Theory of bilinear magneto-electric resistance from topological-insulator surface states

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ABSTRACT

We theoretically investigate a new kind of nonlinear magnetoresistance on the surface of three-dimensional topological insulators (TIs). At variance with the unidirectional magnetoresistance (UMR) effect in magnetic bilayers, this nonlinear magnetoresistance does not rely on a conducting ferromagnetic layer and scales linearly with both the applied electric and magnetic fields; for this reason, we name it bilinear magneto-electric resistance (BMER). We show that the sign and the magnitude of the BMER depends sensitively on the orientation of the current with respect to the magnetic field as well as the crystallographic axes – a property that can be utilized to map out the spin texture of the topological surface states via simple transport measurement, alternative to the angle-resolved photoemission spectroscopy (ARPES).

Keywords: Topological insulator, spin-momentum locking, bilinear magneto-electric resistance, hexagonal warping effect

1. INTRODUCTION

Beyond doubt, the giant magnetoresistance (GMR) effect\textsuperscript{1–3} is one of the most important discoveries in the fruitful field of spintronics, which has found various commercial applications such as magnetic hard disk drives and magnetic memory devices. The building block of these devices is a trilayer structure (also known as a spin valve) which consists of two ferromagnetic metal (FM) layers separated by a nonmagnetic spacer. There is a large variation in the resistance when the magnetizations of the FM layers switch between parallel and antiparallel alignments. When a current is passing through one of the FM layers, the spins of the conduction electrons, due to the strong exchange coupling with the local magnetic moments, will be polarized along the magnetization direction of the FM layer (for this reason, this FM is also called a spin polarizer); the scattering rates of these conduction electrons, when they subsequently propagate through the other FM layer, will depend on their spin direction relative to the magnetization orientation of the FM layer, and so will the total resistance of the spin valve. Therefore, it is the exchange interaction and the spin-dependent scattering that play the key roles in the GMR effect.

In the past decade, both theoretical and experimental endeavors have been dedicated to realizing similar functionalities of a spin valve in magnetic bilayer structures consisting of a ferromagnetic layer and a nonmagnetic layer with strong spin-orbit coupling. The main idea is to use spin-orbit coupling together with structural inversion asymmetry to generate net spin density (or spin accumulation) at the interface through the spin Hall\textsuperscript{4–8} or Rashba-Edelstein effect.\textsuperscript{9–11} Recently, a small change in the longitudinal resistance has been observed in several magnetic bilayer structures\textsuperscript{12–21} by reversing the magnetization direction in the presence of an in-plane current perpendicular to the magnetization, that is to say, $R_l(M,j) \neq R_l(-M,j)$ where $R_l$ is the total longitudinal resistance of the bilayer, $M$ and $j$ are the magnetization and current-density vectors. Note that by symmetry, reversing the magnetization in a magnetic layer is equivalent to reversing the current direction; thus, the magnetoresistance change must be associated with certain nonlinear current response (for this reason, the magnetoresistance effect has been coined in the literature the unidirectional magnetoresistance (UMR)\textsuperscript{22}), which

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makes it distinctly different from other linear magnetotransport phenomena previously studied in magnetic bilayer systems such as the (hybrid) spin Hall magnetoresistance,\textsuperscript{22–25} interfacial spin-orbit magnetoresistance,\textsuperscript{26–28} Hanle magnetoresistance,\textsuperscript{29–31} nonlocal (spin Hall) anomalous Hall\textsuperscript{24,32} and etc. Several different interpretations have been proposed to account for the UMR effect including the interfacial and bulk spin-dependent scattering mechanism\textsuperscript{12,33,34} and the interfacial spin-flip electron-magnon scattering mechanism.\textsuperscript{15–17,20} We note that all these mechanisms rely on one common key ingredient – the current-induced interfacial spin accumulation which in turn alters either the spin asymmetry of the density of the conduction electrons or that of the scattering rate\textsuperscript{a}.

