1. Introduction

Topological insulators (TI) such as Bi$_2$Se$_3$ and Bi$_2$Te$_3$ are characterized by surface states which possess specific characteristics, for instance, a non-trivial Berry phase of $(2n + 1)\pi$, mass-less Dirac fermions, and a spin helical structure under ideal conditions [1, 2]. Time reversal symmetry (TRS) breaking perturbations destroy the topological nature of the surface states and introduce additional contributions that have been experimentally established primarily through angle-resolved photo emission spectroscopy (ARPES) data [3]. Further, the linear dispersion at points away from the Dirac cone is altered by higher order $k$-terms [4] that in turn modify the topologically ordained behaviour [5–8]. An external magnetic field which breaks TRS and higher order $k$-terms that warp the band structure is considered in this work to (1) compute deviations to the Berry phase from the well-known $(2n + 1)\pi$ and (2) evaluate the momentum relaxation time for electrons scattered on the surface of a 3D-topological insulator.

The influence of Berry phase is distinctly noticeable in solid state physics and along with the related Berry curvature, it is of fundamental importance in describing the behaviour and properties of topological insulators (TI). A careful calculation of the Berry curvature which manifests as an orbital magnetization is therefore desirable to fully explain several experimental phenomena emerging in TI structures. These experimental observations which are a direct outcome of Berry curvature mediated effects have far reaching consequences for the design of thermoelectrics, in explaining the anomalous quantum Hall effect, and Nernst conductivity [9].
nature of quantum phase transitions in Floquet TIs [10, 11], which are induced by light dependent perturbations can also be investigated by evaluating the Chern number which is the integral of the Berry curvature over the full Brillouin zone [12, 13]. Similarly, the relaxation time is a useful quantity to explain carriers and thermal transport characteristics on the surface of TIs in the presence of scattering phenomena. The knowledge of these relaxation times also aids in interpreting the measured magneto-resistance data that are obtained probing the TI surface [14, 15].

In this work we intend to address the calculation of Berry phase and Berry curvature for a band gap open TI with higher order band warping. The finite band gap is due to an external magnetic field. We further calculate the carrier relaxation time for such a TI and study the effect of the warping parameter on transport behaviour and compare the result to a pristine topological insulator. The paper is organized as follows: in section 2 we derive an expression for the Berry phase using dispersion and wave functions obtained for a gapped TI film in presence of higher order warping terms. Subsequently, we determine the momentum relaxation time within a linearized Boltzmann equation framework. In section 3 numerical examples based on results computed above are presented in which we estimate the effect of the magnetic perturbations and deviations from linear band structure. Finally, a summary of results and their potential implications concludes the paper.

2. Theory and model

The two-dimensional Dirac Hamiltonian can be written as [16]

\[ H_{\text{surf. states}} = 
\begin{align*}
\nu_f & (\sigma_i k_j - \sigma_j k_i) \\
\end{align*} 
\]  

(1)

where \( \nu_f \) denotes Fermi velocity and \( \sigma_i; i = x, y \) are the Pauli matrices. This form of the Hamiltonian is in principle sufficient to probe the surface states; however, ARPES studies of the Fermi-surface at energies significantly far away from the Dirac point reveals a snow-flake like hexagram structure [17–19] that is markedly different from a simple circular Fermi surface observed by direct application of equation (1). This disagreement with experiment is reconciled by noting that the simple two-dimensional Dirac Hamiltonian fails to account for the underlying crystal symmetries. The deformation of the Fermi surface can be theoretically reproduced if higher order \( k \) terms are incorporated in the Hamiltonian. In the two-dimensional Dirac Hamiltonian must comply with the C\(_{3v}\) point group and time reversal symmetry, the next higher order terms that must be added to the linear Hamiltonian are cubic in \( k \). Consequently, the modified Hamiltonian [20] therefore must have, at least, the following form:

\[ H(k) = e_0(k) + \nu_f (\sigma_i k_j - \sigma_j k_i) + \frac{\lambda}{2} h^2 (k_x^2 + k_y^2) \sigma_z \]  

(2)

where \( e_0(k) \) introduces the particle-hole anisotropy and the cubic terms denote warping. Using equation (2) the surface state spectrum is

\[ e_{\pm}(k) = e_0(k) \pm \sqrt{\nu_f^2 k^2 + \lambda^2 h^6 k^6 \cos^2(\theta)} \]  

(3)

where \( \theta = \tan^{-1} \left( \frac{k_y}{k_x} \right) \). The spectrum contains the lowest order correction to the perfect helicity of the Dirac cone predicted in equation (1). The \( \cos^2(\theta) \) term possesses the symmetry of the C\(_{3v}\) point group and the Hamiltonian can be shown to be time reversal symmetric.

