Influence of helical spin structure on the magnetoresistance of an ideal topological insulator

T Öztürk, R L Field III, Y S Eo, S Wolgast, K Sun and C Kurdak

1 Department of Physics, Selcuk University, Konya, 42075, Turkey
2 Department of Physics, University of Michigan, Ann Arbor, MI 48109, United States of America
E-mail: teozturk@gmail.com

Keywords: helical spin structure, topological insulators, Boltzmann transport, topological enhancement factor

Abstract

In an ideal topological insulator, the helical spin structure of surface electrons suppresses backscattering and thus can enhance surface conductivity. In this study, we investigate the effect of perpendicular magnetic field on the spin structure of electrons at the Fermi energy and define a magnetic-field dependent topological enhancement factor using Boltzmann transport and calculate this factor for different disorder potentials, ranging from short-range disorder to screened Coulomb potential. Within the Boltzmann approximation, the topological enhancement factor reaches its maximum value of 4 for a short-range disorder at zero magnetic field and approaches a value of 1 at high magnetic fields. The topological enhancement factor becomes independent of the nature of the disorder potential at high magnetic fields.

1. Introduction

A topological insulator (TI) is a new class of material with a bandgap in the bulk and gapless surface states arising from the topology of the bulk quantum wavefunctions [1–3]. The surface states are protected by time-reversal symmetry and are expected to dominate conduction at low temperatures. TIs were first predicted in two-dimensional semiconductors [4–6] and later generalized to three-dimensional systems [7, 8], such as Bi1–xSbx, Bi2Se3, Bi2Te3, and Sb2Te3 [9–14]. The presence of topologically protected surface states was first tested using angle-resolved photoemission spectroscopy (ARPES) measurements, which revealed a linear dispersion for these states [11, 13, 14]. In addition to the linear dispersion, the TIs must exhibit a helical spin structure, which is also confirmed by spin-resolved ARPES measurements [15, 16]. However, most experimentally studied TIs such as Bi1–xSbx [17] and Bi2Te3Se [18, 19] exhibit surface conduction which is polluted by defect-assisted bulk transport, thereby presenting challenges to separating the bulk from surface conduction. In contrast, for SmB6, recent experiments reveal that the surface dominant regime has been achieved [20, 21].

The helical spin structure of TIs induces unique transport properties. Most significantly, the locking of spin to the momentum direction inhibits backscattering in the absence of the external magnetic field [15, 22] and this leads to a quantum correction to conductivity, known as weak anti-localization [23, 24]. Also, compared to the classical framework of conductivity for normal metals, the locking of the spins for TIs results in an enhancement of conductivity. Although this enhancement is well-known to the community, the unique response to external magnetic fields is less understood. The role of spin-locking must be theoretically resolved to aid recent experimental magnetoconductivity reports on TIs. Here, we derive a topological enhancement factor using Boltzmann transport equation and calculate the magnetic field dependence of this enhancement factor to conductivity for different types of disorder potentials. We consider the effects of perpendicular magnetic field on the spin structure of surface states for an ideal TI. We find that the helical spin structure leads to an additional positive magnetoresistance at large magnetic fields, which is perpendicular to the surface-conducting layer. Furthermore, the size of the magnetoresistance is found to be greatest for short-range disorder.
2. Helical spin structure

The Hamiltonian of the surface states of an ideal TI is well known in two forms. Considering the surface perpendicular to the $\hat{z}$-direction, the Hamiltonians describing the low-energy physics of the surface states can be expressed as [12, 25]:

\[ H_1 = \hbar v_F \sigma \cdot \mathbf{k}, \]
\[ H_2 = \hbar v_F (\sigma \times \hat{z}) \cdot \mathbf{k}, \]

where $v_F$ is the Fermi velocity, $\sigma$ denotes the vector of the Pauli spin matrices and $\mathbf{k} = (k_x, k_y)$ is the wave vector.

The eigenvalues of these surface Hamiltonians are given by

\[ \varepsilon = \pm \hbar v_F \sqrt{(k_x^2 + k_y^2)} = \pm \hbar v_F k \]

leading to surface states with a Dirac cone type dispersion, as shown schematically in figure 1(a). Here we note that for real 3D TIs, this linear dispersion holds only near the Dirac point. The linear dispersion bends by the intrinsic nature of the bulk. Furthermore, the eigenvectors of these two Hamiltonians (for the derivation, see appendix A) are given by

\[ \Psi_{1\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm e^{-i\phi} \\ 1 \end{pmatrix}, \]
\[ \Psi_{2\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mp ie^{-i\phi} \\ 1 \end{pmatrix}. \]

where $\phi$ is the angle of $\mathbf{k}$ with respect to $k_z$. In both cases the eigenvectors indicate a helical spin structure where the spin direction is tied to the direction of the wave vectors. For the first case the spin direction is parallel to the wave vectors and in the second case the spin direction is perpendicular to the wave vectors as illustrated in figures 1(b) and (c), respectively.