In this work, we theoretically investigate a new kind of nonlinear magnetoresistance originating from the topological insulator surface states, which does not require a magnetic layer. We name this new magnetoresistance effect as bilinear magneto-electric resistance (BM ER) due to its linearity with both the external electric and magnetic fields. At variance with the UMR effect, the BM ER emanates from the conversion of a \textit{nonlinear spin current} to a charge current rather than the current-induced spin density. The physical picture of the BM ER is schematically depicted in Fig. 1 for the surface states of a TI with hexagonal warping.\textsuperscript{42} Due to the spin-momentum locking of the topological surface states, electrons in the \(k\) and \(-k\) states carry opposite spins and have opposite group velocities [i.e., \(v(-k) = -v(k)\)]. When an external electric field \(E\) is applied along certain \(k\) direction, its first-order correction to electron distribution is known to be an accumulation of electrons in the \(k\) states and equal number of electrons depleted in the \(-k\) states, giving rise to a charge current \(j_z = eE\) and a net spin density \(\delta s \sim \hat{z} \times E\) with \(\hat{z}\) denoting the normal vector perpendicular to the surface, while the second-order correction to the electron distribution, which has not been well studied, results in equal number of electrons populated in the surface states with opposite momenta as well as spins and thus induces a \textit{nonlinear pure spin current} \(j_s \sim E^2\). When a magnetic field is applied, both the group velocity and the second-order distribution are shifted in \(k\)-space and then the two fluxes of electrons with opposite spin orientations no longer compensate each other, causing the spin current to be partially converted into a charge current \(\delta j_z \sim E^2\). From an application perspective, the BM ER can be used to map the spin texture of surface states with spin-momentum locking by simple transport measurements, which has been demonstrated experimentally on the conducting surface of the topological insulator \(\text{Bi}_2\text{Se}_3\) and for the two dimensional electron gas on the (111) surface of \(\text{SrTiO}_3\).\textsuperscript{46}

The remainder of the paper is organized as follows. The general formulation of the nonlinear current response of the TI is developed in Sec. 2: We start with the model Hamiltonian for the TI surface states in Sec. 2.1 followed by a discussion of general symmetry considerations of the system and the nonlinear current-response function in Sec. 2.2; then we solve the semi-classical Boltzmann equation up to the second order in the external electric field in Sec. 2.3 and present the detailed derivation of the nonlinear current response function in Sec. 2.4. In Sec. 3.1, we use the general formula for the nonlinear response function to derive an analytical expression for the BM ER from the TI surface states in the presence of hexagonal warping, and then provide more detailed discussions on various aspects of the BM ER effect, including its dependences on the hexagonal warping (Sec. 3.2), the momentum relaxation time (Sec. 3.3) as well as the Berry curvature effect (Sec. 3.4). Finally, we summarize our main results in Sec. 4.

2. GENERAL FORMULATION

2.1 Model Hamiltonian

Let us start with the following model Hamiltonian for a Dirac electron in the topological surface state:

\[
\mathcal{H}_{TI} = \sigma \cdot \left[ h(k) + g\mu_B B \right]
\]

\textsuperscript{a}Previous studies have shown that when an in-plane current is applied in a bilayer consisting of a heavy metal and a ferromagnet, spin accumulation will be induced at the interface due to the spin Hall effect in the heavy metal layer. In the presence of the spin-flip electron-magnon scattering, the spin accumulation may create or annihilate interfacial magnons in the ferromagnetic layer, depending on the way it is aligned with the magnetization (either parallel or antiparallel). If the ferromagnetic layer is conducting, such variation in magnon density will in turn alter the scattering rate of the electrons in the ferromagnetic layer and hence change the total resistance of the bilayer accordingly.\textsuperscript{15–41}

\textsuperscript{1}Similar nonlinear spin current was also proposed\textsuperscript{43,44} recently in other systems with broken inversion symmetry.
Figure 1. Schematics of the physical mechanism of the BMER arising from the TI surface states with hexagonal warping. Panel a: Dirac cone in a 3D TI with hexagonal warping. Panel b: Spin texture of the Fermi contour in the presence of hexagonal warping. Panel c: Variation of the electron distribution in the applied electric field $E$: $f_1$ (blue curve) and $f_2$ (yellow curve) are respectively the corrections to the equilibrium distribution of the first- and second-order in $E$. Solid arrows represent excess of electrons with spins along the arrow direction, and hollow arrows represent depletion of the same. Panel d: When an external electric field $E$ is applied along a certain direction in the momentum space (dash-dotted line), a nonlinear pure spin current $j_s(E^2)$ is generated at the second order in $E$, due to spin–momentum locking. When an external magnetic field $B$ is applied, the nonlinear spin current is partially converted into a charge current $\delta j_e(E^2)$: a high(low)-resistance state can be reached by applying a magnetic field antiparallel (parallel) to the spin direction of the electronic states with $k \parallel E$, as shown in panels e and f respectively.

