

Magneto-optical response of five-septuple-layer MnBi_2Te_4 in spin-flip states

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Magneto-optical (MO) effects like Kerr and Faraday rotations provide a direct probe of topological order in thin films of the magnetic topological insulator (TI) MnBi_2Te_4 (MBT). Motivated by recent experimental studies of spin-flip/flop transitions in MBT thin films, we investigate the interplay between interlayer spin configurations, topological order, and MO response in five septuple-layer (5-SL) MBT using first-principles calculations and a simplified coupled Dirac cone model. Our results reveal that, despite possessing a nonzero out-of-plane magnetization, 5-SL MBT thin films can be either $\mathcal{C} = +1$ TIs or $\mathcal{C} = 0$ topologically trivial insulators depending on the relative spin orientations of the top and bottom SLs. We evaluate the Faraday and Kerr rotation angles using tight-binding models derived from *ab initio* calculations and by comparing our results with those of a simplified coupled Dirac cone model to clarify the macroscopic mechanisms underlying the MO response of spin-flip states. These theoretical findings highlight the tunability of topological and MO properties in MBT thin films and provide microscopic insight into the emergence of complex topological order in layered antiferromagnetic materials.

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I. INTRODUCTION

Time-reversal symmetry breaking can be induced in topological insulators (TIs) by external magnetic fields [1,2], magnetic doping [3,4], or proximity effects [5,6] and detected by measuring their Faraday and Kerr rotation magneto-optical (MO) responses. In intrinsic magnetic TIs such as MnBi_2Te_4 (MBT), magnetization survives down to the few-layer limit in thin films and couples to the topological surface states (TSS) [7–9]. In their ground state (GS), MBT thin films—composed of van der Waals (vdW) gapped and antiferromagnetically (AFM) coupled neighboring septuple layers (SLs)—are Chern insulators exhibiting the quantum anomalous Hall effect (QAHE) for odd SLs [10,11], while for even SLs, they realize the axion insulating phase expected to display the topological magnetoelectric effect [11–13]. Other distinctive even-odd layer-dependent quantum effects have also been actively investigated [14–18].

While transport measurements are commonly used to identify these topological phases [17], MO responses provide a powerful complementary tool for topological characterization of MBT thin films. For example, Qiu *et al.* have confirmed the existence of dynamical axion quasiparticles in six SL (6-SL) MBT using ultrafast optical pump-probe experiments [19]. Quantized magneto-terahertz (THz) effects (Faraday and Kerr rotations) were reported in 6-SL and seven SL (7-SL) MBT

thin films in Ref. [20], and helicity-dependent optical control of AFM order has been demonstrated in 6-SL MBT films [21]. Real-time observation of magnetization and magnon dynamics across different thicknesses are opening routes for ultrafast manipulation of topological and magnetic order in MBT samples [22].

While A-type AFM order with out-of-plane spins is the GS in MBT [7,9], under an applied external magnetic field, thin films exhibit rich and complex spin configurations. The MBT phase diagram includes field-induced spin-flip/flop transitions that modify the spin-wave excitations (magnons) of the AFM-ordered SLs [22–24]. For example, Lian *et al.* have studied the QAHE under spin flips/flops in 7-SL MBT by tuning the gate voltage and the perpendicular magnetic field and have uncovered a cascade of quantum phase transitions [25]. Han *et al.* discussed abrupt magnitude changes in MO response during these transitions, suggesting the possible existence of a Chern insulator state even in 6-SL MBT films under an external magnetic field [20].

Existing theoretical studies on MO properties of TIs [26] and magnetic TIs [27] mostly focus on the GS and discuss layer-dependent Faraday and Kerr rotations and their electric field dependence. The magnetic phase diagram and metamagnetic evolution of few-layer MBT under external magnetic field is discussed in Ref. [28]. Similarly, the emergence of the QAHE in compensated even-layer AFM films with different spin-flip configurations is established in Ref. [29], without investigating their MO response. While these studies provide important insights into the topological and magnetic properties of MBT thin films, they are primarily based on effective low-energy models. A comprehensive first-principles investigation of all-possible spin-flip states, including their relative energetics, electronic structure, topology, and frequency-dependent MO response, remains lacking. Addressing these

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questions is crucial for connecting the rich meta-magnetic phase space of MBT thin films to experimentally accessible optical signatures found in recent experiments [19,21] and forms the primary motivation of the present work.

Hence, we focus specifically on all possible microscopic spin-flip configurations of 5-SL MBT thin films and map out their corresponding relative energy landscape. The interplay between different interlayer spin-arrangements, band gaps, and frequency-dependent transverse and longitudinal conductance and MO responses are discussed using first-principles calculations and compared with a simplified coupled Dirac cone toy model [27]. We argue that, despite possessing a nonzero out-of-plane magnetization, a 5-SL thin film can exhibit either nonvanishing ($C = +1$) or vanishing ($C = 0$) Chern insulating phases. The Chern number of the GS instead depends mainly on the relative spin orientations of the top and bottom SLs. We clarify the merits and the limitations of the coupled Dirac cone model [27] compared with first-principle results in describing the salient transport and MO features of magnetic TI thin films.

