Edelstein effects, spin-transfer torque, and spin pumping caused by pristine surface states of topological insulators

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The Edelstein effect caused by the pristine surface states of three-dimensional topological insulators is investigated by means of a semiclassical approach. The combined effect of random impurity scattering and the spin-momentum locking of the gapless Dirac cone yields a current-induced surface spin accumulation independent from chemical potential and temperature. In a nearby ferromagnet that does not make direct contact with the topological insulator, the bound state nature of the pristine surface state causes a spin-transfer torque that is entirely field-like, whose magnitude is highly influenced by the interface cleanliness and the quantum well state of the ferromagnet. Through incorporating quantum tunneling into Bloch equation, the spin pumping mediated by the pristine surface state is shown to be described by the same spin mixing conductance as the spin-transfer torque, and a semiclassical approach is proposed to explain the inverse Edelstein effect that converts the spin pumping spin current into a charge current. Consistency of these results with various experiments will be elaborated in detail.

I. INTRODUCTION

The peculiar electromagnetic response of three-dimensional (3D) topological insulators (TIs) point to their practical applications, especially to spintronic devices[1]. Of particular interest are the spintronic effects caused by the surface states of 3D TIs, whose low energy sector is described by a two-dimensional (2D) Dirac Hamiltonian[2–4]. For instance, an inverse spin galvanic effect at the TI/ferromagnetic insulator interface due to the gapped surface state has been proposed[5]. Drawing analogy with other 2D parabolic band systems with strong Rashba spin-orbit coupling[6–9], the spin-momentum locking[10–12] of the surface states is expected to yield a spin accumulation in the presence of an electric field or electric current, known as the Edelstein effect. Various experimental evidences indeed point to the existence of Edelstein effect at the surfaces of 3D TIs[13–16]. Exploiting such effect as a mechanism for magnetization switching has been demonstrated in 3D TI and ferromagnetic metal (FMM) hybrid structures[17–19]. In the reciprocal process of what described above, a magnetization dynamics induced by ferromagnetic resonance in the FMM injects a spin current into a nearby TI, a phenomenon known as the spin pumping. Through the inverse Edelstein effect, the spin pumping spin current can be converted into a charge current, which has also been demonstrated and investigated intensively[20–23].

Despite the similarity with conventional 2D parabolic band Rashba systems, experiments reveal several puzzling features for the spin to charge interconversion mediated by the surface state. By varying the chemical potential $\mu$ through the Dirac cone, the efficiency of charge to spin current conversion is found to remain constant in a wide range of $\mu$, except a reduction near the Dirac point[14]. Moreover, the effect is nearly constant of temperature from 0 to 300K[16]. Secondly, the efficiency of the interconversion (see Secs. II B and II B for the definitions) are of the order of nm[14, 22, 24], which awaits a microscopic explanation. Finally, the spin-transfer torque (STT) using the surface spin accumulation is found to be much larger than that induced by spin Hall effect (SHE) in heavy metals, pointing to the fact that the localized surface state may cause a very different spin injection mechanism than the conventional metallic STT based on plane wave states[25, 26].

A significant amount of theoretical effort has been made to understand the current-induced spin torque caused by the surface states, mostly concerning the TI/ferromagnet bilayers or magnetized TI surfaces in which the magnetization gaps out the surface state. Through calculating the transverse spin susceptibility, a Landau-Lifshitz-Gilbert equation has been derived in the presence of the charge current, which renders a negligibly small STT[27]. Within Born approximation and including vortex corrections, the STT in the magnetization perpendicular to the plane configuration is shown to be absent[28]. On the other hand, the diffusion of surface state spin current into the FMM has been proposed as a major mechanism for the experimentally observed large STT[17, 29], and a calculation based on linear response theory reveals a highly anisotropic spin torque[30].

In this work, we elaborate that three important factors, namely the surface disorder, bound state nature of the surface state, and the quantum well state in the FMM, help to understand a number of puzzling experimental results. Focusing on the situations in which the surface state Dirac cone remains gapless, we use a combination of quantum tunneling formalism and semiclassical Boltzmann equation to give a microscopic account for the STT, spin pumping, Edelstein and inverse Edelstein effects, and elaborate how the three factors influence the direction and magnitude of these effects. The difference between the TI-based spintronics and the conventional metallic spintronics will be emphasized, and the agreement with various experimental results, using realistic material parameters[10, 31], will be demonstrated explic-
ity.

This article is structured in the following manner. In Sec. II, we first incorporate the scattering of random surface impurities into a semiclassical approach to demonstrate a temperature and chemical potential independent Edelstein effect, and then combine this calculation with quantum tunneling of nonequilibrium electrons to calculate the STT. Section III first gives a microscopic mechanism for the spin pumping based on quantum tunneling and Bloch equation, and then combine it with a semiclassical approach to demonstrate the inverse Edelstein effect. Section IV summarizes the how the aforementioned three important factors influence these charge to spin interconversion effects.