with $\sigma$ the Pauli spin matrices, $B$ the uniform external magnetic field, $g$ and $\mu_B$ representing the $g$-factor and the Bohr magneton respectively, and

$$h(k) = \alpha \hbar k \times \hat{z} + \lambda \hbar \frac{k^2}{2} (k_x^2 - 3k_y^2),$$

(2)

where $\alpha$ is the Dirac velocity, and the term cubic-in-$k$ describes the hexagonal warping effect. Note that the hexagonal warping term leads to a threefold rotational symmetry $C_3v$, which becomes more transparent when we rewrite $h(k)$ in its angular form as

$$h(k) = \alpha \hbar k (\sin \phi_k \hat{x} - \cos \phi_k \hat{y}) + \left( -\frac{\lambda k^3}{2} \cos 3\phi_k \right) \hat{z},$$

(3)

where $\phi_k$ is the azimuthal angle of the wavevector $k$ with respect to the $x$-axis.

The energy dispersion can be obtained by

$$\varepsilon^s(k) = s |h(k) + g \mu_B B|,$$

(4)

where $s = +1$ and $-1$ correspond to the upper and lower surface bands respectively, and the group velocity is given by

$$v^s(k) = \frac{\partial \varepsilon^s(k)}{\hbar \partial k}.$$

(5)

Note that the group velocity is odd in $k$ in the absence of the external magnetic field. In what follows, we shall assume the Fermi level lies in the upper band ($s = +1$) and thus suppress the superscript for the band index hereafter. Also note that the Berry curvature effects on the density of states and the orbital magnetic moment are not included since they are negligibly small when the Fermi surface is far away from the Dirac point, as we will show in Sec. 3.4.
2.2 Symmetry considerations

In the absence of the external magnetic field, the effective Hamiltonian for the topological surface states, i.e., $\mathcal{H}_{TI}^{(0)} = \mathbf{\sigma} \cdot \mathbf{h}(\mathbf{k})$, is invariant under the following two operations: 1) Mirror reflection about the $y$-$z$ plane, i.e., $M: x \rightarrow -x$, and 2) threefold rotation $C_3$ about the $z$-axis. Here, we are interested in the nonlinear current-density response to the second-order electric field and the first-order magnetic field, i.e.,

$$j^{(2)}_{e,a} = \sum_{bcd} K_{abcd} E_b E_c B_d,$$

where the response function $K_{abcd}$ is a fourth-rank tensor with indices $a, b, c = x$ or $y$ and $d = x, y$ or $z$. For the transport in the surface states, the external electric field is applied in the $x$-$y$ plane (parallel to the surface of the TI) while the magnetic field can be three-dimensional; therefore, the tensor $K_{abcd}$ has 24 elements in total.

As the response function is the property of the unperturbed system, we should expect it to reflect the same symmetries as those of $\mathcal{H}_{TI}^{(0)}$.

First, we note that the mirror symmetry of the unperturbed 2D system requires that the tensor element $K_{abcd}$ must be zero if, under mirror reflection operation $M: x \rightarrow -x$, the corresponding current component $j_{e,a}$ changes sign whereas the product of the external fields $E_b E_c H_d$ is invariant, and vice versa. Without doing any further calculation, we know the following 12 tensor elements are zero, i.e.,

$$K_{xxxx} = K_{xxyy} = K_{xyxy} = K_{xxyy} = K_{xyyx} = 0$$

and

$$K_{yyyy} = K_{yyxx} = K_{yxxy} = K_{yxyx} = K_{yyyz} = K_{yxxz} = 0.$$

The other 12 tensor elements could remain finite. Furthermore, arising from the threefold rotational symmetry about the $z$-axis, some of the remaining 12 tensor elements have equal values, as we will show explicitly below.