Our goal is to include the helical spin structure in the calculation of scattering rates. Typically the spin structure leads to a suppression of scattering rates, which is dependent on the angle of scattering. At zero magnetic field, the total backscattering of electrons is not allowed (from the momentum $\mathbf{k}$ to $-\mathbf{k}$). We should note that since the overall spin angles between the two Hamiltonians at the same momentum consistently differ
by $90^\circ$, the suppression factors are identical for both Hamiltonians; here, we will only focus on the first Hamiltonian for the rest of this paper.

In the presence of an external magnetic field, the surface Hamiltonian of a TI will have an additional Zeeman term:

$$H_{\text{total}} = \hbar v_F \mathbf{\sigma} \cdot \mathbf{k} + g \mu_B \mathbf{\sigma} \cdot \mathbf{B},$$

where $\mathbf{B}$ is an external magnetic field, $g$ is the Lande-$g$ factor and $\mu_B$ is the Bohr magneton. In addition to the Zeeman splitting, the magnetic field also couples to the orbital motion (e.g. via minimal coupling), which plays a crucial role in the understanding of quantum phenomena like quantum interferences and the formation of Landau levels [26, 27]. Here, for simplicity, we will only focus on the Zeeman coupling while the minimal coupling is ignored. This approximation is justified for field parallel to the surface, where the minimal coupling drops out for a 2D system. However, for perpendicular magnetic fields, additional quantum corrections may arise [28], which are beyond the scope of this investigation.

We will first consider the influence of a parallel magnetic field. The Hamiltonian in equation (6) can be written using a parallel magnetic field to the surface:

$$H_{\text{total}||} = \hbar v_F (\sigma_x k_x + \sigma_y k_y) + g \mu_B (\sigma_x B_x + \sigma_y B_y).$$

Using Pauli spin matrices, eigenvalues of $H_{\text{total}||}$ or the dispersion relation in equation (3) is shifted in the presence of a parallel magnetic field:

$$\varepsilon_k = \pm \sqrt{(\hbar v_F k_x + g \mu_B B_x)^2 + (\hbar v_F k_y + g \mu_B B_y)^2}.$$

Thus, for a given $k$, the presence of an external magnetic field alters the direction of the spin. However, if we redefine a new wave number with respect to the position of the Dirac cone, the spin direction of the electron for the shifted wave number would be the same as that of the case of zero magnetic field. For example, the spin structure at the Fermi energy will be identical to the helical spin structure illustrated in figure 1(b). Since, the magnetic field only shifts the position of the Dirac cone without changing the spin structure and the scattering rates would not depend on the magnitude of parallel magnetic field. And therefore, the helical spin structure does not play a role in magnetoresistance in a parallel magnetic field.

Now let us consider the influence of a perpendicular magnetic field. The Hamiltonian in equation (6) can be written as

$$H_{\text{total}\perp} = \hbar v_F (\sigma_x k_x + \sigma_y k_y) + g \mu_B \sigma_z B_z.$$

Unlike the case of parallel magnetic field, the Dirac cone does not survive, as is evident in the modified dispersion relation

$$\varepsilon_k = \pm \sqrt{(g \mu_B B_z)^2 + (\hbar v_F k_x)^2 + (\hbar v_F k_y)^2}.$$

Most significantly, there is an opening of a gap with an energy of $2g \mu_B B_z$ at $k = 0$. The energy dispersion in equation (10) is shown in figure 2(a). We also calculate the eigenvectors which are given as

$$\Psi_{\uparrow} = \begin{pmatrix} -\cos \frac{\eta}{2} e^{-i\theta} \\ -\sin \frac{\eta}{2} \end{pmatrix}, \quad \Psi_{\downarrow} = \begin{pmatrix} \sin \frac{\eta}{2} e^{-i\theta} \\ -\cos \frac{\eta}{2} \end{pmatrix}.$$ (11)

More detailed calculations are given in appendix A. Where $\eta$ is

$$\eta = \tan^{-1} \left( \frac{\hbar v_F k}{g \mu_B B_z} \right).$$ (12)