II. EDELSTEIN EFFECT AND SPIN-TRANSFER TORQUE

A. Edelstein effect

We start by considering the pristine surface state in an isolated, semi-infinite 3D TI of symmetry class AII, described by the Hamiltonian and the spin-momentum locking[11, 32, 33]

$$H = v_F k_x \sigma_x - v_F k_z \sigma_y = d \cdot \sigma.$$  

$$(\sigma)_{k \pm} = (|\psi_{k \pm}| \sigma |\psi_{k \pm}|) = \pm d = \pm x \sin \alpha \mp y \cos \alpha,$$  

where $|\psi_{k \pm}|$ denotes eigenstate of the hole cone with energy $E_{k \pm} = |d| = v_F k$, whereas $|\psi_{k -}|$ is that of the electron cone of energy $E_{k -} = -|d| = -v_F k$. Given the density of states (DOS) $\rho(E) = a^2|E|/2\pi v_F^2$, and a random uncorrelated disorder $\langle (V(r)V(r')) \rangle = n_v \delta^2 (r-r') \equiv \gamma \delta (r-r')$, where $\langle \ldots \rangle$ denotes the impurity averaging, the mean free time[34, 35]

$$\frac{1}{\tau(E)} = a^2 \int \frac{d^2 k'}{(2\pi)^2} \frac{2\pi}{\gamma} \int_{\beta} \langle \langle \psi_{k \beta} | V | \psi_{k \beta} \rangle^2 \rangle \delta(E - E_{k \beta})$$  

$$= \pi \gamma \rho(E)/\hbar.$$  

is inversely proportional to the DOS, a feature very different from other 2D parabolic band systems[7, 8]. In the presence of an electric field $E \parallel \hat{x}$ and at finite chemical potential $\mu$, the semiclassical equation of motion of an electron in the hole cone is $+\beta$ and that in the electron cone $\beta = -\beta$ modifies the Fermi distribution, which can be solved by incorporating the random impurity scattering into Boltzmann equation[35]

$$\frac{d k}{dt} \cdot \nabla f_{\beta} = \frac{2a^2}{\hbar} \int \frac{d^2 k}{(2\pi)^2} \langle \langle \psi_{k \beta} | V | \psi_{k \beta} \rangle^2 \rangle \times \delta(E_{k \beta} - E_{k \beta}) [f_{k \beta} - f_{k \beta}].$$  

The equation may be solved by expanding the distribution function to leading order

$$f_{\beta} = n_{F \beta} + \frac{\partial n_{F \beta}}{\partial E_{k \beta}} \tilde{f}(\alpha),$$  

where $n_{F \beta} = 1/(e^{(E_{k \beta} - \mu)/k_BT} + 1)$. Putting Eq. (4) into Eq. (3), and using $\nabla_{k} E_{k \beta} = \beta v_F k$ and the ansatz $\tilde{f}(\alpha) \propto \cos \alpha$ yield the solution[35]

$$f_{\beta} = n_{F \beta} + \beta \frac{\partial n_{F \beta}}{\partial E_{k \beta}} \frac{4\epsilon E_x}{k^2 \gamma} \cos \alpha.$$  

We have defined a dimensionless variable

$$\tilde{\gamma} = n_v (V \nu / v_F)^2,$$  

that measures the cleanliness of the surface, which is essentially the percentage of disorder multiplied by the square of the disorder potential relative to the Dirac cone energy.

Using Eq. (1), the spin accumulation from each cone can be calculated from the Boltzmann equation

$$\langle \sigma \rangle_{k \beta} = a^2 \int \frac{d^2 k}{(2\pi)^2} f_{\beta} \langle \sigma \rangle_{k \beta}$$  

$$= a^2 \frac{e E_x}{\pi v_F^2} \left[ \beta \delta_{\beta} + \frac{\beta}{e \mu/k_BT + 1} \right] \hat{y},$$  

where the $\hat{x}$ component vanishes due to the angular integration. In Eq. (7), the electron and the hole cone contribute the same sign of spin accumulation because, although the opposite group velocities $\nabla_{k} E_{k \pm} = \pm v_F k$ cause the electron and hole cone to shift in opposite directions in respond to the external field, their spin expectation value along the shift is the same due to the opposite spin chiralities, as shown schematically in Fig. 1 (one may as well define the shift without the group velocity part $\nabla_{k} E_{k \pm}$, then for both cones $\beta = \pm$ it will be along the same direction[14]). This surface spin accumulation occurs only when the external field $E$ has an in-plane component, and it is polarized along the direction perpendicular to the field, in contrast to the bulk magnetoelectric effect (ME) and the Edelstein effect at the TI/ferromagnetic insulator interface that give a magnetization along the field[5, 36]. The total spin accumulation $\sum_{\beta} \langle \sigma \rangle_{\beta} = a^2 e E_x / \pi v_F^2 \hat{y}$ is independent from temperature and chemical potential, and thus manifests even at zero temperature and zero chemical potential, in which case the diverging $\tau(E \rightarrow 0)$ compensates the vanishing Fermi surface. Note that the total spin accumulation $\sum_{\beta} \langle \sigma \rangle_{\beta}$ is not determined by a single mean free time[24] because the energy-dependent $\tau(E_{k \beta})$ in Eq. (2) has been integrated out in Eq. (3), leaving only the cleanliness factor $\tilde{\gamma}$. Our result well explains the temperature-independent surface spin accumulation recently measured in Bi$_2$Se$_3$[37] and spatially modulated electron and hole puddles[38], which may be simulated by a constant and a smoothly varying chemical potential, respectively.