2.3 Second-order nonequilibrium distribution function

Now let us examine the following single-band steady-state Boltzmann equation

$$\frac{E_a}{\hbar} \frac{\partial f}{\partial k_a} = -f - f_0 \tau,$$

where we have assumed, for simplicity, a constant relaxation time $\tau$. Expand the distribution function in powers of the electric field, i.e.,

$$f = f_0 + f_1 + f_2 + ...,$$

where $f_0$ is the equilibrium Fermi distribution, $f_1$ and $f_2$ are the nonequilibrium distribution functions of the first- and second-order in the electric field, i.e., $f_1 \propto E_a$ and $f_2 \propto E_a E_b$. Placing the expansion (8) in the Boltzmann equation (7) and equating terms on the left and right sides of equal order in the electric field, we get

$$\frac{E_a}{\hbar} \frac{\partial f_i}{\partial k_a} = -\frac{f_{i+1}}{\tau},$$

where $i = 0, 1, 2, ...$ By solving the series of equations iteratively, we find the first-order nonequilibrium distribution function takes the familiar form

$$f_1 = -\frac{\tau E_a}{\hbar} \frac{\partial f_0}{\partial k_a},$$

and the second-order nonequilibrium distribution function of interest can be expressed as

$$f_2 = \frac{\tau^2}{2\hbar^2} \sum_{ab} \frac{\partial^2 f_0}{\partial k_a \partial k_b} E_a E_b,$$

where the prefactor $\frac{1}{2}$ eliminates double counting in the summation.
2.4 Nonlinear current response function

The charge current density can be calculated via $j^e = -e \int \frac{d^2 k}{(2\pi)^2} \mathbf{v}(k) f(k)$. It follows that the nonlinear component of the current density of interest can be expressed as

$$j^{(2)}_{e,a} = -e g_B \left(\frac{e \tau}{\hbar}\right)^2 \frac{1}{2} \sum_{k,b,c,d} \left( \frac{\partial^3 f_0}{\partial k_b \partial k_c \partial h_d} v_a + \frac{\partial^2 f_0}{\partial k_b \partial k_c} \frac{\partial v_a}{\partial h_d} \right) E_b E_c B_d,$$

where we have used the relation $\frac{\partial}{\partial B_d} \bigg|_{B=0} = g_B \frac{\partial}{\partial h_d}$ with $h_d (d = x, y, or z)$ the Cartesian components of the vector $\mathbf{h}(k)$ given by Eq. (2). Note that in deriving these results, we have assumed that the linear term in the Hamiltonian tensor. The results for the nonzero tensor elements are

$$K_{abcd} = -e g_B \left(\frac{e \tau}{\hbar}\right)^2 \frac{1}{4} \sum_k f_0' \left( \frac{\partial h}{\partial h_d} \frac{\partial^2 v_a}{\partial k_b \partial k_c} - \frac{\partial h}{\partial k_b} \frac{\partial^2 v_a}{\partial k_c \partial h_d} + \{b \leftrightarrow c\} \right),$$

Performing integration by parts on the r.h.s. of the above equation, we get

$$K_{abcd} = -e g_B \left(\frac{e \tau}{\hbar}\right)^2 \frac{1}{4} \sum_k f_0' \left( \frac{\partial h}{\partial h_d} \frac{\partial^2 v_a}{\partial k_b \partial k_c} - \frac{\partial h}{\partial k_b} \frac{\partial^2 v_a}{\partial k_c \partial h_d} + \{b \leftrightarrow c\} \right),$$

where $f_0' = \frac{\partial f_0}{\partial h}$ with $h = |\mathbf{h}(k)|$, and $\{b \leftrightarrow c\}$ is the shorthand notation of two more terms that are simply the first two terms in the parentheses with the indices $b$ and $c$ interchanged. Note that when the temperature at which the current is measured is much lower than the Fermi temperature, it is a good approximation to replace $f_0'$ with the delta function $-\delta (h - \varepsilon_F)$ and it follows that $\int d^2 k \delta (h - \varepsilon_F) \frac{f(k)}{\varepsilon_F} = \mathcal{F}_{FL} k d \phi \frac{2 F(k)}{\sqrt{\varepsilon_F h}}$. It is straightforward to express the derivatives in the parentheses as those of $h^2$ or $h_a$ with respect to $k_b (a, b = x, y, or z)$ as follows