II. COMPUTATIONAL DETAILS

First-principles calculations were performed using density functional theory (DFT) and the projector augmented-wave method [30,31] as implemented in VASP package [32]. The generalized gradient approximation in the Perdew-Burke-Ernzerhof parametrization was employed for the exchange-correlation potential. The plane-wave cutoff energy was set to a large value of 430 eV. We use a Γ -centered Monkhorst-Pack $9 \times 9 \times 1$ ($12 \times 12 \times 1$) k -mesh for the Brillouin zone integration for structural relaxation (self-consistent calculations). In the iterative solution of Kohn-Sham equations, we ensured a force convergence of 10^{-3} eV/Å and an energy convergence of 10^{-7} eV. DFT-D3 vdW dispersion corrections were employed in all calculations to capture long-range vdW interactions [33]. A vacuum layer of 15 Å was added in the out-of-plane direction to create two-dimensional (2D) structures free from artifacts of the three-dimensional periodic boundary conditions. To correctly describe strong on-site Coulomb interactions of localized Mn d electrons, we used a Hubbard U correction (GGA+ U method) following Dudarev's scheme [34] and fixed the on-site Coulomb (U) and exchange (J) parameters as 3.9 and 0.0 eV, respectively.

A real-space tight-binding (TB) model Hamiltonian was obtained by parametrizing the self-consistent Kohn-Sham Hamiltonian using the WANNIER90 package [35–37]. For this purpose, we used the VASP2WANNIER90 interface and included Mn- d , Bi- p , and Te- p orbitals in generating the Wannier functions. Topological characteristics were computed using the WANNIERTOOLS [38] and WANNIERRBRI packages [39].

For the computation of the optical conductivity, we used the Kubo-Greenwood formula [40,41]

$$\sigma_{xy}(\hbar\omega) = \frac{ie^2}{\hbar} \int \frac{d^2k}{(2\pi)^2} \sum_{nm} \frac{f_{n\mathbf{k}} - f_{m\mathbf{k}}}{E_{n\mathbf{k}} - E_{m\mathbf{k}}} \times \frac{\langle m\mathbf{k} | \partial_{k_x} H_{\mathbf{k}} | n\mathbf{k} \rangle \langle m\mathbf{k} | \partial_{k_y} H_{\mathbf{k}} | n\mathbf{k} \rangle}{E_{n\mathbf{k}} - E_{m\mathbf{k}} - (\hbar\omega + i\eta)}, \quad (1)$$

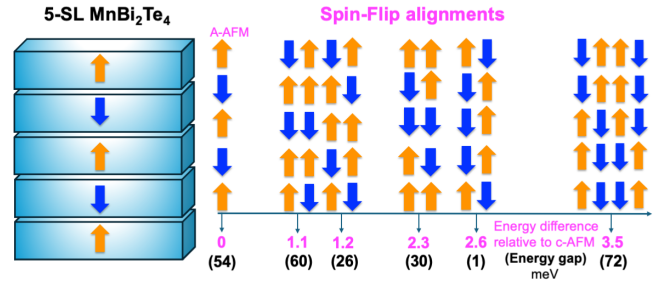


FIG. 1. (left) Schematic of a 5-SL MBT in the AFM GS configuration. (right) Alternate spin-flip configurations with the same net magnetic moment of $5\mu_B$. Energy difference per unit cell (in meV) compared with the AFM GS and band gaps (in meV) are given at the bottom of degenerate cases in magenta and black colors, respectively.

where $f_{n\mathbf{k}}$ is the Fermi-Dirac distribution function giving band occupation probability, ω is the optical frequency, $\hbar$ is the reduced Planck's constant, n, m are band indices, $|n\mathbf{k}\rangle$ and $|m\mathbf{k}\rangle$ are Bloch states, $E_{n\mathbf{k}}$ and $E_{m\mathbf{k}}$ are the corresponding band energies, and η is a phenomenological parameter used for broadening ($\eta = 0.08$ meV).

III. RESULTS AND DISCUSSION

A. Spin configurations in 5-SL MBT thin films

Bulk MBT combines intrinsic magnetism, due to Mn magnetic moments ($\sim 5\mu_B$), and nontrivial band topology characterized by the topological Z_2 invariant [8]. MBT thin films consist of ferromagnetic SL (Te–Bi–Te–Mn–Te–Bi–Te) blocks stacked along the c axis. The GS of a 5-SL thin film has adjacent SLs coupled AFM, with spins pointing along the out-of-plane easy axis, as shown in the left panel of Fig. 1. This thickness was chosen among odd-layer films because it represents an intermediate regime in which surface-state hybridization is reduced compared with thinner films (i.e., 3-SL MBT) while finite-size effects and magnetic-exchange interactions remain significant. At the same time, the film is sufficiently thick to support multiple spin-flip configurations, having distinct relative energies, exchange gaps, and topological phases. Moreover, this thickness allows for a direct comparison between first-principles TB calculations and the coupled Dirac cone model, as both approaches remain computationally feasible. For the AFM GS in 5-SL MBT, TSS display an exchange gap of 54 meV at the Dirac point. From now on, we will consider this value of the energy gap as a zero-energy reference.