The typical experimental current density $j_c \sim 10^7$A/cm$^2$ and conductivity $10^7$S/m correspond to the field strenth $E_z \sim 10^5$N/C. Assuming a lattice constant $a \sim 1$nm and Fermi velocity $v_F \sim eVnm$, the dimensionless spin polarization $a^2 e E_x / 4\pi v_F^2 \tilde{\gamma} \sim 10^{-6}/\tilde{\gamma}$ in units
of \( \hbar \) per unit cell is enhanced by the cleanliness factor in Eq. (6). This conclusion is similar to that for the spin accumulation previously investigated in ultrathin TI films where the top and bottom surface states are coupled[39]. Given a reasonable value, say \( \tilde{\gamma} \sim 0.01 \), the spin polarization is few orders of magnitude larger that that induced by the bulk ME \( \mathbf{M} \sim \alpha a^2 \mathbf{E} \hbar c^2 / \hbar \sim 10^{-7} \)[36]. Such a magnitude should be readily measurable by surface probes such as optical Kerr effect or X-ray magnetic circular dichroism, although existing experiments suggest that the surface magnetization may be highly interfered by the bulk bands contribution[15]. The effect is comparable to or may exceed the inverse spin galvanic effect at the TI/ferromagnetic insulator interface[5], which in the same electric field strength yields an effective magnetic field \( \mathbf{H} = \pm (1/2) (J_{sd}a/v_F \mathcal{S}) \mathbf{E} / \hbar \Rightarrow \mathbf{B} \sim 0.1 \text{T} \) and subsequently a spin polarization \( \mathbf{M} \sim \mu_B \mathbf{B} / \mu_F \sim 10^{-5} \), assuming the proximity induced exchange coupling that gaps out the Dirac cone is \( J_{sd} \sim 0.1 \text{eV} \). In comparison with the spin Hall effect in heavy metals, such as Pt and Ta with a spin Hall angle \( \theta_H \sim 0.1 \), the same current density and field strength produces a surface spin voltage \( \mu_+ - \mu_- \sim 0.01 \text{meV} \) and the corresponding surface spin polarization \( (\mu_+ - \mu_-) / \mu_F \sim 10^{-5} \)[40, 41], which may also be surpassed by the Edelstein effect with sufficiently clean surface. Finally, we remark that the charge current calculated out of this Boltzmann equation approach

\[
j_{\gamma} = -e \sum_{\beta} \langle v_{\gamma} \rangle_{\beta} = -e \sum_{\beta} \langle \psi_{\beta} \rangle_{\gamma} = \frac{\mathcal{E}_x}{\pi \gamma} \left( \frac{q^2 c^2}{\hbar} \right) (8)
\]

is also determined by the surface cleanliness \( \tilde{\gamma} \).

![Figure 1.](image)

**Figure 1.** (a) Schematics of the Edelstein effect. The electron cone and the hole cone of the surface state shift in opposite directions (dotted circles) in the presence of an in-plane electric field \( \mathcal{E} \parallel \hat{x} \) because of their opposite group velocities, yet result in the same spin accumulation \( \langle \sigma \rangle \parallel \hat{y} \) because of their opposite spin chirality (red and green arrows). (b) The TI/NM/FMM trilayer, with an NM of thickness \( \ell_N \) and FMM of thickness \( \ell_F \), and a charge current flowing along \( \hat{x} \). Matching the 2D Fermi surface of the NM (blue sphere) and the 1D Fermi surface of the surface state (black ring) gives the Fermi momentum \( k_{sd} \) relevant in our problem. The \( \hat{z} \) component of \( k_{sd} \) is the \( k_F \) in Eq. (12).

### B. Spin-transfer torque

We proceed to address the STT in the topological insulator/normal metal/ferromagnetic metal (TI/NM/FMM) trilayer. Our motivation to address this particular system is that because the TI is not in direct contact with the FMM, the Dirac cone remains in its gapless pristine condition, so the connection with Sec. II A can be made. Similar to a metal-semiconductor junction, a band banding that shifts the gapped Dirac cone is expected in this system due to the Schottky–Mott rule that aligns the work function of the two materials[42, 43]. As a result, the chemical potential \( \mu \) is likely to reside in either the electron or the hole cone. However, adjusting \( \mu \) through chemical doping has been demonstrated in this trilayer setup[14], so we will treat \( \mu \) as a free parameter.