$$K_{abcd} = \frac{\varepsilon_F^2 g_B}{8\pi^2 h^3} \int_{\text{FL}} \frac{k d \phi_k}{|\nabla_k |} \left\{ \frac{\partial_{abc} h^2}{h} - \frac{2 (\partial_a h^2)(\partial_b h^2) + (\partial_b h^2)(\partial_{ab} h^2) + (\partial_{ab} h^2)(\partial_b h^2)}{4h^3} \right\} h_d$$

$$- \frac{\varepsilon_F^2 g_B}{8\pi^2 h^3} \int_{\text{FL}} \frac{k d \phi_k}{|\nabla_k |} \left( \frac{\partial_{abc} h^2}{h} \right) \frac{2 (\partial_a h_d)(\partial_b h_d)(\partial_c h_d)(\partial_{ab} h^2) + (\partial_{ab} h_d)(\partial_d h_d)(\partial_c h_d)(\partial_{ab} h^2)}{4h^3},$$

where we have used the identities $\frac{\partial h}{\partial h_d} = \frac{h_d}{h}$ and $\partial h \equiv \frac{\partial h}{\partial k_c} = \frac{\partial h^2}{2h}$, and have converted the summation over $k$ to an integral over the Fermi loop (FL) where $h = \varepsilon_F$ is a constant.

3. RESULTS AND DISCUSSIONS

3.1 Bilinear magneto-electric resistance (BMER)

Inserting Eq. (2) into Eq. (15), we can calculate all the elements of the nonlinear current-response function tensor. The results for the nonzero tensor elements are

$$K_{xyyz} = K_{yxyz} = K_{yyxz} = -K_{xxxx} = \frac{3 \kappa_0}{8\pi} \frac{\lambda \varepsilon_F}{(ah)^2}$$

$$K_{gyzz} = K_{xxyz} = K_{xgxz} = -K_{yxyy} = -K_{gyzy} = -K_{gyyy} = \frac{1}{3} K_{yyzz} = -\frac{1}{3} K_{exxy} = \frac{3 \kappa_0}{4\pi} \frac{\lambda^2 \varepsilon_F^3}{(ah)^5},$$

where $\kappa_0 = g_B e^2 \tau^2 / h^3$. All other 12 tensor elements are zero, in agreement with the symmetry analysis that we carried out earlier. Note that in deriving these results, we have assumed that the linear term in the Hamiltonian
for the TI surface states (1), giving rise to the spin-momentum locking, is dominant over the cubic hexagonal warping term.

Having known these tensor elements, we can write the two Cartesian components of the current density as

\[
\begin{align*}
{j^{(2)}_{x,y}} &= -c_\parallel E_y B_x + \frac{2}{3} c_\parallel E_x E_y B_x - \frac{1}{3} c_\parallel E_y E_y B_y - c_\perp (E_x^2 - E_y^2) B_z, \\
{j^{(2)}_{x,z}} &= c_\parallel E_y B_x - \frac{2}{3} c_\parallel E_x E_y B_y + \frac{1}{3} c_\parallel E_x E_x B_x + 2c_\perp E_x E_y B_z,
\end{align*}
\]

where \(c_{\parallel} = \frac{9\lambda^3 e^2}{8\pi^2 v_F^2} \) and \(c_{\perp} = \frac{3\lambda^3 e^2}{8\pi^2 v_F^2} \) with the subscripts “\(\parallel\)" and “\(\perp\)" refer to the terms associated with the in-plane and out-of-plane components of the external magnetic field respectively. The longitudinal resistivity can be calculated via \(\rho_l = E \cdot j_e / |j_e|^2 \) with \(j_e = j_e^{(1)} + j_e^{(2)} + \ldots\) the total current density. Up to the first order in the external electric field, we obtain

\[
\rho_l = \rho_0 - E \left[ \rho_\parallel^{(2)} (B_x \sin \phi_E - B_y \cos \phi_E) - \rho_\perp^{(2)} B_z \cos 3\phi_E \right] + O(E^2),
\]