We should note that $\eta$ has a geometric interpretation. It is instructive to rewrite the Hamiltonian in equation (6) as

$$H_{\text{total}} = g \mu_B \left[ \mathbf{\sigma} \cdot \left( \frac{\hbar v_F \mathbf{k}}{g \mu_B} + \mathbf{B} \right) \right],$$

where the quantity $\frac{\hbar v_F \mathbf{k}}{g \mu_B}$ acts as an intrinsic magnetic field ($\mathbf{B}_{\text{TI}}$) of TI. Then the effective magnetic field becomes the sum of these two fields:

$$\mathbf{B}_{\text{eff}} = \frac{\hbar v_F \mathbf{k}}{g \mu_B} + \mathbf{B}.$$ (14)

When written this way it is clear that spin direction is determined by $\mathbf{B}_{\text{eff}}$. The $\eta$, which is defined in equation (12), is the angle of $\mathbf{B}_{\text{eff}}$ with respect to the $z$-direction. The first term of the above equation acts as an intrinsic magnetic field. At the Fermi energy, the magnitude of this intrinsic magnetic field is written as
The spin structure at the Fermi energy depends on the ratio of perpendicular magnetic field to the magnitude of intrinsic magnetic field of the TI. The spin structures for different values of $B_{z}$ are schematically shown in figures 2(b)–(d): with the increasing magnitude of the perpendicular magnetic field the spins tilt towards the $z$-direction and at $B_{z} = \infty$ (shown in figure 2(d)) the spins would be fully aligned. From the perspective of transport we would expect a positive magnetoresistance and for the backscattering to be enhanced as the magnitude of perpendicular magnetic field increases.

3. Topological enhancement factor

In order to understand the influence of the helical spin structure on transport properties we need to focus on how its spin structure changes the momentum relaxation time. For an ordinary two-dimensional conductor the momentum relaxation time can be written using the Boltzmann transport equation as

$$\frac{1}{\tau} = \int W(k, k')(1 - \cos \theta) d^2k,$$

where $\theta$ is the angle between $k$ and $k'$ and $W(k, k')$ is the scattering rate of these two wave vectors. The detailed derivation of the momentum relaxation time is given in appendix B. For a given disorder potential, the scattering rate can be calculated using Fermi’s Golden Rule. In the case of an ideal TI there would be an addition suppression factor in the transport equation arising from the helical spin structure:

$$\frac{1}{\tau_{TI}} = \int W(k, k')S(s, s')(1 - \cos \theta) d^2k,$$

where $s$ and $s'$ are the spins which correspond to the electrons with a wave number $k$ and $k'$, respectively and $S(s, s')$ is the contribution to the scattering rate due to the spin structure of TI. We note that spin factor $S(s, s')$ is 1 when $s$ and $s'$ are parallel to each other and 0 when $s$ and $s'$ are antiparallel.

For an isotropic conductor the scattering rate and the spin factor would only depend on the angle between $k$ and $k'$, also known as the scattering angle $\theta$: $W(k, k') = W(\theta)$ and $S(s, s') = S(\theta)$. Thus, $\theta$ becomes the
integration variable for the above integrals. Since the spin factor $S(s, s')$ is bounded by 0 and 1, the momentum relaxation time of a TI, $\tau_{TI}$, is always greater than that of an identical electron system without a spin structure, $\tau$.

To quantify the contribution of the helical spin structure to transport we introduce a topological enhancement factor, $\Xi = \frac{\tau_{TI}}{\tau}$, which is defined as the ratio of these two momentum relaxation times. We expect $\Xi$ would be dependent on the nature of the disorder potential as well as the applied magnetic field.

In the absence of external magnetic field, the spin contribution to the scattering rate, $S(s, s')$, can be written as

$$S(s, s') = \cos^2\left(\frac{\theta}{2}\right)$$

Thus, as expected at $\theta = \pi$, the spin dependent scattering rate will be zero and subsequently there is no backscattering. In the presence of an external magnetic field in the $z$-direction, spins are expected to be parallel to the effective magnetic field and can be written as:

$$s = \frac{1}{\sqrt{B_{TI}^2 + B_z^2}} (B_{TI} \cos \phi, B_{TI} \sin \phi, B_z),$$

$$s' = \frac{1}{\sqrt{B_{TI}^2 + B_z^2}} (B_{TI} \cos (\theta + \phi), B_{TI} \sin (\theta + \phi), B_z).$$

$\theta + \phi$ is the angle between $k'$ and x-axis. Defining the angle between these two spins as $\theta_{s'} = \cos^{-1}\left(\frac{s'}{|s|}\right)$, the spin contribution to the scattering rate $S(s, s')$ becomes

$$S(s, s') = \cos^2\left(\frac{\theta_{s'}}{2}\right) = \cos^2\left(\frac{1}{2} \cos^{-1}\left(\frac{B_{TI}^2 \cos \theta + B_z^2}{B_{TI}^2 + B_z^2}\right)\right).$$