Spin configurations involving spin flips between adjacent SLs and thus deviating from the AFM GS configuration are possible, regardless of the mechanism responsible for their formation. Figure 1 (right) illustrates all possible spin alignments for the 5-SL film that preserve a net magnetic moment of $5\mu_B$. This value corresponds to the typical magnetic moment of a single Mn atom in each SL and therefore provides a natural reference for describing spin-flip states in 5-SL MBT. The relative energies of these configurations, calculated per unit cell with respect to the AFM GS energy, are indicated below each alignment in magenta color. The higher-energy spin configurations in Fig. 1 are all metastable and can be realized

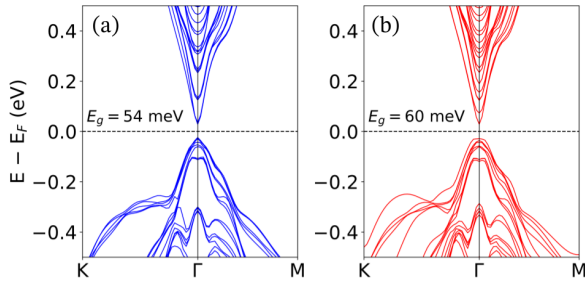


FIG. 2. (a) Band structure of a 5-SL MBT in the AFM GS configuration. (b) Band structure of degenerate spin-flip alignments having 1.1 meV higher energy than the GS.

by cycling applied external magnetic fields and temperatures [25,42–45]. To examine whether our conclusions depend on the magnitude of total magnetization, we also investigated a configuration with a higher net moment of $15 \mu_B$, which will be discussed later.

Spin-reversal processes are energetically costly but become increasingly relevant when the exchange energies between adjacent SLs are comparable with the anisotropy energy [46] or when external perturbations—such as magnetic field, strain, or proximity effects—dominate and lower the barriers separating different magnetic stacking states [47]. Importantly, these deviations from the GS spin configurations have the crucial effect of modifying the TSS gap magnitude and even the topological symmetry of the system. Considerable attention has been paid to how native point and surface defects [48–51] and surface reconstructions [52] affect the TSS energy gap. Our results suggest that the role of domain structures containing local spin-flip magnetic configurations, which has been less investigated, also deserves a careful investigation. The right panel of Fig. 1 shows all spin configurations with the same net magnetization as the GS together with their relative energies and TSS energy gaps (black numbers in parentheses at the very bottom). We do not address the cases of canting, whose topological response has already been discussed in Ref. [53].

We classify all the spin-flip configurations that preserve the same total magnetic moment of the 5-SL MBT GS into two physically distinct categories: (1) configurations in which the spins of the top or bottom SLs are aligned parallel to their adjacent layer(s), thereby modifying the surface magnetization, and (2) configurations in which the parallel spin alignment occurs only within the interior SLs of the 5-SL stack, leaving the surface magnetization comparatively unchanged. Within each category, we identify energetically degenerate configuration pairs, such as the first case when either the top or the bottom two SL spins are aligned in parallel (shown as orange arrows). Here, the energy relative to the AFM GS is only 1.1 meV per unit cell. Interestingly, we observe a flattening of the topmost valence band around the Γ point owing to this change, as shown in Fig. 2(b). Moreover, the TSS energy gap is enhanced to 60 meV in comparison with 54 meV observed for the AFM GS [see also Fig. 2(a)]. In contrast, when the SL spin alignment moves inside the film, the TSS gap decreases to 26 meV, even though the energies of this configuration (1.2 meV) and the previous one (1.1 meV) are essentially the

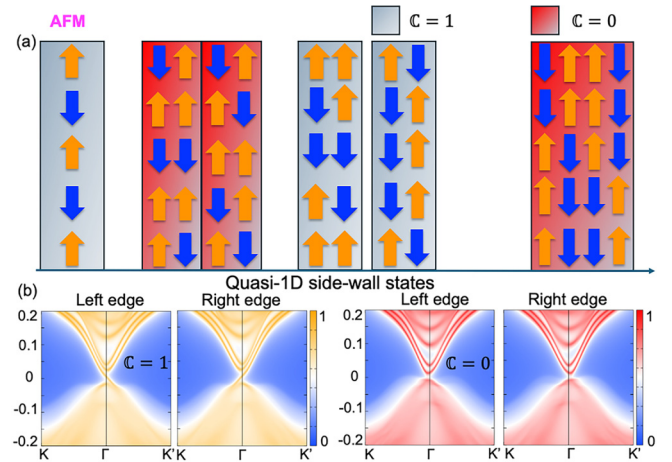


FIG. 3. (a) Topological nature of different spin-flip alignments. Blue columns represent $C = +1$, and red columns show $C = 0$ cases, depending on the spin alignment of the topmost and bottommost SLs. (b) Quasi-1D left and right side-wall edge states of 110 surface, shown for the two representative $C = +1$ and 0 cases, respectively.

