Optical conductivity of topological insulator thin films in a quantizing magnetic field

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Abstract
We determine the optical response of topological insulator thin films in the presence of a quantizing, external magnetic field. We explicitly take into account hybridization between the states of top and bottom surface. The interplay between hybridization and Zeeman energies gives rise to topological and normal insulator phases and phase transitions between them. The optical response in the two phases and at the phase transition point is investigated. We show that the difference in magneto-optical response can be used to distinguish the topological phase from the normal phase of the system. Further, the optical response also allows us to determine the gap generated by hybridization between top and bottom surface states of topological insulator thin films.

Keywords: topological insulator, magneto-optical response, thin film

1. Introduction

Three-dimensional (3D) topological insulators (TIs) are materials that have a bulk bandgap but conducting surface states [1–4]. These materials usually have strong spin–orbit interaction. The conducting surface states are protected by time-reversal symmetry. The surface states have a linear dispersion relation and the quasiparticles (Dirac fermions) at the surface obey the massless Dirac equation. Further, the surface states are helical where intrinsic angular momentum (spin) and translational momentum are locked to each other with the Dirac cone centered at the time-reversal invariant momentum point in the Brillouin zone with spin polarized Berry phase [5–7]. This was confirmed by spin polarized Angle Resolved Photo Emission Spectroscopy (ARPES). These helical Dirac fermions exist on the edge of 3D TIs such as Bi$_2$Se$_3$, Bi$_2$Te$_3$.

The gapless surface states are primarily responsible for transport in TIs. In transport studies of TIs, a major challenge is to separate the bulk contribution from the surface contribution. Since several TIs are layered materials, thin films can be synthesized with the advantage that thin films of TIs have minimum bulk contribution. Experiments on thin films are being actively pursued and it has been demonstrated that they exhibit thermoelectric effect [8], quantum spin Hall [9, 10], quantum anomalous Hall effect [11] and excitonic superfluidity [12]. Additionally, thin films provide an extra tunable degree of freedom which is their thickness. Thin films where states of top and bottom surfaces hybridize exhibit even richer physics. This hybridization can happen for 1–5 quintuple layers with a thickness of the order of 5 nm [11, 13–16]. Fabrication of Bi$_2$Se$_3$ thin film by molecular beam epitaxy [13, 17], as well as its low temperature transport studies, have been reported in [18]. Hybridization leads to opening the gap in the surface state dispersion [19]; in other words, it provides mass to Dirac fermions on the top and bottom surfaces. Further, this gap can be tuned by the application of an external magnetic field. It has been shown that the response of TI thin films in an external magnetic field is highly nontrivial [20–22]. TI thin films exhibit topological phases with phase transition that can be tuned by an external magnetic field. For surface state effects, the Fermi level has to be in the bulk band gap which can be controlled by doping a TI [5, 23] or by a gate potential. Another system that shares similarities with a TI thin film is bilayer graphene. At each valley, there are four parabolic bands in bilayer graphene, two valence and two conduction bands. Two of these meet at the Charge Neutrality Point (CNP) exhibiting no energy gap in pristine bilayer; the remaining two are split from these. Gapless bilayer is a semi-metal, but that can be changed. The gap can be opened and
tuned by an electric field (gate potential) applied perpendicular to bilayer graphene sheets. This is in contrast to a TI thin film where there is a gap when the top and bottom surfaces are coupled, and which can be tuned by an applied magnetic field.

The main question that we address in this work is the effect of hybridization between top and bottom surface states on the magneto-optical response in thin film TIs. For this, we determine the complex frequency dependent longitudinal optical conductivity \( \sigma(\omega) \); its real part gives the absorption as a function of photon energy. This has been carried out for graphene which shows good agreement between theory and experiment [24–28]. Recently in [29] optical properties of TI thin films doped with magnetic impurities has been investigated. The authors include hybridization effects and, for an exchange field that breaks time reversal symmetry, show that the value of Kerr and Faraday rotation angles is large for a wide range of frequencies. Magneto-optical properties of TIs [30] and other single layer material such as MoS\(_2\) [31, 32] and silicene [33] have also been investigated. Landau levels (LLs) are formed in the presence of an external magnetic field. Transitions between the LLs generate absorption lines (LLs) are formed in the presence of an external magnetic field. In section 5, response to circularly polarized light determines the longitudinal conductivity and transverse hall conductivity. In section 4, we consider the topological phase transition in silicene in the presence of normal (band) insulator phase in silicene in the presence of spin orbit interaction and staggered potential. In this paper, we investigate topological phase transition in thin film of a TI where hybridization between top and bottom surfaces is important. This will be done on the basis of information obtained from magneto-optical absorption spectra. We obtain the absorption spectra in both TI phase and normal insulator phase as well as at the CNP.

This paper is organized as follows: in sections 2 and 3 we develop the theoretical model of a thin film TI in a uniform external magnetic field. In section 4, we determine the longitudinal conductivity and transverse hall conductivity. In section 5, response to circularly polarized light is considered. In section 6, the topological phase transition in the semiclassical limit is investigated. In sections 7 and 8, effect of broken inversion symmetry and effect of warping in thin film TI on LLs has been discussed.