Knowing $S(s, s')$ we can now calculate $\Xi$ for different scattering mechanisms that cause disorder potentials. Here we consider two simple disorder potentials: short-range and long-range disorder potentials due to defects and impurities. Also we only discuss the magnetic response to $\Xi$ for short-range and long-range disorder potentials. We note that another scattering mechanism of great interest is magnetic impurities [29] and non-magnetic impurities [30, 31] which are not included in this work. Even for the simplified mean-field approach, a single magnetic impurity additionally deforms the helical spin angles, which have only been calculated numerically [32]. Spin-flip scattering by magnetic impurities, which gives rise to the Kondo effect, can be even more demanding theoretically [33].

### 3.1. Short-range disorder potential

Let us start with the simplest case where the disorder potential is short-range. Examples of short-range disorder include alloy disorder and surface or interface roughness. In all these cases the scattering rate is independent of the scattering angle. Thus, the disorder potential is characterized by a single parameter, $W(k, k') = W_0$ and the calculation of $\Xi(B)$ can be performed analytically. We then obtain an analytical solution for $\Xi(B)$, considering the magnetic-field-dependent spin contribution for a constant scattering rate:

$$\Xi(B) = \int W_0 \frac{(1 - \cos \theta) d^2 k}{\int W_0 \cos^2 \left(\frac{1}{2} \cos^{-1}\left(\frac{B_{TI}^2 \cos \theta + B_z^2}{B_{TI}^2 + B_z^2}\right)\right) (1 - \cos \theta) d^2 k}$$

$$= \frac{4(B_{TI}^2 + B_z^2)}{B_{TI}^2 + 4B_z^2}. \tag{22}$$

As expected the topological enhancement factor decreases from 4 to 1 smoothly with increasing of magnetic field. In the low magnetic field limit, there is a quadratic correction to magnetoconductivity due to $\Xi(B)$.

### 3.2. Long-range disorder potential

We now consider the case of the long-range Coulomb disorder caused by charged impurities. Unless the interfaces are protected by the growth of an epitaxial heterostructure [15], one would expect a large concentration of charged impurities in close vicinity of the two-dimensional topological surface states. In order to write down the disorder potential we need to know the dielectric constant of the material as well as the location of charged impurities. In the calculation below, we will focus on a single impurity located a distance $d$ from the two-dimensional electron system. In this case, the scattering rate can be written as
where, $q = |k - k'| = 2k_F \sin \frac{\theta}{2}$ and $U(q) \propto e^{-q d}/(q)$ is a screened Coulomb potential in Fourier domain \cite{34, 35}. The screening of the Coulomb potential by the two-dimensional electron system can be included in the calculation by the use of the following dielectric function

$$\epsilon(q) = \epsilon_0 \left(1 + \frac{q_{TF}}{q}\right),$$

where $q_{TF}$ is given by the inverse of the Thomas–Fermi (TF) screening length. Then, the scattering rate can be written as

$$W(q, k') \propto \left| \frac{U(q)}{\epsilon(q)} \right|^2,$$

Thus, for Coulomb scattering the topological enhancement factor is expected to depend on both $q_{TF}$ and $d$, which can be calculated numerically. Contour plots of $\Xi$ calculated at $B_z = 0$ and $B_z = B_{TF}$ are shown in figures 3(a) and (b), respectively. Here, the topological enhancement factor for Coulomb scattering is smaller than that for short range disorder.

We should note that there is a special case where $d = 0$ and $q_{TF} = 0$ for which the calculation can be performed analytically. In this special case, the charged impurities would be located at the 2DEG and there would be no screening and thus we can express the potential of a charged impurity as a simplified Coulomb potential \cite{35}. Then, we can write the scattering rate for the impurities in the absence of magnetic field as

$$W(\theta) \propto \frac{e^{-2d|q|}}{(q + q_{TF})^2}.$$
Using this scattering rate along with the spin contribution in equation (21), for the contributions of charged impurities under the influence of an external magnetic field, we obtain an analytical solution for $\Xi(B)$:

$$\Xi(B) = \frac{1}{q^2} \int \frac{1}{q^2} (1 - \cos \theta) dk^2$$

The results of the topological enhancement factor under magnetic field for both short-range and long-range disorder are illustrated in figure 4. In this figure, we assume that $q_{TF}$ and $d$ are proportional to $k_F$, ranging from short-range constant scattering to long-range Coulomb potential. For intermediate cases between short-range and long-range potential, we assume TF screening theory (equation (25)) assuming that $d = 0$, which signifies that the impurity layer is very close to the surface. In the absence of magnetic field, $\Xi(B)$ increases from 2 to 4 as $q_{TF}$ increases from long-range to short-range potential. In all cases, $\Xi(B)$ approaches 1 as $B_z$ increases. So we can say that $\Xi(B)$ becomes independent from the disorder potentials at high magnetic fields. Thus, TF screening theory is consistent with the calculations from long-range and short-range potentials.