Our assumption is that the STT is caused by quantum tunneling of the surface state nonequilibrium electrons into the FMM[44-47]. Consider the TI to occupy the \( z \leq 0 \) half space, the NM \( 0 < z \leq \ell_N \) and the FMM \( \ell_N < z \leq \ell_N + \ell_F \), as shown in Fig. 1. The \( \ell_N \) and \( \ell_F \) are thinner than the spin diffusion length of the materials, relevant to materials such as Cu and Co in nm regime[48]. To simplify the calculation of the injection of a nonequilibrium electron from the surface state, we will rotate the spin quantization axis to be align with that of the injected electron, i.e., \( \langle \sigma \rangle_{k_\beta} \rightarrow (1, 0)^T \cong \hat{z}_F \) following Eq. (1), and write the wave function of the injected electron as

\[
\psi_{k_\beta}(x) = e^{i k_z x} e^{i k_y y} e^{2 \xi A_\beta} \left( \begin{array}{c} 1 \\ 0 \end{array} \right).
\]

with \( A_\beta \) the electric field induced incident amplitude from \( \beta \)-cone, and \( \xi \approx v_F / M \) is the decay length of the surface state set by the bulk gap \( M \) (assuming \( \mu \ll M \), the small momentum dependence of \( \xi \) is ignored for simplicity). The NM and FMM are described by

\[
H_N = \frac{\hbar^2}{2m} \left( k_x^2 + k_y^2 + k_z^2 \right) - \mu_F ,
\]

\[
H_F = \frac{\hbar^2}{2m} \left( k_x^2 + k_y^2 + k_z^2 \right) - \mu_F + J_{sd} \sigma \cdot \mathbf{S} ,
\]

where \( J_{sd} \) is the exchange coupling between the conducting \( s \) electron and the magnetized \( d \) electron. \( \mu_F \) is the energy from the bottom of the parabolic band to the Fermi surface, and the magnetization is given by \( \mathbf{S} = S \left( \sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta \right) \). For an injected nonequilibrium electron with a specific planar momen-
tum $k = (k_x, k_y)$, the corresponding wave functions are
\[
\psi_{N\beta}(r) = e^{i k_x x + i k_y y} \left[ B_\beta e^{i k_F z} + C_\beta e^{-i k_F z} \right] \begin{pmatrix} 1 \\ 0 \end{pmatrix} +
\]
\[
e^{i k_x x + i k_y y} \left[ D_\beta e^{i k_F z} + E_\beta e^{-i k_F z} \right] \begin{pmatrix} 0 \\ 1 \end{pmatrix},
\]
where the upper sign is for spin $\uparrow$ (parallel to $S$) and lower sign for spin $\downarrow$ (antiparallel to $S$).

The wave function at $z > \ell_F$ is assumed to vanish for simplicity. As shown schematically in Fig. 1, matching the 2D Fermi surface of the NM and FMM with the 1D Fermi surface of the surface state determines the momenta
\[
k_F = \sqrt{\frac{2m}{\hbar^2}} \left[ E_{k\beta} + \mu_F \right] - \frac{E_2^2}{v_F},
\]
\[
k_{\beta\uparrow,\downarrow} = \sqrt{\frac{2m}{\hbar^2}} \left[ E_{k\beta} + \mu_F + J_{sd} S \right] - \frac{E_2^2}{v_F},
\]
where the upper sign is for spin $\uparrow$ (parallel to $S$) and lower sign for spin $\downarrow$ (antiparallel to $S$).

Matching the wave function everywhere at the interfaces $z = 0$ and $Z = \ell_N$
\[
\psi_{k\beta}(x, y, 0) = \psi_{N\beta}(x, y, 0), \quad \psi_{N\beta}(x, y, \ell_N) = \psi_{F\beta}(x, y, \ell_N), \quad \partial_z \psi_{N\beta}(x, y, \ell_N) = \partial_z \psi_{F\beta}(x, y, \ell_N),
\]
where we have defined
\[
Z_\pm = \pm \frac{k_{\beta\sigma}}{i k_F} \cos k_{\beta\sigma} \ell_F,
\]
\[
W_\sigma = \frac{e^{i k_F \ell_N}}{2} \left[ Z_\pm - Z_\mp + \frac{k_{\beta\sigma}}{i k_F} \right] \cos k_{\beta\sigma} \ell_F,
\]
Note that the first derivative of the wave function does not have to match at $z = 0$, because the $z = 0^-$ side is described by the Dirac Hamiltonian whose first derivative is given by the bulk gap, whereas the $z = 0^+$ we have the Schrödinger Hamiltonian. Another notable feature is that the surface state wave function in Eq. (9) does not have a spin down component. This is because the spin-momentum locking dictates that shall a spin down component exist, it will have planar momentum $(-k_x, -k_y)$, then the planar component of the wave functions in Eqs. (9) and (11) cannot be matched everywhere at the surface $z = 0$.