2. Theory of topological insulator thin film in an external magnetic field

We consider the Hamiltonian for the surface states in a TI thin film aligned in the x-y plane with hybridization between the surface states. When thin film is subjected to transverse magnetic field \( B = \nabla \times A \), LLs with quantized energies develop in the valence and conduction bands. We employ the minimal substitution \( p \rightarrow p + eA/c \) in the Landau gauge for vector potential \( A = (0, xB, 0) \) and \( c \) is the speed of light. The Hamiltonian of our system takes the form [11]:

\[
\hat{H}_{\sigma \tau} = \frac{v_f}{l_B} \left[ \sigma_z \left( p_y + \frac{eB}{c}x \right) - \tau_z \sigma_y p_x \right] + (\Delta_Z \tau_z + \Delta_H) \sigma_z. \tag{1}
\]

Here \((\sigma_z, \sigma_y, \sigma_x)\) define Pauli matrices acting on real spin space. \(\tau_z = +/−\) represent the symmetric/antisymmetric linear combination of surface states represented by \(|\tau_z \uparrow (\downarrow)\rangle = 1/\sqrt{2}(|\uparrow \uparrow (\downarrow \downarrow)\rangle + \tau_z |\downarrow \uparrow (\downarrow \downarrow)\rangle)\) [11]. Here \(i\) represents the top surface and \(b\) the bottom surface of the thin film. \(v_f\) is the Fermi velocity of Dirac fermions on the surface. Moreover, we have Zeeman energy \(\Delta_Z = g\mu_B B/2\), the effective Lande factor \(g\), the Bohr magneton \(\mu_B\), and \(\Delta_H\) represents the hybridization contribution which is due to the hybridization between upper and lower surfaces of the TI. As \(p_x\) and \(x\) do not commute, we can write the Hamiltonian in terms of dimensionless operators

\[
\hat{H}_{\sigma \tau} = \frac{\hbar v_f}{2l_B} \left[ \sigma_z \left( p_y + \frac{eB}{c}x \right) - \tau_z \sigma_y p_x \right] + (\Delta_Z \tau_z + \Delta_H) \sigma_z, \tag{2}
\]

where \(l_B = \sqrt{c/\epsilon B}\) is the magnetic length. \(\hat{Q} = -i\hbar p_x\) and \(\hat{P} = p_y + \frac{eB}{c}x\) such that \([\hat{Q}, \hat{P}] = i\hbar\). Employing the ladder operators \(a = 1/\sqrt{2\hbar l_B}(\hat{Q} + i\hbar \frac{eB}{c} p_x)\) and \(\hat{a}^\dagger = 1/\sqrt{2\hbar l_B}(\hat{Q} - i\hbar \frac{eB}{c} p_x)\), we may express the Hamiltonian as

\[
\hat{H}_{\sigma \tau} = \frac{\hbar v_f}{2l_B} (i\sigma_z(a^\dagger - a) + \sigma_y, (a^\dagger a)), \tag{3}
\]

which can also be written as

\[
\hat{H}_{\tau_{\tau+1}} = \begin{pmatrix} (\Delta_Z + \Delta_H) & -i\frac{\hbar v_f}{2l_B} a \\ i\frac{\hbar v_f}{2l_B} a^\dagger & -(\Delta_Z + \Delta_H) \end{pmatrix}, \tag{4}
\]

\[
\hat{H}_{\tau_{\tau-1}} = \begin{pmatrix} -(\Delta_Z - \Delta_H) & i\frac{\hbar v_f}{2l_B} a \\ -i\frac{\hbar v_f}{2l_B} a^\dagger & (\Delta_Z - \Delta_H) \end{pmatrix}. \tag{5}
\]

The energy of the LLs is given by

\[
E_n^\tau = \text{sgn}(n) \sqrt{2\hbar v_f eB |n|} + (\Delta_Z + \tau_z \Delta_H)^2. \tag{6}
\]

\[
E_0^\tau = -(\Delta_Z + \tau_z \Delta_H). \tag{7}
\]

\(\omega_B = v_f/l_B\) is the cyclotron frequency of Dirac fermions. \(n = 0, \pm 1, \pm 2, \ldots\) is the Landau level (LL) index. An important feature of the energy spectrum is the splitting of \(n \neq 0\) LLs for non-zero value of Zeeman energy and hybridization between top and bottom surfaces states. This splitting of \(n \neq 0\) requires both Zeeman energy and hybridization to be nonzero. Further, the energy spectrum is electron–hole symmetric in the absence of Zeeman energy \((\Delta_Z = 0)\). For \(\Delta_z < \Delta_H\), with a finite hybridization gap, it is not strictly electron–hole symmetric; the \(n \neq 0\) spectrum maintains this symmetry whereas \(n = 0\) spectrum does not. Note that a quadratic term can appear in the Hamiltonian even in the absence of both Zeeman energy and hybridization [38], if there is no electron–hole symmetry, as shown by angle resolved photoemission spectroscopy. In our case we have not considered a quadratic term in equation (1) as it can be neglected when the system is doped such that the Dirac point is close to the CNP, which is the focus of our work. The \(n = 0\) LL splits only when \(\Delta_H\) is nonzero. The LL energy spectrum carries important information regarding topological phase transition in the system. The \(n = 0\) LL \(E_0^\tau\) changes sign
during the phase transition from normal insulator ($\Delta_z < \Delta_h$) to TI ($\Delta_z > \Delta_h$). For normal insulator phase $E_0$ is hole like and for TI phase it is electron like. This represents an extra filled LL which gives rise to Hall conductivity $e^2/h$ [20]; hence we can write

$$\sigma_{xy} = \frac{e^2}{2h} (\text{sgn}(\Delta_z - \Delta_H) + 1).$$

(8)