where \(E\) is the magnitude of the external electric field \(E\), \(\phi_E\) is the angle between \(E\) and the \(x\)-axis, \(\rho_0 = \frac{4\pi\hbar^2}{e^2 v_F}\) is the linear surface resistivity independent of \(E\), and the coefficients

\[
\rho_\parallel^{(2)} = \left( \frac{36\pi g e B}{e^2 h^4} \right) \frac{\lambda^2 \varepsilon_F}{\alpha^5} \quad \text{and} \quad \rho_\perp^{(2)} = \left( \frac{6\pi g e B}{e^2 h} \right) \frac{\lambda}{\alpha^2 \varepsilon_F}
\]

characterize the magnitudes of the nonlinear surface resistivities for the in-plane and out-of-plane components of the external magnetic fields respectively.

Now we are in a position to provide some remarks on the nonlinear component of the surface resistivity, i.e., the second term on the r.h.s. of Eq. (17). 1) The nonlinear resistivity is linearly proportional to the electric and magnetic fields. 2) The nonlinear resistivity is inversely proportional to \(e\), similar to the regular Hall coefficient; thus one would expect it to change sign as the type of the charge carrier changes from electrons to holes, and vice versa. 3) The nonlinear resistivities associated with the in-plane and out-of-plane components of the magnetic fields exhibit different dependences on the hexagonal warping, i.e., \(\rho_\parallel^{(2)} \propto \lambda^2\) and \(\rho_\perp^{(2)} \propto \lambda\), and both of them vanish when \(\lambda \to 0\), because the in-plane and out-of-plane magnetic fields play different roles in altering the energy dispersion of the surface states. We will elaborate on this point in Sec. 3.2. 4) As shown by Eq. (18), the nonlinear resistivity turns out to be independent of the relaxation time constant \(\tau\) and only depends on the main material parameters of the TI surface states (namely \(\alpha, \lambda\) and \(\varepsilon_F\)). This is somewhat surprising as it indicates that the nonlinear resistivity is independent of scatterings. We note that this finding should be taken with caution due to the constant relaxation time approximation made in our model calculation; we will discuss in more details the validity of the approximation in Sec. 3.3. 5) In addition to the longitudinal component of the nonlinear resistivity, one can also derive its transverse counterpart via \(\rho_t = \hat{z} \cdot (E \times j_e) / |j_e|^2\); in order to concentrate on the BMER effect, we will study this nonlinear Hall effect elsewhere.\(^{47}\)

To evaluate the magnitude of the nonlinear resistivity relative to the linear resistivity \(\rho_0\), we may define the BMER as follows

\[
BMER = \frac{\rho_l (E, B) - \rho_l (-E, B)}{\rho_l (E, B) + \rho_l (-E, B)}.
\]

Placing Eq. (17) in (19) and expanding terms up to the first order in \(E\), we get

\[
BMER = \frac{EB}{\rho_0} \left[ \rho_\parallel^{(2)} \sin \theta_H \sin (\phi_H - \phi_E) + \rho_\perp^{(2)} \cos \theta_H \cos 3\phi_E \right],
\]

where \(\theta_H\) and \(\phi_H\) are, respectively, the polar and azimuthal angles of the magnetic field, and \(B\) is the magnitude of the magnetic field. In Fig. 2, we show the angular dependence of the BMER for magnetic field scans in \(x\)-\(y\), \(y\)-\(z\) and \(z\)-\(x\) planes with the electric field applied along three typical crystallographic axes.
3.2 Dependence of BMER on the hexagonal warping

As we noted earlier that the BMER’s for the in-plane and out-of-plane magnetic fields exhibit different dependences on the hexagonal warping, i.e., $\rho^{(2)}_\parallel \propto \lambda^2$ and $\rho^{(2)}_\perp \propto \lambda$. The two distinct dependences of BMER on the hexagonal warping emanate from the different roles played by the in-plane and out-of-plane magnetic fields to the surface band structure of the TI. This can be seen by rewriting Eq. (4) as follows

$$\varepsilon^s(k) = s\sqrt{\alpha \hbar (k - \delta k) \times \hat{z}}^2 + [\lambda k^3 \cos(3\phi_k) + \Delta_g]^2, \quad (21)$$

where

$$\delta k = \frac{g \mu_B}{\alpha \hbar} \mathbf{B} \times \hat{z} \quad \text{and} \quad \Delta_g = g \mu_B B_z. \quad (22)$$