2.1. Berry phase of gapped Dirac fermions

An expression for the Berry phase of the gapped surface spectrum of a 3D topological insulator was derived in our previous work and can be found in [21]. For example, a finite band gap can be induced either through the proximity effect of a ferromagnet or an s-wave superconductor [22–24]. The final expression for Berry phase for the surface electrons of a topological insulator in presence of a finite band gap \( \Delta \) is found to be

\[ \gamma_{\eta} = \pi \left[ 1 + \frac{\eta \Delta_{\text{pro}}}{\sqrt{\Delta_{\text{pro}}^2 + (\hbar \nu_f)^2}} \right] \]  

(4)

where \( \Delta_{\text{pro}} \) is the band gap split on account of proximity effects and \( \eta = \pm 1 \) denotes the helicity.

The goal of this section is to examine the influence of the warping parameter introduced in equation (2) on the final Berry phase. To begin, we evaluate the wave functions \( \langle \Psi(r; \mathbf{R}) \rangle \) of the warped Hamiltonian solving the Schrödinger equation \( H(\mathbf{R}) \langle \Psi(r; \mathbf{R}) \rangle = E_0(\mathbf{R}) \langle \Psi(r; \mathbf{R}) \rangle \). Note that the Hamiltonian of the quantum mechanical system, which in our case, is a 3D TI can be controlled by external parameters collectively described by the vector \( \mathbf{R} \). The external parameters could be some perturbation brought about by an electric or magnetic field such that the eigen states vary smoothly with \( \mathbf{R} \) in the parameter space manifold. In absence of any external parameter, the vector \( \mathbf{R} \) simply coincides with the crystal momentum space \( \mathbf{k} \). The wave functions for the warped and gapped Hamiltonian \( H(\mathbf{R} = \mathbf{k}) \) are

\[ \psi_{\eta} = \frac{1}{\sqrt{2}} \begin{pmatrix}
\lambda_{\eta}(k) \exp(-i\theta) \\
\eta \lambda_{\eta}(k)
\end{pmatrix} \]  

(5a)

where

\[ \lambda_{\eta}(k) = \sqrt{1 + \frac{\eta \Delta_{\text{pro}}^2}{\sqrt{\Delta_{\text{pro}}^2 + (\hbar \nu_f)^2}}} \]  

(5b)

and

\[ \Delta_{\text{pro}} = \Delta_{\text{pro}} + \frac{\lambda}{2} h^2 (k_x^2 + k_y^2) \sigma_z \]  

(5c)

The warping term effectively augments the band gap splitting originally introduced in the topological insulator. A simple way to induce a band gap is to layer the surface of a TI with a ferromagnet with a magnetization component perpendicular to the surface.
The Berry phase along a closed circuit is defined as [25, 26]

$$\gamma_\eta(C) = i \oint_C \langle \Psi(\mathbf{r}; \mathbf{R}) | \nabla_\mathbf{R} | \Psi(\mathbf{r}; \mathbf{R}) \rangle \, d\mathbf{R}$$  \hspace{1cm} (6)

Note that the closed circuit here refers to a path in momentum space. Expanding the integrand or the Berry connection $A_\eta = \langle \Psi(\mathbf{r}; \mathbf{R}) | \nabla_\mathbf{R} | \Psi(\mathbf{r}; \mathbf{R}) \rangle$ in equation (6) by inserting the wave function expression from equations (5a)–(5c) yields

$$A_\eta = \frac{1}{2} \left( \lambda^a \exp(i\theta) \eta \lambda_{\eta} \left( \frac{\partial \lambda_{\eta} - i \lambda_{\eta} \partial \theta \exp(-i\theta)}{\eta \partial \lambda_{\eta}} \right) \right)$$  \hspace{1cm} (7)