We should note that for most TIs, $B_{TI}$ defined in equation (15) is large, and thus, the corrections to magnetoconductivity are expected to be small. For example, Bi$_2$Se$_3$ [13, 36] has a single Dirac cone with a Fermi velocity $v_F = 5 \times 10^5$ ms$^{-1}$ and a Fermi wavevector $k_F \approx 1$ nm$^{-1}$, leading to a $B_{TI} \approx 2842$ T. Similarly, for the topological Kondo insulator SmB$_6$, Fermi velocity and Fermi wavevector have been measured for three different Fermi pockets in recent experiments [37]. The first Fermi pocket has a Fermi velocity of $\sim 2.90 \times 10^5$ ms$^{-1}$ and Fermi wavevector of $k_F \approx 0.30$ nm$^{-1}$, so $B_{TI} \approx 4947$ T. For the second Fermi pocket, $v_F = 8.45 \times 10^5$ ms$^{-1}$ and $k_F \approx 0.941$ nm$^{-1}$, leading to a $B_{TI} \approx 4521$ T and the third Fermi pocket has a Fermi velocity of $\sim 6.50 \times 10^5$ ms$^{-1}$ and Fermi wavevector of $k_F \approx 1.080$ nm$^{-1}$, so $B_{TI} \approx 3991$ T. For sufficiently large g factors [38], reasonable results of $B_{TI}$ can be obtained. Even in such high carrier density two-dimensional systems, the quadratic correction to magnetoconductivity due to $\Xi(B)$ can have a measurable effect and should be included in the analysis of high field data [39]. On the other hand, if we can realize topological conducting states with a very low Fermi wavevector, we could reach a regime where $B_z / B_{TI}$ is large and there is a total suppression of the topological enhancement factor.

4. Conclusion

In conclusion, we have studied theoretically the magnetoresistance of an ideal TI surface utilizing Boltzmann transport. We investigate conductivity enhancement in the presence of a perpendicular magnetic field. By finding the angle deflection of the helical spins by the Zeeman effect, the enhancement is calculated within the

$$W(k, k') = \frac{1}{q^2}.$$ (26)
classical scattering theory. For short-range disorder in the absence of magnetic field, \( \Xi(B) \) is equal to 4. With increasing magnetic field the topological enhancement factor decreases from 4 to 1 smoothly as given by the analytical function of equation (22). For Coulomb disorder with no screening, the topological enhancement factor is equal to 2 in the absence of the magnetic field. In the presence of magnetic field the topological enhancement factor is suppressed by the analytical function given in equation (27). We also investigated the effect of the screening using TF screening theory. The results are relevant for all high field magnetotransport measurements performed on TIs. The corrections to magnetoconductivity are small for high carrier density systems such as conducting electrons on the surface of SmB\(_6\), but are expected to be more significant for TIs with lower carrier density of electrons.

Acknowledgments

This work is supported by TUBITAK (The Scientific and Technological Research Council of Turkey) and by the National Science Foundation through DMR-1006500, DMR-1441965 and PHY-1402971.

Appendix A

In the absence of magnetic field, the Hamiltonians in equations (1) and (2) can be written using \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) and \( \mathbf{k} = (k_x, k_y) \)

\[
H_1 = \begin{pmatrix} 0 & \hbar v_F k_x - i\hbar v_F k_y \\ \hbar v_F k_x + i\hbar v_F k_y & 0 \end{pmatrix}, \quad (A.1)
\]

\[
H_2 = \begin{pmatrix} 0 & -\hbar v_F k_y - i\hbar v_F k_x \\ -\hbar v_F k_y + i\hbar v_F k_x & 0 \end{pmatrix}. \quad (A.2)
\]

The eigenvalues of \( H_1 \) and \( H_2 \) are \( \varepsilon = \pm \hbar v_F \sqrt{(k_x^2 + k_y^2)} = \pm \hbar v_F k \) which were mentioned in equation (3). The eigenvectors of \( H_1 \) and \( H_2 \) are easily calculated and given as respectively:

\[
\Psi_{1\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm \frac{k_x - ik_y}{\sqrt{k_x^2 + k_y^2}} \\ 1 \end{pmatrix}, \quad (A.3)
\]

\[
\Psi_{2\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mp \frac{(k_x + ik_y)}{\sqrt{k_x^2 + k_y^2}} \\ 1 \end{pmatrix}. \quad (A.4)
\]

