_0(n_k)]_{kk}^{mm} = \frac{2\pi}{\hbar} \sum_{m',k'} \left\langle U_{kk}^{m'm'} U_{kk}^{m'm'} \right\rangle \left[ \rho_{kk}^{m'm'} - n_{kk}^{m'm'} \right] \delta(e_k^m - e_{k'}^{m'}). \tag{33}
\]

According to equation (32) and \( \nu = (1/\hbar)\partial e_k^m / \partial k = k/m \), we can calculate \( n_k(e_k^m) \) in the electric field.

We assume transport time is angular-independent or \( k \) direction independent. Substituting the above equation in equation (33) and assuming an elastic scattering \( \bar{\epsilon}_{k'} = \bar{\epsilon}_k \) when the direction of electrical field is \( k \), the transport time obtains as

\[
\frac{1}{\tau_T(k)} = \frac{2\pi}{\hbar} \sum_{m',k'} \left\langle U_{kk}^{m'm'} U_{kk}^{m'm'} \right\rangle [1 - \cos(\theta_k - \theta_{k'})] \delta(e_k^m - e_{k'}^{m'}). \tag{34}
\]

As discussed in [72], \( S_{kk}^{m'm'} \) starts as order 0 based on an expansion in the small parameter \( \hbar/(\epsilon_F T) \). The kinetic equation for the off-diagonal density matrix is written as

\[
\frac{\partial S_{kk}^{(0)}_{ek}}{\partial t} + \frac{i}{\hbar} \left[ H_{ek}, S_{kk}^{(0)}_{ek} \right] = D_E + D'_E,
\]

where \( D \) is the intrinsic driving term and \( D' \) is the anomalous driving term, containing disorder renormalizations of the response which are in part equivalent to vertex corrections.

Having solved the above equation, the intrinsic and extrinsic contributions are defined as

\[
[S_{kk}^{(0)}_{ek}]_{m'm'}^{mm} = \frac{\hbar D_{kk}^{m'm'}}{i(e_k^m - e_{k'}^{m'} - \eta)}, \tag{36}
\]

\[
[S_{kk}^{(0)}_{ek}]_{m'm'}^{mm} = \frac{\hbar D_{kk}^{m'm'}}{i(e_k^m - e_{k'}^{m'} - \eta)}. \tag{37}
\]

**ORCID iDs**

Reza Asgari ✉️ https://orcid.org/0000-0001-5163-4765
Dimitri Culcer ✉️ https://orcid.org/0000-0002-2342-0396

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