same. Hence, we conclude that the distinction between the two classes is consequential, as the TSS gap is predominantly governed by the spin alignments of the surface and adjacent interior SLs. Contiguous SLs at the surface with parallel spin configurations are more effective in increasing the TSS energy gap than contiguous SLs with parallel spin configurations located inside the film.

Extending this analysis to the last two cases (2.6 and 3.5 meV energy difference relative to AFM GS) when three inner (outer) SLs are aligned parallel, we observe a TSS gap of 1 meV (72 meV), respectively. These findings are in line with the recent experimental work in Ref. [25]. Since the Dirac-like surface states are spatially localized largely in the top and bottom SLs only, we notice that parallel-spin SLs on the surfaces increase the local surface magnetization which, in turn, produces a larger exchange field and is responsible for an increase in the TSS gap. On the other hand, parallel spin SL pairs in the interior reduce the effective surface exchange field, thus yielding a smaller TSS gap. This behavior demonstrates that the TSS gap in MBT thin films is controlled primarily by the local top and bottom SL spin alignments rather than by the global magnetization of the sample.

B. Topological properties of MBT 5-SL thin films

Next, we examine the topological character of the spin-flip states in a 5-SL MBT thin film. Since we have already established that the relative spin orientations of the top and bottom surface SLs play a crucial role in determining the TSS gap, it is natural to classify all cases into two groups: (1) configurations in which the surface SL spins are parallel and (2) those in which they are antiparallel. This distinction proves to be decisive in determining the topological nature of spin-flip states by computing Chern number for each case. Interestingly, when the topmost and bottommost SL spins are aligned in the same direction, we obtain a nontrivial Chern insulating phase with $C = 1$, as shown in blue color in Fig. 3(a). In contrast, when the surface SL spins are oppositely oriented, we find that the

Chern number vanishes ($\mathcal{C} = 0$), as shown in the panels with red color in Fig. 3(a). This argument is valid for a thicker 7-SL thick MBT film as well, as shown in the Supplemental Material [54]. In other words, the topological response mirrors our earlier conclusion that a global magnetization of the sample ($5 \mu_B$ for 5-SL MBT) does not necessarily imply a nonzero Chern number characterizing a Chern insulating state; rather, it is the relative orientation of the top and bottom SLs which dictates the topology of MBT thin films. We further confirm this by looking at a higher net magnetization of $15 \mu_B$, as shown in Fig. S1 in the Supplemental Material [54].

Additionally, we compute quasi-one-dimensional (1D) side-wall edge states of the 110 surface for two representative cases, with $\mathcal{C} = 1$ and 0 , respectively, as shown in Fig. 3(b) (left). For the $\mathcal{C} = 1$ case, we observe spin-polarized counter-propagating chiral edge states on the left and right side walls (orange), as expected for a quantized Chern insulating state. On the other side, the $\mathcal{C} = 0$ case shows gapped side-wall edge states (red), which is typical of an axion insulating state. It should be mentioned that, in a recent experiment, Han *et al.* pointed to the presence of a possible Chern insulator state in an even 6-SL MBT film under an external magnetic field [20]. According to our theoretical results, this finding can be explained by a magnetic field-induced spin-flip transition, where the SL spins on the top and bottom surfaces are parallel. Finally, the coexistence of $\mathcal{C} = 0$ and 1 spin-flip states at fixed nonzero magnetization provides insight into the existence of complex topological order present in MBT thin films.