Simplifying the above expression,

$$A_\eta(k) = \frac{1}{2} \left( \lambda^a \partial \lambda_{\eta} - i \lambda_{\eta} \partial \theta + \lambda^a \partial \lambda_{\eta} \right)$$

$$= \frac{1}{2} \lambda^a \partial \lambda_{\eta}$$  \hspace{1cm} (8)

The last expression has been condensed by observing that $\partial \lambda_{\eta}$ evaluates exactly as $\partial \lambda_{\eta}$ with sign reversed, therefore taken together they are equal to zero. $\partial \lambda_{\eta}$ is worked out.

$$\partial \lambda_{\eta}(k) = \frac{\eta \Delta_{\text{pro}}}{\sqrt{\Delta_{\text{pro}}^2 + (\hbar v_k)^2}}$$  \hspace{1cm} (9)

The final expression for Berry connection in matrix notation is therefore

$$A_\eta = \frac{1}{2} \left( 1 + \frac{\eta \Delta_{\text{pro}}}{\sqrt{\Delta_{\text{pro}}^2 + (\hbar v_k)^2}} \right) \frac{1}{k} \begin{pmatrix} -k_y \\ k_x \end{pmatrix}$$  \hspace{1cm} (10)

In deriving equation (10), the angular derivatives $\partial_\theta \eta(k) = -\frac{k_y}{k}$ and $\partial_\theta \lambda(k) = \frac{k_x}{k}$ were used. Inserting equation (10) in equation (6) and integrating over a closed path in $k$-space gives

$$\gamma_\eta = \oint_C dk_x \cdot A_\eta(k) + \oint_C dk_y \cdot A_\eta(k)$$  \hspace{1cm} (11)

Since the energy contour under the influence of warping is no longer a circle but has a dependence on $(k, \theta)$, the usual relations $k_x = k \cos(\theta)$ and $k_y = k \sin(\theta)$ are modified to $k_x = k(\theta) \cos(\theta)$ and $k_y = k(\theta) \sin(\theta)$. The angular derivatives are therefore

$$\frac{dk_x}{d\theta} = \frac{dk}{d\theta} \cos(\theta) - k \sin(\theta)$$  \hspace{1cm} (12a)

and

$$\frac{dk_y}{d\theta} = \frac{dk}{d\theta} \sin(\theta) + k \cos(\theta).$$  \hspace{1cm} (12b)

The Berry phase with warping using equation (11) and substituting for angular derivatives from equation (2.1) gives

$$\gamma_\eta = \frac{1}{2} \oint_C dk \left( 1 + \frac{\eta \Delta_{\text{pro}}}{\sqrt{\Delta_{\text{pro}}^2 + (\hbar v_k)^2}} \right) \frac{-k \sin(\theta)}{k^2}$$

$$+ \frac{1}{2} \oint_C dk \left( 1 + \frac{\eta \Delta_{\text{pro}}}{\sqrt{\Delta_{\text{pro}}^2 + (\hbar v_k)^2}} \right) \frac{k \cos(\theta)}{k^2}$$  \hspace{1cm} (13)

Collecting terms, one obtains

$$\gamma_\eta = \frac{1}{2} \int_0^{2\pi} d\theta \left( 1 + \frac{\eta(\Delta + \hbar^2 v_k^2 \cos(3\theta))}{\sqrt{(\Delta + \hbar^2 v_k^2 \cos(3\theta))^2 + (\hbar v_k)^2}} \right)$$  \hspace{1cm} (14)

A closed form solution of the integral in equation (14) is not possible and a numerical evaluation will be presented in section 3. The integral, as evident, consists of the topological contribution of $\pi$ and the non-topological part shown in equation (15). The warping term effectively increases the proximity induced band gap and the non-topological component of the Berry phase.

$$\gamma_{\text{non-top}} = \frac{\Delta + \hbar^2 v_k^2 \cos(3\theta)}{\sqrt{(\Delta + \hbar^2 v_k^2 \cos(3\theta))^2 + (\hbar v_k)^2}}$$  \hspace{1cm} (15)

It is useful to underscore the ‘non-topological’ nomenclature. In a pristine TI, the Berry phase of $\pi$ is purely on account of the metal-like surface states, attributable to the topological phase transition at the boundary of an inverted and normal ordered material or vacuum. On the other hand, the mass and warping terms introduced in equation (2) do not have a topological origin. The ‘mass’ term $\Delta$ is a scalar quantity controllable in an experimental set up, while warping denotes the higher order description in momentum space of electronic bands. This justifies the ‘non-topological’ classification for the additional term described by equation (15) and solely constituted of $\Delta$ and $\lambda$. Note that this term vanishes as $\Delta, \lambda \rightarrow 0$, reducing the Berry phase to the topologically ordained value of $\pi$.