At $\Delta_z = \Delta_H$, $E_0$ has exactly zero energy and is at the CNP. If the chemical potential is tuned to CNP, this zeroth LL will be partially filled. The plot of LLs with respect to magnetic field is shown in figure 1 with $g = 60$ and $\mu_B = 5.788 \times 10^{-6} \text{ eV T}^{-1}$. Similar to graphene all $n \neq 0$ LLs scale as $\sqrt{B}$. But unlike graphene $n = 0$ LLs do not sit at zero energy when $\Delta_z \neq \Delta_H$. The energy of one of the $n = 0$ LLs becomes zero for $\Delta_z = \Delta_H$. At that point $\Delta_H = 4 \text{ meV}$ with magnetic field $B = 2.3 \text{ T}$. This represents the topological phase as shown in figure 1.

Using equations (4) and (5), the states are

$$|\tilde{n}\rangle_{\tau_z,+1} = \left( \frac{A_n}{B_n} \frac{|n - 1\rangle}{|n\rangle} \right),$$

(9)

and

$$|\tilde{n}\rangle_{\tau_z,-1} = \left( \frac{A_n}{B_n} \frac{|n\rangle}{|n - 1\rangle} \right),$$

where $|n\rangle$ is an orthonormal Fock state of the harmonic oscillator and

$$A_n = \frac{1}{\sqrt{v}} \left( 1 + \text{sgn}(n) \frac{(\Delta_z + \tau_z \Delta_H)}{|E_n^i|} \right)^{1/2}, \quad n \neq 0,$$

(10)

and

$$B_n = \frac{1}{\sqrt{v}} \left( 1 - \text{sgn}(n) \frac{(\Delta_z + \tau_z \Delta_H)}{|E_n^i|} \right)^{1/2}, \quad n \neq 0,$$

(11)

3. Density of states

To shed further light on the energy spectrum of our system, we determine the Dirac fermion density of states. The Green’s function associated with our Hamiltonian is

$$G(\omega, n, \tau_z) = \sum_{\tau_z} \frac{1}{\omega - \text{sgn}(n) \sqrt{2v^2 f \mu B} |n| + (\Delta_z + \tau_z \Delta_H)^2 + i\eta},$$

(12)

From which we can compute the density of states $D(\omega)$ as

$$D(\omega) = \left[ \frac{1}{2\pi^2 l_B^2} \right] \sum_{n = -\infty}^{\infty} \sum_{\tau_z} \text{Im} G(\omega, n, \tau_z) + \sum_{\tau_z} \text{Im} G(\omega, 0, \tau_z),$$

(13)

which can be expressed as

$$D(\omega) = \frac{1}{2\pi^2 l_B^2} \left[ \sum_{n = -\infty}^{\infty} \sum_{\tau_z} \delta(\omega - \text{sgn}(n) \sqrt{2v^2 f \mu B} |n| + (\Delta_z + \tau_z \Delta_H)^2) + \sum_{\tau_z} \delta(\omega + (\Delta_z + \tau_z \Delta_H)) \right].$$

(14)

This yields

$$D(\omega) = \left[ \frac{1}{2\pi^2 l_B^2} \right] \sum_{n = -\infty}^{\infty} \sum_{\tau_z} \delta(\omega - \text{sgn}(n) \sqrt{2v^2 f \mu B} |n| + (\Delta_z + \tau_z \Delta_H)^2) + \sum_{\tau_z} \delta(\omega + (\Delta_z + \tau_z \Delta_H)).$$

(15)
The plot of density of states $D(\omega)$ is shown in figure 2 as a function of energy. We used $B = 1$ T and $\eta = 0.12/\Delta_{\text{HI}}$; $\eta$ is the scattering rate which results in broadening of the states. The two $n = 0$ LLs are located at $\omega = -(\Delta_{Z} + \Delta_{\text{HI}})$ and $\omega = -(\Delta_{Z} - \Delta_{\text{HI}})$. At $\Delta_{Z} = \Delta_{\text{HI}}$ we have peak at CNP representing partial filled LL. Peak at CNP shifts to the hole region by increasing Zeeman energy or it shifts to the electron region by decreasing Zeeman energy relative to the hybridization as shown in figures 2(a) and (c).

4. Magneto-optical conductivity

We determine the magneto-optical conductivity within the linear response regime using the Kubo formula [28, 39]

$$\sigma_{\alpha\beta} = \frac{i}{2\pi B} \sum_{\tau_{z}=\pm 1} \sum_{nm} \left( f_m - f_n \right) \frac{\langle \hat{j}_\alpha \hat{n}_m | \hat{n}_n \rangle \langle \hat{n}_n | \hat{j}_\beta \hat{n}_m \rangle}{\hbar \omega + \epsilon_m - \epsilon_n + i\eta},$$

(16)

where $\hat{j}_\alpha = e \frac{\partial H}{\partial \alpha}$ and $f_m = 1/[1 + \exp(\beta(\epsilon_m - \mu))]$ is the Fermi distribution function with $\beta = 1/k_B T$, $\epsilon_m$ is the energy of $m$th LL and $\eta$ is scattering rate taken as constant. We will take states $m$ to be occupied and $n$ as unoccupied LLs. The selection rule for LLs transition is $|n| = |m| \pm 1$ determined by the evaluation of matrix elements. At zero temperature we can drop the absolute value of $n$ and all transition to negative LLs are Pauli blocked. For longitudinal magneto-optical conductivity with $\hat{j}_x = ev_f (-\tau_z \sigma_y)$, the matrix element for symmetric eigenstates is determined as

$$\langle \hat{n}_m | \hat{j}_x \hat{n}_n | \hat{n}_m \rangle = v_f^2 e^2 \left[ \frac{\left( A_m B_n \right)^2 \delta_{n,m-1}}{\epsilon_m - \epsilon_n} + \frac{\left( A_n B_m \right)^2 \delta_{n,m+1}}{\epsilon_m - \epsilon_n} \right],$$