C. MO properties

Experimentally, quantum transport and MO measurements are the two most convenient ways of studying the topological properties [2–4]. To elucidate the underlying mechanisms of the quantized response in characterizing a specific topological state, we first analyze the longitudinal and transverse optical conductivities. Using the expression of the optical conductivity tensor given in Eq. (1) calculated with a TB model obtained from *ab initio* methods, we present results for the two cases ($\mathcal{C} = 0$ and 1). In Fig. 4, we plot the real (Re, blue line) and imaginary (Im, red line) parts of the transverse [Figs. 4(a) and 4(c)] and longitudinal [Figs. 4(b) and 4(d)] optical conductivities for $\mathcal{C} = 1$ and 0 , respectively. In this figure, the dashed vertical line marks the position of the TSS gap. At photon energies much smaller than the TSS gap value ($\hbar\omega \ll E_{\text{gap}}$), we find $\text{Re}\sigma_{xy}$ to be quantized in units of e^2/h (Hall plateau), which is characteristic of the Chern insulating ($\mathcal{C} = 1$) state [see Fig. 4(a)]. On the other hand, $\text{Im}\sigma_{xy}$ remains zero throughout the gapped region. As the frequency increases and approaches the threshold of $\hbar\omega \approx E_{\text{gap}}$, photons have enough energy to excite electrons across the gap. In the region of $\hbar\omega > E_{\text{gap}}$, $\text{Re}\sigma_{xy}$ increases beyond the quantized value, and $\text{Im}\sigma_{xy}$ becomes greater than zero. As shown in Fig. 4(b) for the $\mathcal{C} = 1$ case, the real part of the longitudinal conductivity ($\text{Re}\sigma_{xx}$) remains zero inside the gapped region due to the absence of interband transitions, signaling absence of dissipation, whereas in the same region, $\text{Im}\sigma_{xx}$ decreases linearly. These findings are in qualitative agreement with the

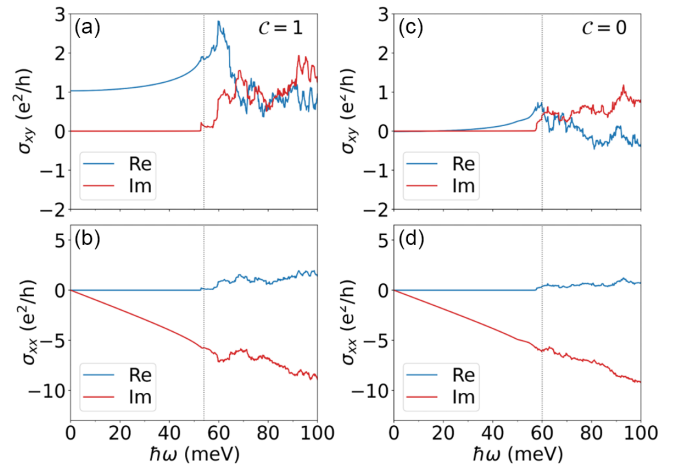


FIG. 4. Frequency-dependent optical conductivity (in units of e^2/h) for the two representative spin-flipped 5-SL MBT cases. (a) and (c) Transverse (Hall) conductivity (σ_{xy}) and (b) and (d) longitudinal conductivity (σ_{xx}) for the representative $\mathcal{C} = +1$ and 0 . In each case, real and imaginary parts are shown in blue and red colors, respectively. The TSS gap is shown as a dotted line.

results in Ref. [27] based on a simplified coupled Dirac cone model.

It is pertinent to mention that a nonzero Berry curvature acts as an effective magnetic field in momentum space, generating an anomalous transverse velocity and thus a Hall response in the gapped TSS. The quantization of $\text{Re}\sigma_{xy}$ in the parallel spin-alignment configuration of the top and bottom SL layers, where each surface contributes to half-quantized Hall conductance, is a signature of the QAHE in the zero frequency limit. In the $\mathcal{C} = 0$ state, i.e., when the surface SL spins are aligned in the antiparallel direction, both $\text{Re}\sigma_{xy}$ and $\text{Im}\sigma_{xy}$ are zero in the TSS gap region, leading to the so-called zero-Hall plateau of the zero-frequency Hall conductance in the axion insulating phase [55]. Alternatively, a nonzero $\text{Re}\sigma_{xy}$ reflects the asymmetric optical response of the material to right- and left-circularly polarized light in systems where time-reversal symmetry is broken, thereby producing a rotation of the plane of light polarization.

Since MBT thin films intrinsically break time-reversal symmetry through their internal magnetic order, MO measurements provide an indirect probe to confirm these transport features. Indeed, the coupling between circularly polarized incident light and spin-flip states should lead to a distinct MO response in the two phases, in the form of Faraday rotation (θ_F) and Kerr rotation (θ_K) angles, corresponding to the rotation of the polarization plane of transmitted and reflected light from MBT samples. This behavior can be described using a simple electrodynamic model. If a thin film of thickness d ($d \ll \lambda$, with λ being the wavelength of incident light) is placed between two dielectrics with refractive indices $n_1 = \sqrt{\epsilon_1}$ (top) and $n_2 = \sqrt{\epsilon_2}$ (bottom), the MO response is characterized by 2D conductive layers with surface conductivity σ (measured in units of e^2/h). Imposing the boundary conditions allows us to determine the transmission field ($E_{x/y}^t$) and reflection field ($E_{x/y}^r$).