In the absence of the hexagonal warping effect (i.e., $\lambda = 0$), we can see that an in-plane magnetic field shifts the Dirac cone rigidly in the $k_x-k_y$ plane, whereas an out-of-plane magnetic field opens up a band gap of $2\Delta_g$ at the Dirac point. Consequently, without the cubic hexagonal warping term, applying an in-plane magnetic field would not alter the current provided the system has translational symmetry in the $x$-$y$ plane, and likewise an out-of-plane magnetic field wouldn’t do so as long as the Fermi level lies far away from the gap opened by $B_z$ (note that the gap is about 2 meV for $B_z = 10$ T and $g = 2$).

In the presence of the hexagonal warping effect, however, a magnetic field not only shifts the Dirac cone and/or open up a gap, but also deforms the snow-flake-like Fermi contour accordingly, as shown in Fig. 3. It follows that both the group velocity and the second-order distribution function are shifted in $k$-space in a way that the two fluxes of electrons with opposite spin orientations no longer compensate each other, giving rise to the BMER effect.

3.3 Dependence of BMER on the momentum relaxation time

As we have pointed out in the end of Sec. 3.1, the nonlinear longitudinal resistivity turns out to be independent of the relaxation time $\tau$. Here we want to emphasize that this result relies on two approximations that we made in our calculation: 1) constant relaxation time approximation and 2) single-band contribution to the conductivity. The constant relaxation time approximation is valid when the scattering potential is isotropic and short-ranged. However, when there are multiple bands contributing to the conduction, the nonlinear resistivity would still depend on the relaxation time of each band even if the relaxation times are momentum independent. To see this, let us consider a simple case of two bands with constant relaxation times $\tau_a$ and $\tau_b$. The total current density is the sum of the contributions from the two bands (neglecting interband transition); for a simple 1-D problem in which an electric field is applied in the $x$-direction, the total current density is given by

$$j_x = j_{a,x} + j_{b,x} = (c_a,1\tau_a + c_b,1\tau_b)E_x + (c_a,2\tau_a^2 + c_b,2\tau_b^2)E_x^2 + O(E_x^3), \quad (23)$$
Figure 3. Magnetic-field induced deformation of the surface energy dispersion $\varepsilon(k)$. The top panels show the Dirac cones in the absence of the hexagonal warping ($\lambda = 0$), and the bottom panels show those in the presence of the hexagonal warping ($\lambda \neq 0$). In each panel, the Dirac cone in the absence of the external magnetic field is depicted in blue color, whereas that in the presence of the external magnetic field is depicted in orange color.

We see that the $\tau$-dependence of $\rho_{xx}$ disappears in the single-band case when either $c_{a,i}$ or $c_{b,i}$ ($i = 1, 2$) are set to zero; however, the nonlinear resistivity (i.e., the term linear in $E_x$) in general depends on the relaxation times in the two-band case when both $c_{a,i}$ and $c_{b,i}$ remain finite. The same conclusion holds for multiple-band ($i > 3$) cases.

### 3.4 Influence of the Berry phase effect on BMER

Hitherto we have not considered the influence of the Berry curvature of the surface bands on the nonlinear transport, which we shall justify below. Qualitatively speaking, the BMER effect relies on the hexagonal warping term which becomes important when the Fermi level lies far away from the Dirac point, as we have discussed in Sec. 3.2, whereas the Berry curvature effect is profound when the Fermi level is close to Dirac point. For the Bi$_2$Se$_3$ investigated in the recent experiment, the Fermi level lies far away from the Dirac point, and hence the Berry curvature effect on the BMER is negligible. Below, we will perform an order-of-magnitude estimation to confirm this.