Here, \( 1/\sqrt{2} \) comes from the normalization. We can write the trigonometric values of \( \phi \) which is defined before as the angle of \( \mathbf{k} \) with respect to \( k_x \)

\[
\sin \phi = \frac{\hbar v_F k_y}{\sqrt{\left((\hbar v_F k_x)^2 + (\hbar v_F k_y)^2\right)}} = \frac{k_y}{\sqrt{(k_x)^2 + (k_y)^2}}, \quad (A.5)
\]

\[
\cos \phi = \frac{\hbar v_F k_x}{\sqrt{\left((\hbar v_F k_x)^2 + (\hbar v_F k_y)^2\right)}} = \frac{k_x}{\sqrt{(k_x)^2 + (k_y)^2}}. \quad (A.6)
\]

So, using these definitions in equations (A.3) and (A.4), we obtain the eigenvectors of \( H_1 \) and \( H_2 \) as mentioned in equations (4) and (5), respectively:

\[
\Psi_{1\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm (\cos \phi - i\sin \phi) \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm e^{-i\phi} \\ 1 \end{pmatrix}, \quad (A.7)
\]

\[
\Psi_{2\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mp (\sin \phi + i\cos \phi) \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mp ie^{-i\phi} \\ 1 \end{pmatrix}. \quad (A.8)
\]

If the magnetic field is perpendicular to the surface of the TI (\( \hat{z} \)-direction), the Hamiltonian in equation (6) can be written as

\[
H_{\text{total,}\perp} = \begin{pmatrix} g\mu_B B_z & \hbar v_F k_x - i\hbar v_F k_y \\ \hbar v_F k_x + i\hbar v_F k_y & -g\mu_B B_z \end{pmatrix}. \quad (A.9)
\]

The eigenvalue of \( H_{\text{total,}\perp} \) is easily calculated and given in equation (10) as

\[
\varepsilon_{\perp} = \pm \sqrt{(g\mu_B B_z)^2 + (\hbar v_F k_x)^2 + (\hbar v_F k_y)^2}. \quad (A.10)
\]

The normalized eigenvectors of \( H_{\text{total,}\perp} \) are given as
We defined the angle between \( \mathbf{k} \) and perpendicular magnetic field as \( \eta \) in equation (12), so we obtain that trigonometric definitions:

\[
\sin \eta = \frac{\sqrt{(\hbar v_F k_x)^2 + (\hbar v_F k_y)^2}}{\sqrt{(\hbar v_F k_x)^2 + (\hbar v_F k_y)^2 + (g \mu_B B_z)^2}},
\]

\[
\cos \eta = \frac{g \mu_B B_z}{\sqrt{(\hbar v_F k_x)^2 + (\hbar v_F k_y)^2 + (g \mu_B B_z)^2}}.
\]

Using equations (A.5), (A.6), (A.12) and (A.13) with \( \varepsilon_{\perp +} \), we reach that equations:

\[
g \mu_B B_z = \varepsilon_{\perp +} \cos \eta,
\]

\[
(\hbar v_F k_x)^2 + (\hbar v_F k_y)^2 = \varepsilon_{\perp +} \sin \eta,
\]

\[
\hbar v_F k_x = (\hbar v_F k_x)^2 + (\hbar v_F k_y)^2 \cos \phi = \varepsilon_{\perp +} \sin \eta \cos \phi,
\]

\[
\hbar v_F k_y = (\hbar v_F k_x)^2 + (\hbar v_F k_y)^2 \sin \phi = \varepsilon_{\perp +} \sin \eta \sin \phi
\]

with these equations, equation (A.10) can be written as

\[
\Psi_{\perp +} = \frac{\cos \eta - 1}{\sqrt{\sin^2 \eta + (\cos \eta - 1)^2}} \left( \frac{-\sin \eta \cos \phi - i \sin \phi}{(\cos \eta - 1) - i \sin \eta} \right).
\]

Defining \( \cos \eta - 1 = -2 \sin^2(\eta/2) \) and \( \sin \eta = 2 \sin(\eta/2) \cos(\eta/2) \), we can write the equation (A.18) as

\[
\Psi_{\perp +} = \begin{pmatrix}
-\cos \frac{\eta}{2} e^{-i\phi} \\
-\sin \frac{\eta}{2}
\end{pmatrix}.
\]