(17)

and for antisymmetric eigenstates, it is

$$\langle \hat{n}_m | \hat{j}_x \hat{n}_n | \hat{n}_m \rangle = v_f^2 e^2 \left[ \frac{\left( A_m B_n \right)^2 \delta_{n,m-1}}{\epsilon_m - \epsilon_n} + \frac{\left( A_n B_m \right)^2 \delta_{n,m+1}}{\epsilon_m - \epsilon_n} \right].$$

(18)

Therefore, we obtain

$$\sigma_{xx} = \frac{2i v_f^2 e^2 \hbar B}{\pi} \sum_{\tau_{z}=\pm 1, mn} \frac{\left( A_m B_n \right)^2 \delta_{n,m-1} + \left( A_n B_m \right)^2 \delta_{n,m+1}}{(E_n - E_m)(\hbar \omega + E_n^0 - E_m^0 + i\eta)}.$$
where $\sigma_o = e^2/4\hbar$. From the above result it is clear that for possible transitions we must have $n = |m| \pm 1$. Using the selection rule $n = |m| \pm 1$ we can write

\[
\frac{\sigma_{xx}(\omega)}{\sigma_o} = \frac{2v_f^2 e^2}{\pi} B \times \sum_{\tau_z=\pm1,m} \frac{(A_{|m|+1} B_m)^2}{(E_{|m|+1} - E_m)(\hbar \omega + E_m - E_{|m|+1}^e + \eta)} + \frac{(A_m B_{|m|-1})^2}{(E_{|m|-1} - E_m)(\hbar \omega + E_m - E_{|m|-1}^e + \eta)} \Bigg] \times \sum_{\tau_z=\pm1,m} \frac{(A_{|m|+1} B_m)^2 \times \eta}{(E_{|m|+1} - E_m)(\hbar \omega + E_m - E_{|m|+1}^e + \eta^2)} + \frac{(A_{|m|-1} B_m)^2 \times \eta}{(E_{|m|-1} - E_m)(\hbar \omega + E_m - E_{|m|-1}^e + \eta^2)} \Bigg].
\]

(20)

For transverse Hall conductivity $\hat{j}_x = ev_f (\tau_z \sigma_y)$ and $\hat{j}_y = ev_f (\sigma_y)$. The matrix elements are evaluated to yield

\[
\frac{\sigma_{xy}}{\sigma_o} = \frac{2v_f^2 e^2}{\pi} \times \sum_{\tau_z=\pm1,m} \tau_z \bigg[ \frac{(A_{|m|+1} B_m)^2}{(E_{|m|+1} - E_m)(\hbar \omega + E_m - E_{|m|+1}^e + \eta)} \bigg] = \frac{2v_f^2 e^2}{\pi} \times \sum_{\tau_z=\pm1,m} \tau_z \bigg[ \frac{(A_{|m|-1} B_m)^2}{(E_{|m|-1} - E_m)(\hbar \omega + E_m - E_{|m|-1}^e + \eta)} \bigg].
\]

(21)

Using selection rule $n = |m| \pm 1$ we can write

\[
\frac{\sigma_{xy}}{\sigma_o} = \frac{2v_f^2 e^2}{\pi} \times \sum_{\tau_z=\pm1,m} \bigg[ \frac{(A_{|m|+1} B_m)^2}{(E_{|m|+1} - E_m)(\hbar \omega + E_m - E_{|m|+1}^e + \eta)} \bigg] = \frac{2v_f^2 e^2}{\pi} \times \sum_{\tau_z=\pm1,m} \bigg[ \frac{(A_{|m|-1} B_m)^2}{(E_{|m|-1} - E_m)(\hbar \omega + E_m - E_{|m|-1}^e + \eta)} \bigg].
\]

(22)

This is the general expression for transverse Hall conductivity representing transition from $m$ to $|m| \pm 1$ state. We can also
Figure 4. Imaginary part of the transverse conductivity $\sigma_{xy}(\omega)$ of thin film topological insulator in units of $e^2/h$ as a function of $h\omega$ in eV compared in (a) TI regime, (b) at CNP and (c) NI regime. The scattering rate is $\eta = 0.15\Delta H$ and $\mu = 0$.

determine $\text{Im}\sigma_{xy}/\sigma_o$ as

$$\frac{\text{Im}\sigma_{xy}}{\sigma_o} = \frac{2\nu^2 e^2 h B}{\pi^2} \sum_{\tau_\tau=\pm 1} \left[ \frac{-\tau_\tau (A_m B_{m\tau})^2 \times \eta}{(E_{E_{m\tau}} - E_0)\left[(h\omega + E_{E_{m\tau}} - E_{E_{m\tau}})^2 + \eta^2\right]} \right] \left[ \frac{\tau_\tau (A_m B_{m\tau})^2 \times \eta}{(E_{E_{m\tau}} - E_0)\left[(h\omega + E_{E_{m\tau}} - E_{E_{m\tau}})^2 + \eta^2\right]} \right] .$$