The Berry phase which is analogous to a magnetic vector potential induces an orbital magnetic field [27, 28] whose magnitude can be determined by evaluating $\mathbf{V} \times A_\eta$. Setting the warping term to zero to keep the algebra tractable, we obtain

$$B_{\text{orb}} = \frac{1}{2} \left( \frac{\hbar^2 v_k^2 \Delta_{\text{pro}}}{\sqrt{(\Delta_{\text{pro}}^2 + (\hbar v_k)^2)^2}} \right)$$  \hspace{1cm} (16)

The electron wave packet acquires an additional (anomalous) velocity given by $v_{\text{an}} = \frac{e}{\hbar} \times \mathbf{B}_{\text{orb}}$ transverse to the electric field and gives rise to the intrinsic Hall current. Writing $\frac{dx}{dt} = \frac{-e}{\hbar} \mathbf{E}$, the corresponding Hall current is

$$j_{\text{Hall}} = -e \sum_\sigma \int_{\text{BZ}} \frac{dk}{4\pi^2} f(k)v_{\text{an}}$$  \hspace{1cm} (17a)

$$= -\frac{e^2}{\hbar} \sum_\sigma \mathbf{E} \times \int_{\text{BZ}} \frac{dk}{4\pi^2} f(k)B_{\text{orb}}$$  \hspace{1cm} (17b)
The Hall conductivity \([29, 30]\) is \(\sigma_{xy} = \frac{\partial J_{xy}}{\partial B}\), therefore evaluating the expression \(\frac{\partial}{\partial \theta}(\mathbf{E} \times \mathbf{B}) = B_{\text{orb}}\) gives
\[
\sigma_{xy} = \frac{e^2}{h} \int_{BZ} \frac{d\mathbf{k}}{4\pi^2} \delta(E_k - \epsilon_v) |(1 - \cos \theta)|
\]
(17c)
where \(f(k)\) is the electron distribution of the given band.

The anomalous velocity \([31, 32]\) in equation (17b) induced by the Berry phase, gives rise to an orbital magnetization \(\langle \mathbf{B}_{\text{orb}} \rangle\) that manifests as Hall current flowing transverse to the electric field. In a pristine TI with massless Dirac fermions \((\Delta = 0)\), the anomalouos velocity proportional to the Berry curvature vanishes as can be easily seen by setting \(\Delta\) to zero in equation (10) and performing a direct algebraic evaluation of the curl of the Berry vector potential. The curl which is \(\mathbf{B}_{\text{orb}}\) evaluates to zero. However, in presence of a proximity effect induced band gap, and further augmented by warping, the anomalous velocity is finite, and as a consequence of this we have an intrinsic anomalous Hall conductivity. This anomalous Hall conductivity is therefore band gap and warping dependent.

2.2. Momentum relaxation time

The surface of a topological insulator is generally impure with impregnated foreign atoms carried over from the fabrication process. Transport measurements provide key insights into the arrangement of electronic states, mobility, and related phenomenon like weak anti-localization on the surface of a topological insulator \([33, 34]\). In this section of the paper, we derive expressions to determine the reciprocal of the relaxation time in Boltzmann equation \([35, 36]\). Several approximations are made to keep the calculations tractable such as (1) system is homogeneous (2) impurities are dilute and random and (3) there is no interference between successive scatterings. The inverse of relaxation time under these approximations is given by
\[
\frac{1}{\tau} = \beta \int \frac{d^3 k}{8\pi^3} \delta(E_k - \epsilon_v) |(1 - \cos \theta)|
\]
(18)
where \(\chi_{\mathbf{k}} = \langle \Psi^\dagger \Psi \rangle \zeta(s, s')\). The additional spin-scattering factor \([37]\) \(\zeta(s, s')\) takes into account the helical spin structure of the TI surface states. If the external magnetic field is sufficiently large, such that the spins are aligned parallel to it, \(\zeta(s, s')\) can be set to unity. \(\beta\) is a constant determined from the scattering time expression derived in equation (18) differentiates the relaxation time in Boltzmann equation from the corresponding time between two scattering events \([38]\). It can be considered as an additional factor to ‘measure’ the effectiveness of scattering. For small angle scattering, the \((1 - \cos \theta)\) term is insignificant and contributes little to \(1/\tau\), however, for a scattering event that deflects the carrier (surface electron) by a large angle, relaxation time and resistivity are tangibly affected. Finally, the constant \(\beta\) in equation (18) is usually defined to be equal to \(2m_e n_i\), where \(n_i\) is the concentration of impurities. Since we compute the ratio of relaxation times for the trivial \((\Delta \neq 0)\) and topological insulator, an exact value for \(n_i\) is not needed for our purpose.