Similarly, for \( \varepsilon_{\perp -} \), we obtain

\[
\Psi_{\perp -} = \begin{pmatrix}
\sin \frac{\eta}{2} e^{-i\phi} \\
-\cos \frac{\eta}{2}
\end{pmatrix}.
\]

### Appendix B

The transport properties of an ideal TI can be calculated using the Boltzmann equation. We will first introduce the quantity \( f_k(r, t) \) which is defined as the occupation probability of electrons at time \( t \) around point \( r \) with a crystal momentum \( \mathbf{k} \). The time dependence of \( f_k(r, t) \) will be due three different processes: diffusion, drift and scatterings. The contributions from these three effects are written separately below:

\[
\left( \frac{\partial f_k}{\partial t} \right)_{\text{diff}} = -v_k \nabla f_k,
\]

\[
\left( \frac{\partial f_k}{\partial t} \right)_{\text{drift}} = -\frac{1}{\hbar} \mathbf{F} \nabla f_k,
\]

\[
\left( \frac{\partial f_k}{\partial t} \right)_{\text{scat}} = -\sum_{k'} \left[ W(k, k') f_{k'}(1 - f_{k'}) - W(k', k) f_k(1 - f_k) \right].
\]

\( \mathbf{F} \) is the external force, \( v_k \) is the velocity of electrons with a crystal momentum \( \mathbf{k} \), and \( W(k, k') \) is the scattering rate between the states \( \mathbf{k} \) and \( \mathbf{k}' \). At the steady state, the total rate of change of \( f_k(r, t) \) must be zero.

\[
\left( \frac{\partial f_k}{\partial t} \right)_{\text{diff}} + \left( \frac{\partial f_k}{\partial t} \right)_{\text{drift}} + \left( \frac{\partial f_k}{\partial t} \right)_{\text{scat}} = 0.
\]
If the system is not driven far from equilibrium, the scattering term can be written in terms of a relaxation time:

\[
\left( \frac{\partial f_k}{\partial t} \right)_{\text{scat}} = - \frac{f_k - f^0}{\tau} = - \frac{g_k}{\tau}.
\]  

(B.5)

where \( \tau \) is the relaxation time and \( f^0 \) is the occupation probability in equilibrium. It is instructive to introduce a new quantity \( g_k \), which is given by the departure of \( f_k \) from its equilibrium value \( f^0 \). Also \( f^0 \) is given by the Fermi–Dirac distribution function.

In equation (B.3), in the symmetric scattering, we can write

\[
W_{kk} = \frac{g_k}{g_k'} = \frac{1}{1 + \cosh \theta}.
\]  

(B.6)

So equation (B.5) can be written as

\[
\frac{1}{\tau} = \sum_{k'} W(k, k') \left[ 1 - \frac{g_k'}{g_k} \right].
\]  

(B.7)

For the uniform translation invariance, diffusion term vanishes in Boltzmann transport equation in equation (B.4) and it becomes as

\[
\frac{1}{\hbar} F \nabla f_k = - \frac{g_k}{\tau}.
\]  

(B.8)

Using the chain rule of derivative,

\[
g_k = - \tau F \nabla f_k = - \tau F v_k \frac{\partial f_k}{\partial E}.
\]  

(B.9)

Here \( E \) is the energy and \( v_k \) is velocity and defined as using the group velocity

\[
v_k = \frac{\partial W}{\partial k} = \frac{\partial}{\partial k} \left( \frac{E}{\hbar} \right) = \frac{1}{\hbar} \left( \frac{\partial E}{\partial k} \right).
\]  

(B.10)

We consider only small field intensities so we can replace \( f_k \) by its equilibrium \( f^0 \) in \( \frac{\partial g_k}{\partial E} \) [41]. Using the ratio of \( g_k \) and \( g_k' \) in equation (B.7), we obtain

\[
\frac{1}{\tau} = \sum_{k'} W(k, k') \left[ 1 - \frac{v_k'}{v_k} \right].
\]  

(B.11)

If we multiply the fraction in the square brackets with \( v_k \) and using the scalar product [42], we reach

\[
\frac{1}{\tau} = \sum_{k'} W(k, k') [1 - \cos \theta].
\]  

(B.12)

Using the integral instead of the sum, we get equation (16):

\[
\frac{1}{\tau} = \int W(k, k')(1 - \cos \theta) d^2k.
\]  

(B.13)