(24)

Figure 3(c) shows $\text{Re}\sigma_{xy}(\omega)/\sigma_o$ as a function of frequency in normal insulator phase showing absorption line for interband transitions with $\nu^2 e^2 h B = 1.6 \times 10^{-2}$ for magnetic field of 1 Tesla and $\mu = 0$. The transition energy is determined from the energy gap between LLs satisfying the selection rule for allowed transitions. The first two absorption peaks correspond to $E_{-1} \rightarrow E_{0}^+$ and $E_{0}^+ \rightarrow E_{1}^+$ transitions. These transitions involve zeroth LL. The energy of first peak is $E_{0}^+ - E_{-1}$ and for the second peak it is $E_{1}^+ - E_{0}^+$. Each of these peaks represents single transition. The absorption peaks for allowed transitions which involve LLs other than $E_0^+$ represent the sum of absorption peaks of two transitions in the absence of hybridization($\Delta_H = 0$), one transition for $E_{-n} \rightarrow E_{n+1}$ and another transition for $E_{-(n+1)} \rightarrow E_{n}$. However, for finite hybridization $\Delta_H$, each peak splits into two peaks for $\tau_\tau = +1$ and $\tau_\tau = -1$. The first peak represents $E_{-1}^+ \rightarrow E_{n+1}^+$ and $E_{n+1}^+ \rightarrow E_{-1}^+$ transitions. The second peak represents $E_{-n}^+ \rightarrow E_{n+1}^+$ and $E_{-(n+1)}^+ \rightarrow E_{n}^+$ transitions. For a fixed hybridization, the splitting between these peaks depends on the applied magnetic field; the energy gap is $(\Delta Z + \tau_\tau \Delta H)$. Further, the spacing between absorption peaks also depends on the broadening parameter $\eta$; we have taken its value to be $\eta = 0.15\Delta H$ estimated from experimental findings [40]. Moreover, at low magnetic fields, in the NI phase, the splitting between $\tau_\tau = -1$ and $\tau_\tau = -1$ is very small, as shown in figure 3(c). Figure 3(b) shows the real part of $\sigma_{xx}(\omega)$ at CNP. For the first peak two transitions, represented by arrows, $E_{0}^+ \rightarrow E_{1}^+$ and $E_{-1}^+ \rightarrow E_{0}^+$ contribute; while the second peak represents $E_{0}^+ \rightarrow E_{1}^+$ transition. The value of Zeeman interaction is large enough that it can open a gap between LLs of different $\tau_\tau$ but the same Landau index $n$ resulting in splitting of absorption peaks; this is clearly seen in the third peak. Figure 3(a) shows $\text{Re}\sigma_{xx}(\omega)/\sigma_o$, as a function of frequency in the TI phase with broken particle-hole symmetry for interband transitions. The first absorption peak represents the transition $E_{0}^+ \rightarrow E_{-1}^+$, while the second peak represents the $E_{0}^+ \rightarrow E_{1}^+$ transition. An important feature of the absorption spectra is that the $E_{0}^+ \rightarrow E_{-1}^+$ has replaced the $E_{-1}^+ \rightarrow E_{0}^+$ transition.
which was allowed in normal insulator phase, but Pauli blocked in TI phase. Another difference arises in absorption peaks for \( \tau_z = -1 \) and \( \tau_z = +1 \) respectively. These differences not only decrease the height of absorption peaks but they also create oscillations in absorption peaks for Im\( \sigma_y(\omega)/\sigma_o \) in the topological insulator phase. For example the terms for the first peak in equation (24) for \( \tau_z = -1 \) have \( E_{-1} \rightarrow E_0^- \) and \( E_{-2} \rightarrow E_1^- \) transitions. Both of these transitions have opposite signs but have same transition energy. So these terms decrease the height of absorption peaks. Similar behavior is seen for \( \tau_z = +1 \). The amplitude for the transition with \( m \rightarrow |m| + 1 \) will always be greater than the amplitude of transition \( m \rightarrow |m| - 1 \) for \( \tau_z = -1 \) in both TI and normal insulator phase. At CNP, the contribution to absorption peak in Im\( \sigma_y(\omega)/\sigma_o \) resulting from transitions involving \( \tau_z = -1 \) are absent. At \( \Delta_\text{H} = \Delta_\text{H} \) all transitions resulting from \( \tau_z = -1 \) cancel out and the contribution to absorption peaks is given by transition between LLs with \( \tau_z = +1 \). The first peak in figure 4(b) represents the transition \( E_0^+ \rightarrow E_1^- \) while for the second case, two transitions contribute i.e. \( E_{-1}^+ \rightarrow E_0^+ \) and \( E_{-2}^+ \rightarrow E_1^+ \) transitions. Figure 4(a) represents the absorption peaks for Im\( \sigma_y(\omega)/\sigma_o \) in TI phase. At \( \Delta_\text{H} > \Delta_\text{H} \) the absorption peaks has negative and positive amplitudes. The first negative peak results from the transition \( E_0^- \rightarrow E_1^- \), while the second positive peak represents the \( E_0^+ \rightarrow E_1^+ \) transition.