The scattering matrix in equation (18) can be calculated as follows
\[
T(k, k') = \left[\frac{1}{2} \left( \lambda_+(k) \exp(i\theta) - \lambda_-(k) \right) \left( \lambda_+(k') \exp(-i\theta) - \lambda_-(k') \right) \right]^2
\]
(19a)
where \(\lambda_\pm\) is given by equation (5b). Expanding the inner product gives
\[
T(k, k') = \frac{1}{4} \left[ (\lambda_+^2 \cos \theta + \lambda_-^2) + \lambda_+^2 \sin \theta \right]
\]
(19b)

Simplifying equation (19a), one obtains
\[
T(k, k') = \frac{2(\Delta^2 + (h\nu k)^2)(1 + \cos \theta)}{2(\Delta^2 + (h\nu k)^2)}
\]
(19c)

In deriving equation (19b), it is assumed that scattering takes place between two equi-energetic states such that \(|k| = |k'|\). Further, the states are assumed to be of positive helicity and \(\exp(i\theta)\) is set to unity for the initial wave function \(\theta = 0\). The relaxation time can now be evaluated by multiplying equation (19b) by the factor \((1 - \cos \theta)\) and integrating over all angles
\[
\frac{1}{\tau} = \beta \int_0^\pi T(k, k')(1 - \cos \theta) d\theta
\]
\[
= \frac{\pi \beta}{4} \left( \frac{(h\nu k)^2 + 4\Delta^2}{\Delta^2 + (h\nu k)^2} \right)
\]
(20)

Setting \(\Delta\) to zero for a pristine 3D-topological insulator, the relaxation time reduces to \(\frac{1}{\tau} = \frac{\Delta}{4}\). The ratio of the relaxation time is therefore
\[
\frac{\tau_{\text{rel}}}{\tau} = \frac{(h\nu k)^2 + 4\Delta^2}{(h\nu k)^2 + \Delta^2} = \frac{1 + 4\kappa}{1 + \kappa}
\]
(21)
where \(\tau_{\text{rel}}\) denotes the individual relaxation time for a topological(trivial) insulator and \(\kappa = \frac{\Delta}{(h\nu k)^2}\). If \(\kappa \gg 1\) when a large magnetic field is impressed, the ratio is approximately equal to four. The scattering time for a topological insulator with a band gap is therefore reduced by a factor of four over its zero-gap counterpart. This can be explained by simply noting that this corresponds to a change in the magneto-resistance; a gapped TI offers more resistance over a pristine sample which is spin-protected to have zero back scattering.

When the warping term is explicitly included, the band gap \(\Delta\) must be modified to \(\Delta_{\text{warp}} = \Delta + h^2 \lambda \cos 3\theta k^2\). Using \(\Delta_{\text{warp}}\), the scattering time expression in equation (20) changes to
\[
\frac{1}{\tau} = \beta \int_0^\pi \frac{2(\Delta_{\text{warp}})^2(1 - \cos \theta) + (h\nu k)^2 \sin^2 \theta}{2(\Delta_{\text{warp}})^2 + (h\nu k)^2} d\theta
\]
(22)

The integral in equation (22) is numerically evaluated in section 3.