To calculate the torque, it is customary to use the rotated reference frame $[25, 26, 44, 45] (x_2, y_2, z_2)$ defined by unit vectors $z_2 \parallel \hat{S}, y_2 \parallel \hat{S}_{T1} \times \hat{S}$, and $x_2 \parallel -\hat{S} \times (\hat{z}_{T1} \times \hat{S})$, and write the FMM wave function as
\[
\psi_{F\beta}(z) = \begin{pmatrix} B_\beta \sin k_{\beta\sigma}(z - \ell_N - \ell_F) \\ C_\beta \sin k_{\beta\downarrow}(z - \ell_N - \ell_F) \end{pmatrix},
\]
where $\langle \sigma \rangle k_\beta = \hat{z}_{T1}$. In this reference frame, the Pauli matrices $\sigma^{x_2, y_2, z_2}$ take the usual form, which yield a finite spin expectation value $\langle \psi_{F\beta}(z) \sigma^{x_2, y_2, z_2} \psi_{F\beta}(z) \rangle = \langle \sigma^{x_2} \rangle_{F\beta}$. whereas $\langle \psi_{F\beta}(z) \sigma^{y_2} \psi_{F\beta}(z) \rangle = \langle \sigma^{y_2} \rangle_{F\beta} = 0$. Defining the function that integrates over the FMM slab
\[
g_\beta(k_{\beta\sigma}, \ell_F) = \frac{4 m J_{sd} S}{\hbar^2} a^2 \int_{\ell_N}^{\ell_N + \ell_F} dz \sin [k_{\beta\sigma}(z - \ell_N - \ell_F)] + \sin [k_{\beta\downarrow}(z - \ell_N - \ell_F)]
\]
\[
= \frac{a^2}{W_\uparrow W_\downarrow} \left[ k_{\beta\uparrow} \cos k_{\beta\downarrow} \ell_F \sin k_{\beta\downarrow} \ell_F - k_{\beta\downarrow} \cos k_{\beta\uparrow} \ell_F \sin k_{\beta\uparrow} \ell_F \right],
\]
and consider the Landau-Lifshitz dynamics, the spin torque contributed from this nonequilibrium electron is
\[
\tau_{k_\beta} = \frac{J_{sd} S}{\hbar} \langle \sigma^{x_2} \rangle_{F\beta} \hat{x}_{2} \times \hat{S}
\]
\[
= \frac{A^2}{4m} g_\beta(k_{\beta\sigma}, \ell_F) \langle \sigma \rangle_{k_\beta} \times \hat{S}
\]
\[
= \frac{\hat{y}_2}{4im} \left[ \psi_{F\beta}(z) \sigma^{y_2} \partial_z \psi_{F\beta}(z) - h.c. \right]_{z = \ell_N} \hat{y}_2 a^2 j_{z_2} \psi_{F\beta} \langle \sigma^{x_2} \rangle_{F\beta}.
\]
The last line of Eq. (18) indicates that the torque is equal to the spin current at the NM/FMM interface, so angular momentum is conserved in this approach.

Unlike the plane wave states in metallic STT systems that sustain a spin phase difference between the incident and reflected waves$[25, 26, 44, 47]$ which usually yields both field-like and damping-like torques, the bound state wave function in Eq. (9) has no reflected amplitude and does not support such a spin phase difference. As a result, the STT is entirely field-like, of the form $\langle \sigma \rangle_{k_\beta} \times \hat{S}$.

To connect Eq. (18) of a single injected electron with the total spin accumulation caused by the Edelstein effect in Eq. (7), we identify the incident amplitude $|A_\beta|^2$ with the nonequilibrium electron density induced by the external electric field in Eq. (5)
\[
|A_\beta|^2 = \frac{1}{a^2} \frac{\partial E_{\beta}}{\partial E_{k_\beta}} \frac{2 \epsilon E_x v_F}{\hbar} \tau(E_{k_\beta}) \cos \alpha.
\]
The total torque contributed from the two cones is then
\[
\tau = \sum_{\beta} a^2 \int \frac{d^2k}{(2\pi)^2} \kappa_{k\beta} = \frac{\hbar e\mathcal{E}_\sigma}{4\pi m v_F \gamma} G_i \hat{S} \times \hat{y}, \tag{20}
\]
with the dimensionless spin mixing conductance
\[
G_i = \sum_{\beta} \int_0^\infty dk v_F \frac{\partial n_{\beta k}}{\partial E_{k\beta}} \left[ \frac{1}{a} \gamma g_{\beta}(k_{\beta\sigma}, \ell_F) \right]. \tag{21}
\]
The torque is measured in units of the prefactor in Eq. (20). In a typical experimental current density \(j_c \sim 10^7\) A/cm² and the corresponding field \(\mathcal{E}_x \sim 10^4\) N/C, the prefactor in Eq. (20) is \(\hbar e\mathcal{E}_x/4\pi m v_F \gamma \sim \text{GHz}/\gamma\), where we see that the cleanliness factor \(\gamma\) dramatically enhances the torque. This may explain the puzzling large STT obtained experimentally in a similar TI/FMM bilayer setup[17]. The total torque is entirely field-like, along the cross product of the magnetization and the net spin accumulation \(\mathbf{S} \times \hat{y}\), due to the same reason stated after Eq. (18).