A schematic diagram which helps us to understand the behavior of the absorption lines that we have described is shown in figure 5 for NI, in figure 6 at CNP, and in figure 7 in TI phase. On the left side we show the Landau index \( n \) with energy define by equation (6). The blue lines represent the LLs with \( \tau_z = -1 \) while red lines represent LLs for \( \tau_z = +1 \). The bold black line gives the possible values of chemical potential \( \mu = 0 \). The possible optical transitions are indicated by vertical arrows and they connect the levels \( m \) to \( |m| \pm 1 \) only. Moving from left to right in figure 5 in NI phase we see first two single transitions with different transition energy from \( E_{-1}^- \rightarrow E_0^- \) and \( E_{-2}^+ \rightarrow E_1^- \), then a pair of interband transitions from \( E_{-1}^- \rightarrow E_2^- \) and \( E_{-2}^+ \rightarrow E_1^- \) followed by another pair \( E_{-1}^+ \rightarrow E_2^- \) and \( E_{-2}^- \rightarrow E_1^- \). The difference between the transition energy of these two pairs is very small in NI phase showing small splitting in absorption peak of Re\( \sigma_y(\omega)/\sigma_o \). For TI the schematic of allowed transitions is shown in figure 7. The main difference in the TI and NI phase arises in the first transition. The transition \( E_{-1}^- \rightarrow E_0^- \) in NI is replaced by the transition \( E_0^- \rightarrow E_1^- \) in TI. The 2nd transition is from \( E_0^+ \rightarrow E_1^- \). It is followed by a pair of transitions from \( E_{-1}^- \rightarrow E_2^- \) and \( E_{-2}^- \rightarrow E_1^- \) followed by another pair \( E_{-1}^+ \rightarrow E_2^- \) and \( E_{-2}^+ \rightarrow E_1^- \). The absorption peaks of the two pairs are well separated in the response function of Re\( \sigma_y(\omega)/\sigma_o \), as shown in figure 3(a). At CNP, the allowed transitions are shown in figure 6. The first two transitions involve partially filled LL \( E_{0}^- \). These transitions are \( E_0^- \rightarrow E_1^- \) and \( E_{-1}^- \rightarrow E_0^- \). These have the same transition energy. These transitions are followed by \( E_0^+ \rightarrow E_1^+ \), then a pair of transitions the same as described previously. Figures 8 and 9 represent Re\( \sigma_y(\omega)/\sigma_o \) which resulted from allowed transitions in NI and TI phases respectively for \( \mu = 0.02 \text{eV} \). The red peak represents the absorption lines contributed by intraband transitions; while the black peaks represent the allowed interband transition splited in TI phase at high magnetic field. A schematic diagram for allowed transition with nonzero value chemical potential is shown in figure 10 for low magnetic field (NI) and in figure 11 for high magnetic field (TI) showing inter and intra band transitions.
5. Circularly-polarized light

For circularly Polarized light the conductivity is written as $\sigma_{xx}(\omega) \pm i \sigma_{xy}(\omega)$ with (+) representing the right-handed polarization and (−) representing left-handed polarization. The circularly polarized light shows different behavior in normal insulator and in topological insulator phase. The absorptive part of conductivity is

$$\text{Re} \sigma_{\pm} = \text{Re} \sigma_{xx}(\omega) \mp i \text{Im} \sigma_{xy}(\omega)$$

For normal insulator

$$\frac{\text{Re} \sigma_{+}(\omega)}{\sigma_0} = \frac{2v_f^2e\hbar B}{\pi} \times \sum_{m=0}^{\infty} \left[ (A_{|m+1|}B_m)^2 \times \frac{\eta}{(E_{|m+1|}^+ - E_m^+)(\hbar\omega + E_m^+ - E_{|m|+1}^+ + \eta^2)} \right. \right.$$

$$\left. + \frac{(A_mB_{|m|-1})^2 \times \eta}{(E_{|m|-1}^- - E_m^-)(\hbar\omega + E_m^- - E_{|m|-1}^- + \eta^2)} \right]$$

and

$$\frac{\text{Re} \sigma_{-}(\omega)}{\sigma_0} = \frac{2v_f^2e\hbar B}{\pi} \times \sum_{m=0}^{\infty} \left[ (A_{|m+1|}B_m)^2 \times \frac{\eta}{(E_{|m+1|}^+ - E_m^+)(\hbar\omega + E_m^+ - E_{|m|+1}^+ + \eta^2)} \right. \right.$$

$$\left. + \frac{(A_mB_{|m|-1})^2 \times \eta}{(E_{|m|-1}^- - E_m^-)(\hbar\omega + E_m^- - E_{|m|-1}^- + \eta^2)} \right]$$

For topological insulator

$$\frac{\text{Re} \sigma_{+}(\omega)}{\sigma_0} = \frac{2v_f^2e\hbar B}{\pi} \times \sum_{m=0}^{\infty} \left[ (A_{|m+1|}B_m)^2 \times \frac{\eta}{(E_{|m+1|}^+ - E_m^+)(\hbar\omega + E_m^+ - E_{|m|+1}^+ + \eta^2)} \right. \right.$$

$$\left. + \frac{(A_mB_{|m|-1})^2 \times \eta}{(E_{|m|-1}^- - E_m^-)(\hbar\omega + E_m^- - E_{|m|-1}^- + \eta^2)} \right]$$

and

$$\frac{\text{Re} \sigma_{-}(\omega)}{\sigma_0} = \frac{2v_f^2e\hbar B}{\pi} \times \sum_{m=0}^{\infty} \left[ (A_{|m+1|}B_m)^2 \times \frac{\eta}{(E_{|m+1|}^+ - E_m^+)(\hbar\omega + E_m^+ - E_{|m|+1}^+ + \eta^2)} \right. \right.$$

$$\left. + \frac{(A_mB_{|m|-1})^2 \times \eta}{(E_{|m|-1}^- - E_m^-)(\hbar\omega + E_m^- - E_{|m|-1}^- + \eta^2)} \right]$$
Figure 8. Real part of the longitudinal conductivity $\sigma_{xx}(\omega)$ of thin film topological insulator in units of $e^2/h$ as a function of $\hbar\omega$ in eV in normal insulator phase. The scattering rate is $\eta = 0.15\Delta_H$ and $\mu = 0.0225$ and $B = 2$ T. Red peak represents absorption peak for intraband transition while black peaks represent absorption peaks for interband transitions.