The scattering time expression derived in equation (22) can be inserted in a Boltzmann equation and solved under the
relaxation time approximation to determine the response of the two-dimensional electronic system through the magneto-conductivity tensors $\sigma_{xx}$ and $\sigma_{xy}$. The magneto-conductivity tensors are evaluated with an external magnetic field directed along the $z$-axis and an electric field that is confined to the $x$–$y$ plane. The electric current in terms of Boltzmann transport equation per spin is therefore

$$J = \frac{e}{4\pi^2} \int d^2k v_k \delta f_k$$  \hspace{1cm} (23)$$

where $\delta f_k$ is the deviation from the Fermi–Dirac distribution, $v_k = v_F(\cos\theta, \sin\theta)$ and $\theta = \tan^{-1}\left(\frac{y}{x}\right)$. $v_F$ is the Fermi-velocity. The Boltzmann equation under no spatial variation is

$$\frac{df(r, k, t)}{dt} + \frac{dk}{dt} \cdot \frac{\partial f(r, k, t)}{\partial k} = 0 \hspace{1cm} (24a)$$

where $f(r, k, t)$ is the distribution function written as a sum of the equilibrium distribution and deviation under an electric and magnetic field $f(r, k, t) = f_0(r, k, t) + \delta f(r, k, t)$. Since $\frac{dk}{dt} = -q(E + v \times B)$, equation (24a) can be written as

$$\frac{df}{\tau} - q(E + v_k \frac{df}{dk} + (v \times B) \cdot \frac{\partial f}{\partial k}) = 0 \hspace{1cm} (24b)$$

In writing equation (24b), $\frac{df(r, k, t)}{dt}$ is approximated as $\frac{\delta f}{\tau}$ using the relaxation time approximation. $E$ is the electric field on the surface of the TI and $\tau$ is carrier relaxation time. Solving equation (24b) and inserting $\delta f$ in equation (23), yields the magneto-conductivity tensors

$$\sigma_{xx} = \frac{e^2|f|_s}{\pi \hbar^2} \frac{\tau}{1 + \omega_k^2 \tau^2} \hspace{1cm} (25a)$$

$$\sigma_{xy} = \frac{e^2|f|_s}{\pi \hbar^2} \frac{\omega_k \tau}{1 + \omega_k^2 \tau^2} \hspace{1cm} (25b)$$

The ratio of the longitudinal and transverse conductivity tensors for a pristine and gapped topological insulator is therefore

$$\frac{\sigma_{xx}^{nt}}{\sigma_{xx}^{0}} = \frac{\tau_0(1 + \omega_k^2 \tau^2)}{\tau(1 + \omega_k^2 \tau_0^2)} \hspace{1cm} (26a)$$

and

$$\frac{\sigma_{xy}^{nt}}{\sigma_{xy}^{0}} = \frac{\tau_0^2(1 + \omega_k^2 \tau^2)}{\tau^2(1 + \omega_k^2 \tau_0^2)} \hspace{1cm} (26b)$$

where $\omega_k = eB/\hbar c$ is the cyclotron frequency for Dirac fermions at a certain energy $E$.

3. Results and discussion

In this section we quantitatively calculate the influence of the non-topological component on the Berry phase and impurity induced momentum relaxation time on a TI surface. We utilize expressions derived in section 2. Figure 1 shows the electronic structure of a pristine TI (left panel) and also in the presence of a ferromagnet which furnishes the non-topological component. The surface state of the TI at the Dirac point ($\Gamma = 0$) is gapped due to the proximity effect due to a ferromagnet. The ferromagnet with an out-of-plane magnetization component breaks time reversal symmetry. Note that while an in-plane magnetization violates time reversal symmetry, the Dirac cone on each surface at $\Gamma$ are not gapped but simply shifted in $k$-space.