The total torque \(\tau\) is the spin mixing conductance \(G_i\) shown in Fig. 2, of the order of \(1 \sim 10\), multiplied by the unit \(\hbar e\mathcal{E}_x/4\pi m v_F \gamma \sim \text{GHz}/\gamma\). Owing to the quantum well state wave function in Eq. (11), \(G_i\) shows periodic resonances with FMM thickness \(\ell_F\)[14, 46, 47]. These resonances are expected to survive even if spin diffusion is incorporated, as suggested by a recent work that incorporates the spin diffusion effect into quantum tunneling by means of a nonhermitian Hamiltonian[49]. The torque increases with the exchange coupling in the FMM in the experimentally relevant regime \(0 < J_{sd} < 0.3\), and is roughly constant of temperature. In a large region of positive chemical potential \(\mu > 0\), the STT stays roughly constant, and shows a sign change at \(\mu\) close to the Dirac point, and eventually recovers at \(\mu < 0\). In comparison with the Edelstein effect in an isolated TI described by \(\sum_{\beta} g_{\beta}(\ell_{sd}, \mu, T)\) factor in the integration of Eq. (21), which represents the quantum tunneling effect into the FMM. Finally, we should remark that in a realistic TI/NM/FMM trilayer, STT is only part of the total torque, since the current flowing in the FMM will induce a spin-orbit torque.

Because the STT is equal to the total interface spin current \(\tau = a^2 j_0\), we may combine it with Eq. (8) to obtain the momentum \(\mu_{EE}\) that represents the efficiency of charge to spin current conversion in the Edelstein effect[14, 24]
\[
\mu_{EE} = \frac{\tau}{\sum_{\beta} (v_{z\beta})_\beta} = \frac{\hbar^2}{m v_F a^2} |G_i|. \tag{22}
\]
The prefactor of \(\mu_{EE}\) is of the order of \(\hbar^2/m v_F a^2 \sim 1/\text{nm}\), and the spin mixing conductance \(G_i\) is that presented in Fig. 1 of the order \(1 \sim 10\), yielding a \(\mu_{EE}\) close to that obtained experimentally[14]. Remarkably, \(\mu_{EE}\) calculated out of this quantum tunneling theory is independent of the surface cleanliness \(\gamma\), and depends on \(\{\ell_{F}, J_{sd}, \mu, T\}\) through the spin mixing conductance \(G_i\). The dependence of \(|G_i|\) on \(\mu\) shown in Fig. 2 is in accordance with the \(\mu_{EE}\) extracted experimentally[14], which remains constant in a wide range of positive \(\mu\). The reduction of \(\mu_{EE}\) near the Dirac point may be attributed to certain quantum corrections omitted in our approach, such as weak anti-localization[35] or Berry phase effects[50–52].

III. SPIN PUMPING AND INVERSE EDELSTEIN EFFECT

A. Spin pumping

We now formulate the spin pumping within the quantum tunneling formalism. The principle is to solve the Bloch equation of the conduction electron spin in the FMM[44, 53]
\[
\frac{\partial \langle \sigma \rangle_{F\beta}}{\partial t} + \partial_z \mathbf{j}_{\beta z} = \frac{J_{sd}}{\hbar} \mathbf{S} \times \langle \sigma \rangle_{F\beta} - \mathbf{\Gamma}_{\beta sf}, \tag{23}
\]
in the presence of a magnetization dynamics \(d\mathbf{S}/dt\), where \(\mathbf{\Gamma}_{\beta sf}\) is a spin relaxation term. To apply the Bloch equation to the dynamical magnetization, we assume that in equilibrium and at zero time \(t = 0\) where
the magnetization is static, there is an equilibrium spin density parallel to the magnetization
\[ \langle \sigma(z, 0) \rangle_{F\beta} = \langle \sigma(z, 0) \rangle_{F\beta 0} \parallel \hat{S} \parallel \hat{z}_2. \]  
(24)

After the magnetization starts moving \(d\mathbf{S}/dt \neq 0\), the spin density starts to deviate from its equilibrium value by
\[ \langle \sigma(z, \delta t) \rangle_{F\beta} = \langle \sigma(z, 0) \rangle_{F\beta 0} + \delta \langle \sigma(z, \delta t) \rangle_{F\beta}. \]  
(25)

We use the rotated coordinate \((x_2, y_2, z_2)\) that moves with the magnetization[44]
\[ \dot{x}_2 = \frac{1}{|d\mathbf{S}/dt|} \frac{d\mathbf{S}}{dt}, \quad \dot{y}_2 = \frac{1}{|d\mathbf{S}/dt|} \hat{S} \times \frac{d\mathbf{S}}{dt}, \]  
(26)
as shown in Fig. 3. After the small time lapse \(\delta t\), the angle that the magnetization makes with its equilibrium direction is
\[ \lim_{\delta t \rightarrow 0} \sin \theta' = \theta' = \left. \frac{d\hat{S}}{dt} \right|_{\delta t} \frac{1}{\hat{S}} \left| \frac{d\mathbf{S}}{dt} \right| \delta t. \]  
(27)