Figure 9. Real part of the longitudinal conductivity $\sigma_{xx}(\omega)$ of thin film topological insulator in units of $e^2/h$ as a function of $\hbar\omega$ in eV in topological insulator phase. The scattering rate is $\eta = 0.15\Delta_H$, $\mu = 0.0225$ and $B = 4$ T. All peaks represent absorption peaks for interband transitions.

Figure 12 shows absorption peaks for right-handed circularly polarized light for $\text{Re}\sigma_{xx}(\omega)/\sigma_0$ versus $\omega$. The right-handed circularly polarized light in normal insulator phase only gives $m \rightarrow |m|+1$ transition for $\tau_z = -1$ and $m \rightarrow |m|−1$ transition for $\tau_z = +1$. In both cases $m \leq -1$ if $\mu = 0$ while for TI phase it gives $m \rightarrow |m|+1$ transition for $\tau_z = -1$ with $m \leq 0$ for $\mu = 0$ and for $\tau_z = +1$ it gives $m \rightarrow |m|−1$ transition with $m \leq -1$. The plot for TI phase is shown in figure 12(a).

Figure 13 shows absorptive peaks which resulted from the left-handed circularly polarized light for $\text{Re}\sigma_{-xx}(\omega)/\sigma_0$ versus $\omega$. Left-handed circularly polarized light gives $m \rightarrow |m|+1$ for $\tau_z = +1$ and $m \rightarrow |m|−1$ for $\tau_z = -1$ transitions with $m \leq 0$ for $\mu = 0$ in both cases. While in TI it gives $m \rightarrow |m|+1$ for $\tau_z = +1$ with $m \leq 0$ and $m \rightarrow |m|−1$ for $\tau_z = -1$ transition with $m \leq -1$ for $\mu = 0$.

6. Semiclassical limit

The semiclassical limit is valid when the quantization between LLs is unimportant. It is the case when chemical potential...
the transition between and the last pair at the lowest energy represents the transition between Landau levels of same $B = 1$ T and $\mu = 0.02$. Orange arrows represent intraband transition and black arrows represent interband transitions.

$\mu \gg E_1$ [12]. For large $\mu$ all transitions will be intraband. The energy of intraband transitions is given by $\delta E = E_{n+1} - E_n$, which is approximated to give

$$\delta E = \frac{\hbar \omega_B e B}{\sqrt{2N}\hbar \omega_B e B + (\Delta Z \pm \Delta H)}$$

(30)

The chemical potential $\mu$ falls exactly between $N$ and $N + 1$ with $N \gg 1$, so we can write $\mu \approx E_N$, we obtain

$$\delta E = \frac{\hbar \omega_B e B}{\mu},$$

(31)

so for $n$ to $n + 1$ transitions the Re$\sigma_{xx}(\omega)$ in semiclassical limit is written as

$$\text{Re} \sigma_{xx}(\omega) = \frac{\mu}{2\pi} \sum_{\tau_z = \pm 1} \langle A_{m+1} | B_m \rangle^2 \times \frac{\eta}{[\mu \omega - \hbar \omega_B e B + (\Delta Z \pm \Delta H)]^2 + \eta^2}.$$  

(32)

The real part of the frequency dependent longitudinal optical conductivity Re$\sigma_{xx}(\omega)$ versus $\hbar\omega$ in units of $e^2/h$ in the semiclassical limit is shown in figure 14 with $E_o < \mu < E_{n+1}$. The first pair starting from the right side represents the transition between $n = 5$ to $n = 6$ while the second pair represents the transition between $n = 11$ and $n = 12$ LLs and the last pair at the lowest energy represents the transition between $n = 20$ and $n = 21$ LLs. The dashed peak gives the transition between $\tau_z = -1$ LLs and solid peaks represent transitions for $\tau_z = +1$ LLs. We observe that as the chemical potential increases the spectral weight increases.

7. Broken inversion symmetric TI thin film

Thin film TIs are usually grown on a substrate which breaks inversion symmetry. In this case, the effective Hamiltonian in the symmetric and antisymmetric basis, equation (1), will be augmented by a term $V \sigma_z$ that breaks inversion symmetry. $V$ represents the magnitude of inversion asymmetry. The Hamiltonian becomes

$$\hat{H}_{\sigma_z} = \sqrt{\hbar \omega_B} \left( i \sigma_z (a^+ - a) + \tau_z \sigma_z (a + a^+) \right) + \Delta Z \tau_z + \Delta H \sigma_z + V \sigma_z.$$  

(32)