**ORCID iDs**

T Ozturk @ https://orcid.org/0000-0002-5002-5412

**References**

[1] Hasan M Z and Kane C L 2010 Rev. Mod. Phys. 82 3045
[2] Moore J E 2010 Nature 464 194
[3] Qi X-L and Zhang S-C 2011 Rev. Mod. Phys. 83 1057
[4] Kane C L and Mele E J 2005 Phys. Rev. Lett. 95 146802
[5] Kane C L and Mele E J 2005 Phys. Rev. Lett. 95 226801
[6] Bernevig B A, Hughes T L and Zhang S-C 2006 Science 314 1757
[7] Fu L, Kane C L and Mele E J 2007 Phys. Rev. Lett. 98 106803
[8] Moore J E and Balents L 2007 Phys. Rev. B 75 121306(R)
[9] Fu L and Kane C L 2007 Phys. Rev. B 76 045302
[10] Murakami S 2007 New J. Phys. 9 356
[11] Hsieh D, Qian D, Wray L, Xia Y, Hor Y S, Cava R J and Hasan M Z 2008 Nature 452 970
[12] Zhang H, Liu C-X, Qi X-L, Dai X, Fang Z and Zhang S-C 2009 Nat. Phys. 5 438
[13] Xia Y et al 2009 Nat. Phys. 5 398
[14] Chen Y L et al 2009 Science 325 178
[15] Roushan P, Soo J, Parker C V, Hor Y S, Hsieh D, Qian D, Richardella A, Hasan M Z, Cava R J and Yazdani A 2009 Nature 460 1106

10
[16] Hsieh D et al 2009 Nature 460 1101
[17] Taskin A A and Ando Y 2009 Phys. Rev. B 80 085303
[18] Ren Z, Taskin A A, Sasaki S, Segawa K and Ando Y 2010 Phys. Rev. B 82 241306(R)
[19] Xiong J, Petersen A C, Qu D, Hor Y S, Cava R J and Ong N P 2012 Physica E 44 917
[20] Wolgast S, Kurda C, Sun K, Allen J W, Kim D-I and Fisk Z 2013 Phys. Rev. B 88 180405(R)
[21] Kim D J, Thomas S, Grant T, Botimer J, Fisk Z and Xia J 2013 Sci. Rep. 3 3150
[22] Zhang T et al 2009 Phys. Rev. Lett. 103 266803
[23] He H-T, Wang G, Zhang T, Sou I-K, Wong G K L, Wang J-N, Lu H-Z, Shen S-Q and Zhang F-C 2011 Phys. Rev. Lett. 106 166805
[24] Liu M et al 2012 Phys. Rev. Lett. 108 036805
[25] Adam S, Hwang E H and Das Sarma S 2012 Phys. Rev. B 85 235413
[26] Tkachov G and Hankiewicz E M 2013 Phys. Status Solidi B 250 215
[27] Bardarson J H and Moore J E 2013 Rep. Prog. Phys. 76 056501
[28] Tahir M and Schwingerenschlogl U 2013 Europhys. Lett. 102 37001
[29] Cha J J, Williams J R, Kong D, Meister S, Peng H, Bestwick A J, Gallagher P, Goldhaber-Gordon D and Cui Y 2010 Nano Lett. 10 1076
[30] Lu J, Shan W-Y, Lu H-Z and Shen S-Q 2011 New J. Phys. 13 103016
[31] Seshadri R and Sen D 2014 Phys. Rev. B 89 235413
[32] Liu Q, Liu C-X, Xu C, Qi X-L and Zhang S-C 2009 Phys. Rev. Lett. 102 156603
[33] Xin X and Yeh M-C 2013 J. Phys.: Condens. Matter 25 286001
[34] Hwang E H, Adam S and Das Sarma S 2007 Phys. Rev. Lett. 98 186806
[35] Culcer D, Hwang E H, Stanescu T D and Das Sarma S 2010 Phys. Rev. B 82 155457
[36] Cao H, Xu S, Miotkowski I, Tian J, Pandey D, Hasan M Z and Chen Y P 2013 Phys. Status Solidi RRL 7 133
[37] Li G et al 2014 Science 346 1208
[38] Analytis J G, McDonald R D, Riggs S C, Chu J-H, Boebinger G S and Fisher I R 2010 Nat. Phys. 6 960
[39] Wolgast S et al 2015 Phys. Rev. B 92 115110
[40] Singh J 2004 Modern Physics for Engineers (Weinheim: Wiley) p 359
[41] Seeger K 2004 Semiconductor Physics: An Introduction 9th Edition (Berlin: Springer) p 50
[42] Ferry D K, Goodnick S M and Bird J 2009 Transport in Nanostructures 2nd Edition (Cambridge: Cambridge University Press) p 88