According to that calculated in Sec. II.B, as long as the magnetization makes an angle \(\theta'\) with the equilibrium spin, the wave functions will yield a spin deviation
\[ \delta \langle \sigma \rangle_{F\beta} = \langle \sigma^\prime \rangle_{F\beta} \hat{x}_2 \]
\[ = -|A_\beta|^2 \sin \theta' \left[ \sin k_{\beta\ell}(z - \ell_N - \ell_F) \right] \times \sin k_{\beta\ell}(z - \ell_N - \ell_F) \hat{x}_2 \]
\[ = -|A_\beta|^2 \frac{\delta t}{\tau_{sd}} \frac{d\mathbf{S}}{dt} \times \left[ \sin k_{\beta\ell}(z - \ell_N - \ell_F) \right] \hat{x}_2. \]  
(28)

The three terms in Eq. (23) then read
\[ \frac{\partial \langle \sigma \rangle_{F\beta}}{\partial t} = \frac{\delta \langle \sigma \rangle_{F\beta}}{\delta t} = \left. \frac{d\hat{S}}{dt} \right|_{\delta t} \frac{1}{\hat{S}} \left| \frac{d\mathbf{S}}{dt} \right| \delta t, \]
\[ \frac{J_{sd}}{\hbar} \mathbf{S} \times \langle \sigma \rangle_{F\beta} = \frac{\delta t}{\tau_{sd}} \frac{d\mathbf{S}}{dt}, \]
\[ \mathbf{\Gamma}_{sf} = \frac{\delta \langle \sigma \rangle_{F\beta}}{\delta t} = \frac{\delta \langle \sigma \rangle_{F\beta}}{\tau_{sf}} \frac{d\mathbf{S}}{dt}. \]  
(29)

where \(\tau_{sd} = \hbar/J_{sd}\) and \(\tau_{sf}\) is the spin relaxation time. Since the last two terms in Eq. (29) are proportional to \(\delta t\) and vanish in the \(\delta t \rightarrow 0\) limit, the Bloch equation reduces to the left hand side of Eq. (23), whose integration over the FMM slab yields the spin current flowing towards the TI
\[ a^2 j_{\beta 0} = a^2 j_{\beta \ell_N} = a^2 \int_{\ell_N}^{\ell_N + \ell_F} \frac{d\mathbf{S}}{dt} \cdot \frac{\partial \langle \sigma \rangle_{F\beta}}{\partial t}, \]
\[ = -|A_\beta|^2 \frac{d\mathbf{S}}{dt} \frac{N_F \hbar^2}{4 \pi m a^2} g_\beta(k_{\beta\ell}, \ell_F) = \frac{d(\langle \sigma \rangle_{k\beta})}{dt}. \]  
(30)

We have used the fact that the NM part does not consume spin, so \(a^2 j_{\beta 0} = a^2 j_{\beta \ell_N}\), and in the last line we have used angular momentum conservation to identify the spin current flowing into the TI with the time rate of the surface state spin. We see that the surface state spin expectation value \(\langle \sigma \rangle_{k\beta}\) at momentum \(k\) changes because of the magnetization dynamics \(d\mathbf{S}/dt\), manifesting spin pumping. Moreover, at a time \(t\) when the magnetization dynamics is a specific \(d\mathbf{S}/dt\), the time rate of such change is the same for all momenta \(k\) of the surface state that have the same energy \(E_{k\beta}\). Finally, because \(|A_\beta|^2\) represents the equilibrium spin density in the FMM induced by the exchange coupling \(J_{sd}\mathbf{S} \cdot \sigma\) in Eq. (10), we use the Pauli paramagnetic susceptibility and identify
\[ |A_\beta|^2 \approx \frac{N_F J_{sd} a^2}{a^2}, \]  
(31)
which is approximated as momentum independent, with \(N_F\) the DOS of the FMM at the Fermi surface.

Figure 3. (a) The rotated coordinate used in the spin pumping calculation. (b) Schematics of the inverse Edelstein effect caused by an instantaneous magnetization dynamics \(d\mathbf{S}/dt \parallel \hat{y}\) in the FMM. The generalized spin force \(d\mathbf{S}/dt\) must project to the spin-momentum locked \(\langle \sigma \rangle_{k\beta}\) in order to increase the population of \(\langle \sigma \rangle_{k\beta}\), which yields a shift of the Fermi surface (dotted circle, assumed to be at the hole cone) and hence a charge current along \(\hat{x}\).