This is the inversion symmetry broken thin TI Hamiltonian given in equation (3) of [11], without the exchange field for ferromagnetic ordering but including an applied magnetic field. The single-particle eigenstates of the above Hamiltonian have the following form:

$$| n, \tau_z, \text{sgn}(n) \rangle = u_{n\tau_z=+1}^{\text{sgn}(n)} | n \rangle \downarrow, \tau_z = +1 \rangle$$

$$+ u_{n\tau_z=+1}^{\text{sgn}(n)} | n \rangle \uparrow, \tau_z = +1 \rangle$$

$$+ u_{n\tau_z=-1}^{\text{sgn}(n)} | n \rangle \downarrow, \tau_z = -1 \rangle$$

$$+ u_{n\tau_z=-1}^{\text{sgn}(n)} | n \rangle \uparrow, \tau_z = -1 \rangle.$$  

(33)
$u_{\sigma z}^{\text{sign}(n)}$ are the complex four-component spinor wave functions. The LL spectrum can be obtained by diagonalizing the following Hamiltonian

$$
\begin{pmatrix}
\Delta_Z + \Delta_H & -i\sqrt{2\hbar v_f}a & 0 & V \\
i\sqrt{2\hbar v_f}a & (\Delta_Z + \Delta_H) & V & 0 \\
0 & V & -(\Delta_Z - \Delta_H) & i\sqrt{2\hbar v_f}a^2 \\
V & 0 & -i\sqrt{2\hbar v_f}a & \Delta_Z - \Delta_H
\end{pmatrix}
$$

(34)

Diagonalizing equation (34), we find the following LL spectrum:

$$
E_{\tau z}^n = \text{sgn}(n)\left[2\hbar v_f^2 eB |n| + V^2 + \Delta_Z^2 + \Delta_H^2 + \tau_z \sqrt{2V^2\hbar v_f^2 eB |n| + \Delta_Z^2 + \Delta_H^2 + V^2}\right]^{1/2}
$$

(35)

$$
E_{\tau z}^0 = -(\Delta_Z + \tau_z \sqrt{\Delta_Z^2 + V^2}).
$$

(36)

In the inversion symmetry broken system, the phase transition from normal insulator to TI phase now occurs at $\Delta_Z = \sqrt{\Delta_H^2 + V^2}$. This shows that the phase transition is pushed to higher magnetic fields. For $V = 0$ the system is decoupled for $\tau_z = \pm 1$. As a result of inversion symmetry breaking, symmetric and antisymmetric hybridized states become coupled to each other and there can be allowed transitions between them. An additional feature is that broken inversion symmetry gives rise to crossing of LLs $n$ with $\tau_z = +1$ and $n+1$ with $\tau_z = -1$ at certain values of magnetic field, as shown in figure 15. This will allow additional transitions between LLs with $\tau_z = +1$ and LLs with $\tau_z = -1$. Recently, one photon and two photon absorption was investigated in TI thin films with broken inversion symmetry [41], in the absence of a magnetic field. It was observed that additional transition channels open when inversion symmetry is not present.

8. Effect of hexagonal warping on Landau levels and magneto-optical conductivity

ARPES data suggests that there is warping effect on the band structure of Bi$_2$Te$_3$. To take this effect into account, Fu [42] added a cubic correction term in the Hamiltonian of a TI. This induces an anisotropic effect on the bands in momentum space whose strength is set by the parameter $\lambda$. The Hamiltonian of TI thin film in a magnetic field with a warping term is

$$
\hat{H}_{\sigma z} = \hat{H}_{\sigma z} - \frac{2\lambda \hbar^2}{l_B^3} [(a^\dagger)^3 + (a)^3] \sigma_z \tau_z,
$$

(37)
Figure 13. \( \text{Re} \sigma_{\text{xx}}(\omega)/\sigma_0 \) as a function of frequency for left handed circularly-polarized light in (a) topological insulator phase (b) at CNP (c) normal insulator phase.

Figure 14. The semiclassical limit of the real part of the longitudinal conductivity \( \text{Re} \sigma_{\text{xx}}(\omega)/\sigma_0 \) in units of \( \frac{e^2}{\hbar} \) in eV.

where \( \hat{H}_{\sigma \tau} \) is given in equation (3). Analytical diagonalization of the above Hamiltonian is not possible. However, if warping is treated as a perturbation, then effect of warping on LLs can be evaluated [43]. These results show that the primary effect of warping on the LL spectrum is that slope of LLs increases with increasing magnetic field. This has implications on our work; warping affects the gap between LLs with optical transitions shifting to higher \( \hbar \omega \). This effect will be more significant at higher magnetic fields.

9. Summary and conclusions
We have studied the effect of hybridization between the top and bottom surface states on the magneto-optical conductivity
in a thin film TI. Hybridization induces a gap in the Dirac spectrum. Each LL splits into two with the same Landau index representing LLs for symmetric and antisymmetric hybridized states. At a critical magnetic field the system makes a quantum phase transition from the NI phase to a TI phase. This has a signature in the magneto-optical absorption spectra, both \( \text{Re}\sigma_{xx}(\omega) \) and \( \text{Im}\sigma_{xy}(\omega) \). \( \text{Re}\sigma_{xx}(\omega) \) peak for \( E_{n-1} \to E_0 \) transition in NI phase is replaced by \( E_0 \to E_1 \) peak in TI phase. More significant signature for the quantum phase transition is found in absorption spectra for \( \text{Im}\sigma_{xy}(\omega) \). It shows negative peaks in the TI phase which are absent in the absorption spectra in NI phase. The signature in circularly polarized light is the splitting and shifting of the absorption peaks in TI phase relative to the NI phase.

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