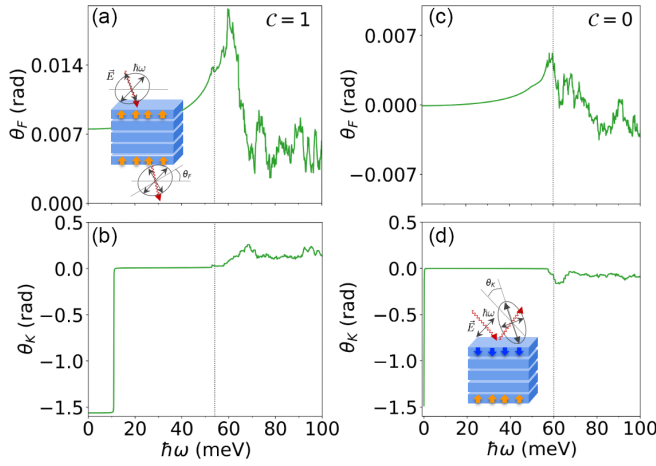


FIG. 5. MO response of two representative spin-flipped 5-SL MBT cases. (a) and (c) Faraday rotation angle and (b) and (d) Kerr rotation angle (in rad) against optical frequency (ω) for the representative $C = +1$ and 0 cases.

We then express these fields in a linear polarization basis

$$\begin{pmatrix} E_x^t \\ E_y^t \end{pmatrix} = \frac{1}{N} \begin{pmatrix} 2n_1(n_1 + n_2 + 2\alpha\sigma_{xx}) \\ -4\alpha n_1\sigma_{xy} \end{pmatrix}, \quad (2)$$

$$\begin{pmatrix} E_x^r \\ E_y^r \end{pmatrix} = \frac{1}{N} \begin{pmatrix} n_1^2 - (n_2 + 2\alpha\sigma_{xx})^2 - (2\alpha\sigma_{xy})^2 \\ -4\alpha n_1\sigma_{xy} \end{pmatrix}, \quad (3)$$

where $N = (n_1 + n_2 + 2\alpha\sigma_{xx})^2 + (2\alpha\sigma_{xy})^2$.

Using Eqs. (2) and (3) together with the optical conductivity tensor computed via the Kubo-Greenwood formula in Eq. (1), we finally obtain expressions for the angles θ_F and θ_K as follows:

$$\theta_F = \frac{1}{2}(\arg E_+^t - \arg E_-^t), \quad \theta_K = \frac{1}{2}(\arg E_+^r - \arg E_-^r), \quad (4)$$

where $E_{\pm}^{t,r} = E_x^{t,r} \pm i E_y^{t,r}$.

We use these expressions to calculate the MO response of spin-flip states, focusing on the θ_F and θ_K angles for $C = +1$ and 0 cases, as shown in Fig. 5. In the limit $\hbar\omega \ll E_{\text{gap}}$ (dotted black line), θ_F acquires the quantized value of $\theta_F = C \tan^{-1}\alpha$ (α is the fine structure constant) for the $C = +1$ case, whereas it vanishes for the $C = 0$ case, as shown in Figs. 5(a) and 5(c). These observations can be explained by the specifics of the measurements to underlying physical processes, as depicted schematically in the inset of Fig. 5(a). For the $C = +1$ case, the spins on the top and bottom SLs are parallel. Since θ_F is proportional to the sum of the Hall conductivities along the light propagation direction, the contributions of both surfaces to the Faraday angle add up, resulting in a finite rotation of the polarization plane. Conversely, for $C = 0$, the spins on the top and bottom surfaces are oppositely oriented. As a consequence, the polarization-plane rotation induced at the top surface is compensated by an opposite rotation at the bottom surface, leading to a vanishing net θ_F in the gapped region, as shown in Fig. 5(c). Importantly, the distinction between the $C = +1$ and 0 spin-flip states is qualitative rather than quantitative, as only the former exhibits a low-frequency quantized θ_F plateau.

On the other hand, light reflection from MBT spin-flip states can be characterized through the Kerr rotation angle (θ_K), as shown in Figs. 5(b) and 5(d). Several experiments using THz and far-infrared spectroscopy techniques on thin films and bulk MBT have reported the observation of MO Kerr signals [15,22,56]. Refer to Fig. 5(b), spin-flip states corresponding to $C = 1$ [panels with blue color in Fig. 4(a)] are characterized by nonzero value of θ_K . In the DC limit ($\omega \rightarrow 0$), neglecting dissipation terms ($\text{Im}\sigma_{xy}$ and $\text{Re}\sigma_{xx}$), we can estimate $\theta_K \simeq -\pi/2$, in agreement with the results for odd-numbered MBT films in Ref. [27]. Notice that the value of θ_K remains constant—generating the flat plateau visible in Fig. 5(b)—but drops sharply to zero at a finite frequency. Importantly, the θ_K sudden jump to zero obtained from the realistic TB model does not correlate with the TSS energy gap but occurs at a considerably smaller threshold of $\hbar\omega \approx 10$ meV. For spin-flip states leading to $C = 0$ [panels with red color in Fig. 4(a)], the decay is rapid and does not exhibit a robust low-frequency plateau, as given in Fig. 5(d). This behavior of θ_K differs from the results in Ref. [27], where the size of the flat plateau was controlled by the TSS energy gap. In other words, in the description of the Kerr dynamics [$\theta_K(\omega)$], we find a discrepancy between the microscopic TB model approach and the coupled Dirac cone model, although both models correctly capture the topological phase of the system. The reason for this discrepancy is explained below. Nevertheless, the spectral range of θ_F and θ_K in this work is experimentally accessible, and predicted MO signals are well within the detection capabilities of current state-of-the-art MO and THz spectroscopy techniques [56].