### B. Inverse Edelstein effect based on spin pumping

We proceed to discuss the charge current generated at the TI surface by the spin pumping in the TI/NM/FMM trilayer, i.e., the inverse Edelstein effect based on spin pumping. Our starting point is that the time rate of the surface state spin, \(d(\langle \sigma \rangle_{k\beta})/dt\) in Eq. (30), serves as a generalized spin force and yields the Boltzmann equation
\[ \frac{d(\langle \sigma \rangle_{k\beta})}{dt} = \frac{2\pi a^2}{\hbar} \int \frac{d^2k}{(2\pi)^2} \langle \langle \psi k\beta | V | \psi k\beta \rangle \rangle^2 \times \delta(E_{k\beta} - E_{k\beta}) [f_{k\beta} - f_{k\beta}]. \]  
(32)

In essence, we treat \(\langle \sigma \rangle_{k\beta}\) as part of the phase space of the Boltzmann equation. The derivative \(\nabla_{\langle \sigma \rangle}\) is interpreted as the gradient along the direction that the population of \(\langle \sigma \rangle_{k\beta}\) increases without changing the orientation of \(\langle \sigma \rangle_{k\beta}\). It is given by
\[ \nabla_{\langle \sigma \rangle} f_\beta = \langle \sigma \rangle_{k\beta} \frac{\beta \partial f_\beta}{\partial k} = \langle \sigma \rangle_{k} \frac{v_F}{a} \frac{\partial f_\beta}{\partial E_{k\beta}}. \]  
(33)
because first the generalized spin force \( d(\sigma)_{k\beta}/dt \) in Eq. (32) has to project to \((\sigma)_{k\beta}\) to be accommodated by the state at \(k\), and because of the spin momentum locking, the increase of population of \((\sigma)_{k\beta}\) is in the radial direction but opposite between the electron and the hole cone \(\beta \partial \beta / \partial k\), with \(1/\alpha\) inserted to keep the derivative dimensionless.

Without loss of generality, and for the sake of comparing with Sec. II A, we assume that at a specific moment \(t\) the magnetization dynamics is along \(dS/dt \parallel \hat{y}\). Using the same expansion and ansatz as Eq. (4), and the identification in Eq. (31), the solution to the distribution function is

\[
 f_{\beta} = n_{F\beta} - \left. \frac{d\hat{S}}{dt} \right|_{(2\pi)^2} \frac{N_F h^3}{a^3 m k_\gamma^2} g_\beta(k_{\beta\sigma}, \ell_F) \frac{\partial n_{F\beta}}{\partial E_{k\beta}} \cos \alpha, \tag{34}
\]

which yields a nonzero average velocity along \(\hat{x}\) direction

\[
 \sum_\beta \langle v_x \rangle_\beta = \sum_\beta a^2 \int \frac{d^2k}{(2\pi)^2} f_\beta \frac{v_F}{h} \beta \cos \alpha
 = -\frac{N_F h^2}{4\pi m v_G} \left. \frac{d\hat{S}}{dt} \right|_{G_i}, \tag{35}
\]

whereas the current in the \(\hat{y}\) direction \(\langle v_y \rangle_\beta\) vanishes because of the angular integration. Notice that Eq. (35) and Eq. (21) are described by the same spin mixing conductance \(G_i\), indicating that the response coefficients are the same. Thus we see that a spin dynamics \(dS/dt\) along \(\hat{y}\) generates a charge current along \(\hat{x}\), a reciprocal process of the field-like STT in Sec. II B. Since their response coefficients are the same and the directions are reciprocal, the Onsager relation between STT and spin pumping is deliberately satisfied in our approach[54], and the spin pumping has the same \(\{\ell_F, J_{sd}, \mu, k_B T\}\) dependence as that of the STT shown in Fig. 1.

We argue the total spin current in the TI caused by spin pumping by noticing that the nonequilibrium part of Eq. (34) generates a spin accumulation

\[
 \sum_\beta \langle \sigma \rangle_\beta = \sum_\beta a^2 \int \frac{d^2k}{(2\pi)^2} f_\beta \langle \sigma \rangle_{k\beta}
 = \hat{y} \frac{N_F h^3}{4\pi m v_F} \left. \frac{d\hat{S}}{dt} \right|_{G_i}, \tag{36}
\]

In the presence of a phenomenological spin relaxation time \(\tau_{sf}\), approximated as momentum independent, the total spin current is identifiable with \(\sum_\beta \langle \sigma \rangle_\beta / \tau_{sf}\). This total spin current and (35) allow to define the length scale that characterizes the efficiency of the spin current to charge current conversion in the inverse Edelstein effect[22, 24]

\[
 \lambda_{IEE} = \left| \sum_\beta \langle v_x \rangle_\beta / \tau_{sf} \right| = \frac{v_F \tau_{sf}}{h}, \tag{37}
\]

which takes the same form as a previous investigation[24], and is independent from the interface cleanliness, chemical potential, and temperature. To obtain the experimental value \(\lambda_{IEE} \sim nm\) requires \(\tau_{sf} \sim 10fs\), which also agrees with the experimental value[22].

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