In the presence of an external magnetic field, the Berry curvature alters the transport property in two ways: 1) a correction to the density of states \cite{48, 49} as

$$
\bar{D}(k) \equiv 1 + \frac{e}{\hbar} \Omega(k) \cdot B
$$

and 2) a correction to the total band energy due to the orbital magnetic moment, \cite{49}, i.e.,

$$
\varepsilon_M(k) = \varepsilon(k) - m(k) \cdot B.
$$
From the full Hamiltonian of the surface states (1), we can derive the following general expression for the Berry curvature
\[
\Omega(k) = -\frac{\alpha \hbar^2}{2 |\varepsilon(k)|^3} \left[ \alpha (g \mu_B B_z - 2 \lambda k^3 \cos 3\phi_k) + 3\lambda k^2 g \mu_B (B_x \sin 2\phi_k + B_y \cos 2\phi_k) \right] \hat{z}.
\] (27)

And for the two-band model, one can easily show that the orbital magnetic moment is proportional to the product of the energy dispersion and the Berry curvature, i.e.,
\[
m(k) = \frac{e}{\hbar} \varepsilon(k) \Omega(k),
\] (28)

where the energy dispersion of the upper band, \(\varepsilon(k)\), is given by Eq. (4) with \(s = 1\).

Equipped with Eqs. (25) - (28), we are ready to estimate the sizes of Berry curvature effects on the BMER. Using the following material parameters relevant to the experiments: \(\alpha = 5 \times 10^5 \text{ m/s}, \lambda = 165 \text{ eV} \cdot \text{Å}^3, \varepsilon_F = 0.256 \text{ eV}, g = 2, B_x = B_y = B_z = 5 \text{ T}, \text{ and } k_F \sim \frac{\varepsilon_F}{\alpha \hbar} \approx 7.8 \times 10^8 \text{ m}^{-1}\), we obtain
\[
\max \left( \left| \frac{e}{\hbar} \varepsilon(k) \cdot B \right| \right) \sim 0.003 \ll 1
\]
and
\[
\max (|m(k) \cdot B|) \sim 0.001 \text{ eV} \ll \lambda k_F^3 < \alpha \hbar k_F \simeq \varepsilon_F,
\]
where \(\lambda k_F^3 \sim 0.08 \text{ eV}\). We thus conclude that the influence of the Berry curvature on the BMER can be neglected in our present case of interest.

4. SUMMARY AND CONCLUSION

In this paper, we have developed a transport theory for a new kind of nonlinear magnetoresistance on the surface of three dimensional TIs. At variance with the UMR effect in magnetic bilayers, the nonlinear magnetoresistance does not require the presence of a conducting ferromagnetic layer and scales linearly with both the applied electric and magnetic fields; for this reason, we name it bilinear magneto-electric resistance (BMER). We have also shown that the sign and the magnitude of the BMER depends sensitively on the orientation of the current with respect to the magnetic field as well as the crystallographic axes – a property that can be utilized to map out the spin texture of the topological surface states via simple transport measurement.

The physical origin of the BMER is a partial conversion from the nonlinear spin current to charge current in the presence of an external magnetic field. An analytical expression of the BMER is derived based on a semiclassical Boltzmann transport theory in the relaxation time approximation, which allows us to further examine various aspects of the BMER. We find that, in addition to the spin-momentum locking of the topological surface states, the cubic hexagonal warping term also plays a crucial role in generating the BMER – the BMER vanishes in the absence of the hexagonal warping since in this case the external magnetic field can no longer deform the Fermi contour (provided that the Fermi level is not too close to the Dirac point). Also, we have shown that, the Berry curvature effect is unimportant when the Fermi level is far away from the Dirac point in which case the hexagonal warping effect is profound.

Acknowledgments

We are grateful to Pan He, Hyunsoo Yang, Guang Bian, Axel Hoffmann, Olle Heinonen, Shufeng Zhang and Albert Fert for helpful discussions. The theoretical framework for the BMER was developed by S. S.-L. Zhang and G. Vignale at the University of Missouri and was supported by NSF Grants DMR-1406568. Detailed analysis of various aspects of the BMER as well as the manuscript preparation was done by S. S.-L. Zhang at Argonne National Laboratory and was supported by Department of Energy, Office of Science, Materials Sciences and Engineering Division through Materials Theory Institute.
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