We first address the sharp change from $-\pi/2$ to 0 of θ_K [presented in Fig. 5(b)] and the decrease in the width of the plateau below the TSS gap found in the microscopic TB model. For this, it is necessary to start from Eq. (4), which gives the Kerr angle θ_K in as the difference of $\arg z = (\arg E_+^r - \arg E_-^r)$. Here, $\arg z$ is the phase of the complex number z in the interval $(-\pi, \pi)$. The phase of a complex number z can, in principle, be expressed as the inverse tangent of the ratio ($\text{Im}z/\text{Re}z$). Note, however, that a naive calculation of $\arctan(\text{Im}z/\text{Re}z)$ would only yield an angle in the interval $(-\pi/2, \pi/2)$. To get the full range of the phase, it is necessary to consider the signs of ($\text{Re}z$) and ($\text{Im}z$) separately, which allows us to determine the quadrant on which the complex number resides. As shown in detail in the Supplemental Material [see Eqs. (S4)–(S7)] [54], this is conveniently done by means of the two-argument function $\text{atan2}(\text{Im}z, \text{Re}z)$ [57]. This algorithm uniquely specifies the argument of z in the interval $-\pi$ to π and thereby correctly reproduces branch switches caused by the sign changes of ($\text{Re}z$) and ($\text{Im}z$), which are ultimately responsible for the sharp change in θ_K .

By writing θ_K in terms of the atan2 function, we finally obtain the following expression:

$$\theta_K = \frac{1}{2}\text{atan2}\{\text{Im}[E_+^r(E_-^r)^*], \text{Re}[E_+^r(E_-^r)^*]\}. \quad (5)$$

Calculating $\text{Im}[E_+^r(E_-^r)^*]$ and $\text{Re}[E_+^r(E_-^r)^*]$ in the TSS-gapped region ($\text{Re}\sigma_{xx} = 0$ and $\text{Im}\sigma_{xy} = 0$) and using the piecewise definition of the atan2 function (see Eqs. (S9) and (S10) in the Supplemental Material [54]), one can directly track how the conductivity components control the behav-

ior of θ_K . Inside the gap, $\text{Re}\sigma_{xy}$ remains constant, whereas $|\text{Im}\sigma_{xx}|$ increases monotonically with ω . As a result, the complex quantity $z(\omega) = E_+^r(E_-^r)^*(\omega)$ evolves continuously in the complex plane, and the Kerr angle $\theta_K(\omega) = \frac{1}{2} \arg z(\omega)$ decreases toward zero as the relative phase between the reflected circular components E_+^r and E_-^r is reduced by the growing longitudinal reactive response. The sharp steplike crossover toward $\theta_K \simeq 0$ occurs at the point where the reactive longitudinal contribution becomes comparable with the Hall term, causing $\text{Re}z(\omega) = 0$ to vanish and change sign. This produces a rapid phase shift of the corresponding reflected circular component, i.e., a rapid change of the relative phase $\arg[E_+^r(E_-^r)^*]$ by approximately $\pm\pi$, which translates into a change of θ_K by $\pm\pi/2$. In the atan2 representation, this phase shift appears as the branch switching discussed in Figs. S2 and S3 in the Supplemental Material [54]. The apparent abruptness of the step is set by how quickly this compensation is reached, which we discuss in more detail in the next section.

D. Comparison with the coupled Dirac cone model

To interpret the characteristic features of the MO response in different regimes, we use the coupled Dirac cone model introduced in Ref. [45] and based on the theoretical formalism developed earlier in Ref. [26]. Therein, the properties of MBT thin films are modeled by coupled Dirac cones originating from the top and bottom SLs and are described by the following Hamiltonian:

$$H = \sum_{\mathbf{k}_\perp, i, j} \{ [(-1)^i \hbar v_D (\hat{\mathbf{z}} \times \boldsymbol{\sigma}) \cdot \mathbf{k}_\perp + m_i \sigma_z] \delta_{ij} + \Delta_{ij} (1 - \delta_{ij}) \} c_{\mathbf{k}_\perp, i}^\dagger c_{\mathbf{k}_\perp, j}. \quad (6)$$