3.1. Numerical evaluation of Berry phase with warping

The combined influence of warping and a finite band gap on the Berry phase is computed numerically using equation (14). The warping term $h^2/(2m L^2)$ and the band gap $\Delta$ are varied while $|k|$ is held constant at 0.03 $1\text{ Å}^{-1}$. $|k|$ is chosen to be in close proximity of the charge neutral Dirac point at $\Gamma$. The accumulated Berry phase for a surface electron with positive spin helicity ($\eta = 1$) in presence of proximity induced magnetic field and higher order warping terms is shown in figure 2. As the strength of the warping term and band gap increases, the deviation from the topologically determined value of $\pi$ is more pronounced. The ’non-topological’ contribution arising purely on account of warping in absence of a band gap can be computed by setting $\Delta$ to zero in equation (15). The Berry phase provides a direct measurement of the intrinsic Hall current and the corresponding quantized Hall conductivity. The quantized conductivity [39] can be theoretically determined as illustrated by equation (17). We underscore the importance of external terms like $\Delta$ and $\lambda$ that break time-reversal and spatial inversion symmetry to result in a finite Berry curvature or orbital magnetic field that is revealed through an additional velocity. The additional velocity comes from the Lorentz force on an electron due to the effective Berry phase magnetization. In fact, this provides the third mechanism (external magnetic field and spin–orbit coupling are the other two) that gives rise to the now well-recognized quantum anomalous Hall effect. While the deviation as seen from figure 2 is indeed small, an experimentally observable quantum anomalous Hall current can be measured [28, 40] and constitutes a key evidence for the Berry phase.

We quantitatively now show the ’non-topological’ increase in the Berry curvature (equation (16)) which is the geometric
analog of a real magnetic field. Figure 3 plots the dependence of the dimensionless ratio of the Berry curvature to square of the magnetic length \( \frac{\alpha}{L_B^2} \) as a function of an external magnetic field. The magnetic length is approximated as 25.0 nm/\( B \) and the band gap \( \Delta \) is calculated using the Zeeman splitting \( gB \). The \( g \)-factor is set to 20 [42] for electrons on surface of a TI. The Fermi velocity for surface electrons in Bi\(_2\)Te\(_3\) is assumed to be \( 5 \times 10^5 \text{ m s}^{-1} \) and the \( k \)-vector is 0.3 1 Å\(^{-1}\). As can be easily seen from figure 3, the Berry curvature depends on the non-topological contribution of the external magnetic field that splits the surface states, an increased magnetic field therefore enhances the overall Berry curvature. The Berry curvature in equation (16) does not include the warping term, which has been ignored to write a more compact expression.

We point out that warping contribution to the overall Berry phase calculation becomes dominant when the cubic terms of the Hamiltonian are comparable in energy to the linear component. The warping terms can then no longer be treated as a perturbation; to provide an approximate energy scale where this transition could happen, we set the linear energy term equal to the cubic contribution such that \( \hbar v_k c \cos(3\theta) \). Assuming \( \cos(3\theta) = 0.5 \), the warping term [41] to be equal to 200 eV Å\(^3\), and the Fermi velocity \( v_F = 5 \times 10^5 \text{ m s}^{-1} \), gives \( k = 0.18 \text{ Å} \). This roughly corresponds to an energy equal to 0.4 eV for the surface states. This in a way also determines a cut-off energy beyond which the warped Hamiltonian is the dominant component and outweighs the linear contribution.

The Berry phase expression in this case changes to
\[
\gamma = \frac{1}{2} \int_0^{2\pi} d\theta \left( 1 \pm \frac{1}{\sqrt{2}} \right) \tag{27}
\]
which integrates to \( 1.292\pi \) for a positive helicity electron.

### 3.2. Momentum relaxation time

The ratio of momentum relaxation times for the case of an ungapped topological insulator to a gapped sample is roughly four times if \( \kappa = \frac{\Delta}{\hbar v_F B} \) in equation (21) is significantly larger than unity. The gap \( \Delta = g\mu_B B \) is computed by assuming an externally impressed magnetic field. Figure 4 shows the relaxation time ratio \( t_r/\tau_0 \) as a function of the warping strength. The corresponding ratio for a reasonably strong magnetic field equal to 50 T without warping is also indicated as a constant. For relatively small values of the magnetic field, the linearly dispersing surface-state energy \( \hbar v_k c \) dominates the Zeeman splitting term. For instance, with \( B = 50 \text{ T} \) along the \( z \)-axis, and a \( g \)-factor equal to 20, the Zeeman-induced band gap is roughly 0.0579 eV while the surface energy contribution at \( k \)-point = 0.3 1 Å\(^{-1}\) is 6.2 eV. The surface energy therefore masks the Zeeman split and brings the ratio of scattering times for a topological and trivial insulator close to unity. For \( k \)-points

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**Figure 2.** The Berry phase \( (\gamma) \) magnitude plotted as function of the warping strength. \( \gamma \) increases with greater warping thus magnifying the non-topological contribution to the standard value of \( \pi \). The overall phase is shown for two values of the band gap indicated on the sub-plots. As warping increases, the band gap contribution diminishes and the curve flattens out.

**Figure 3.** The ratio of Berry phase induced orbital magnetic field (Berry curvature) to magnetic length is plotted against an externally applied magnetic field. The Berry curvature is augmented as the magnetic field strength increases. Warping effects are ignored in this calculation.

**Figure 4.** The relaxation time ratio \( t_r/\tau_0 \) as a function of the warping strength.
sufficiently close to the Dirac point, which is a low energy case, for example, at \( k = 5e - 3 \) \( \text{Å}^{-1} \), the ratio changes to 1.71. The overall validity of a surface state energy contribution limited to a linear Hamiltonian holds only when the \( k \)-point is chosen close to the charge neutral Dirac point at \( \Gamma \).

The ratio of scattering times in states characterized by wave vectors farther away from \( \Gamma \) is more correctly represented through a numerical evaluation of equation (22). The warping term usually dominates the band gap split induced by the magnetic field and a marked deviation in the ratio of scattering times from the non-warped case is seen in figure 4. At higher warping strength, a significant shift in the ratio leads to a departure from unity for cases where the topological insulator is pristine or the higher-order \( k \) terms have limited contribution.

It must be emphasized here that a direct connection exists between the Berry phase and scattering time. As the warping strength increases, the shift in Berry phase from \( \pi \) is more pronounced as shown above. A Berry phase of \( \pi \) which gives rise to weak anti-localization [33, 43] is reduced under warping: a consequence of which is enhanced forward resistance manifest as a higher scattering time shown in figure 4.

The ratio of longitudinal and transverse conductivity tensors without warping is evaluated by using equation (26a) and equation (26b) under a sufficiently strong magnetic field of 10 T at 0.2 eV. The cyclotron frequency is 1.25 GHz; the ratio \( \sigma_{\text{xx}}/\sigma_{\text{xy}} \) by approximating \( 1 + \omega_{\text{c}}^2 \tau_{\text{nt}}^2 \) as \( \omega_{\text{c}}^2 \tau_{\text{nt}}^2 \) is \( \tau_{\text{tt}}/\tau_{\text{nt}} \). The transverse conductivity under these conditions is almost close to unity. As mentioned above, at points in proximity to \( \Gamma \), such as \( k = 5e - 3 \) \( \text{Å}^{-1} \), the longitudinal conductivity tensor ratio is 1.71. The longitudinal conductivity tensor therefore exhibits the same behaviour as the scattering times noted above.

4. Conclusion

In this work we have presented a theoretical and numerical study of the effect of a time reversal symmetry (TRS) breaking magnetic field that opens a band gap at the surface of a topological insulator and of higher order terms defined as warping of the eigen energy spectrum. The influence of time reversal symmetry (TRS) breaking magnetic field that opens a band gap at the surface and higher order terms defined by a warping of the eigen energy spectrum alter the topological Berry phase of \( (2n + 1)\pi \) and any related phenomenon that characterize the transport parameters of the carriers at the surface.

It is found that the Berry phase increases from the topologically determined value of \( \pi \) to a larger value due to an additional component that depends on the band gap split (TRS breaking) and the warping strength. Furthermore, for a given band gap induced by an external magnetic field, the Berry phase increases with the warping strength. The modification in Berry phase for a finite gap topological insulator described by a warped Hamiltonian also gives rise to an anomalous Hall velocity through the orbital magnetization. The carrier relaxation time values computed within the Boltzmann transport equation formalism (assuming spins aligned to the external magnetic field) are also warping dependent. Higher values of warping offsets the magnetic field induced splitting and becomes the dominant term in the relaxation time expression.

Finally, it is worthy to mention that to study a more accurate model, relaxation times should be computed for charged impurities with screening. Additional processes that involve spin-flip scattering by magnetic impurities, namely the Kondo-effect [44] must also be taken into account. In this work, the spin scattering factor, which has been chosen as unity to simplify calculations, should be evaluated by including a scattering angle dependent quantity. This will be done in a future work.

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