Here, $\mathbf{k}_\perp$ is the in-plane two-dimensional quasimomentum, and $c_{\mathbf{k}_\perp, i}^\dagger$ and $c_{\mathbf{k}_\perp, j}$ are the electron creation and annihilation operators in the i th and j th Dirac cones, respectively. Indexes i and j are numbered for each SL; odd index corresponds to the upper surface and the even index to the lower surface. The Dirac kinetic term $\hbar v_D (\hat{\mathbf{z}} \times \boldsymbol{\sigma}) \cdot \mathbf{k}_\perp$ describes the linear dispersion of surface states, and the factor $(-1)^i$ considers the opposite sign of the Dirac term for the upper and lower surfaces. The mass term $m_i \sigma_z$ determines the exchange splitting of the corresponding Dirac cone, where m_i is formed as the sum of contributions from nearby Mn magnetic layers within the same SL (J_S parameter) and from neighboring SLs (J_D parameter). The off-diagonal elements Δ_{ij} describe the hybridization between different Dirac cones. Specifically, we use Δ_S to indicate the coupling between upper and lower cones within a SL and Δ_D the coupling between cones across the gap between adjacent SLs. Thus, an N -layer film is reduced to a quasi-2D system with $4N$ bands. The following set of parameters are used in our model calculations: $v_D = 5 \times 10^5$ m/s, $\Delta_S = 84$ meV, $\Delta_D = -127$ meV, $J_S = 36$ meV, and $J_D = 29$ meV. We employed the Kubo-Greenwood formula [Eq. (1)] to obtain the components of conductivity tensor. Finally, Eqs. (2)–(5), used above for the DFT TB model, are also used here to calculate the Kerr and Faraday rotation angles.

The conductivity plots for this model are shown in Figs. 6(a), 6(b), 6(e), and 6(f). We notice that the coupled

Dirac cone model captures qualitatively the behavior of the TB model, with two main differences:

(i) The main peaks appear exactly at the threshold set by energy gap TSS E_{gap} , whereas in the TB model they appear at frequencies exceeding $E_{\text{gap}}/\hbar$.

(ii) The imaginary part of the conductivity $\text{Im}\sigma_{xx}$ is approximately constant and small inside the TSS gap region [Figs. 6(b) and 6(f), red line] before developing a sharp cusp at $\omega = E_{\text{gap}}/\hbar$, in contrast with the linear decrease with a relative large negative slope displayed by the TB model [see Figs. 4(b) and 4(d)]. This is observed to occur for both $C = 1$ and 0. It turns out that this qualitative and quantitative difference between the two models is responsible for the remarkably different behavior of their corresponding Kerr angles, for the $C = 1$, displayed in Figs. 6(b) and 6(c) (blue line), respectively. For both models, θ_K starts at $-\pi/2$ for $\omega = 0$, forming a flat plateau, whose width, however, is different for the two cases. Using the coupled Dirac cone model, the threshold is exactly equal to the TSS gap, while for the TB model, the value is considerably smaller than the gap. Beyond this threshold, θ_K for the TB model is just a step function sharply dropping to zero and remaining so until the $\hbar\omega \approx$ TSS gap. For the coupled Dirac cone model, θ_K smoothly tends to zero after a small sharp step up.

Point (ii) exposes the main limitation of the minimal continuum description of the finite-frequency MO response. The 4N-band coupled Dirac cone model captures the topological Hall response correctly, but it does not contain the full multi-band reactive longitudinal response present in the microscopic TB calculation.

Indeed, the band structure of the former, shown in Fig. 2, contains many more bands than the latter, which for a 5-SL MBT film consists of only 20 bands. (Remember that, in this model, an N -SL thin film is reduced to a quasi-2D system with $4N$ bands.) Indeed, the considerably more complex band structure of the TB model allows many more transitions when calculating $\text{Im}\sigma_{xx}$ (the reactive response term of σ_{xx} given by the principal value), leading to linear behavior with a large slope within the TSS gap region [58].

To demonstrate this point, we plot the conductivity tensor components (σ_{xx} and σ_{xy}) together with the corresponding Kerr and Faraday rotation angles in Fig. 7, calculated for a 31-SL coupled Dirac cone model and whose electronic structure now consists of 124 energy bands that account for an increased number of transitions. We can see that the transverse component (σ_{xy}) shows good agreement with the results of the TB model [see Fig. 4(a)]. Hence, θ_F remains unchanged and retains its quantized value, as shown in Fig. 7(c). In addition, the imaginary part of the longitudinal conductivity ($\text{Im}\sigma_{xx}$) now exhibits a steeper slope in contrast with the model calculation shown in red color in Fig. 6(b).

A steeper (more negative) slope of $\text{Im}\sigma_{xx}(\omega)$ implies a faster growth of the reactive longitudinal response inside the gap. This accelerates the evolution of the complex quantity $z(\omega) = E_+^r(E_-^r)^*$ in the complex plane and brings it to the branch-switching condition $\text{Re}z(\omega) = 0$ at a lower frequency (see Eq. (S10) and Figs. S2 and S3 in the Supplemental Material [54]). This corresponds to reaching the point where the longitudinal reactive contribution becomes comparable with the Hall term, so that the relative phase between the reflected

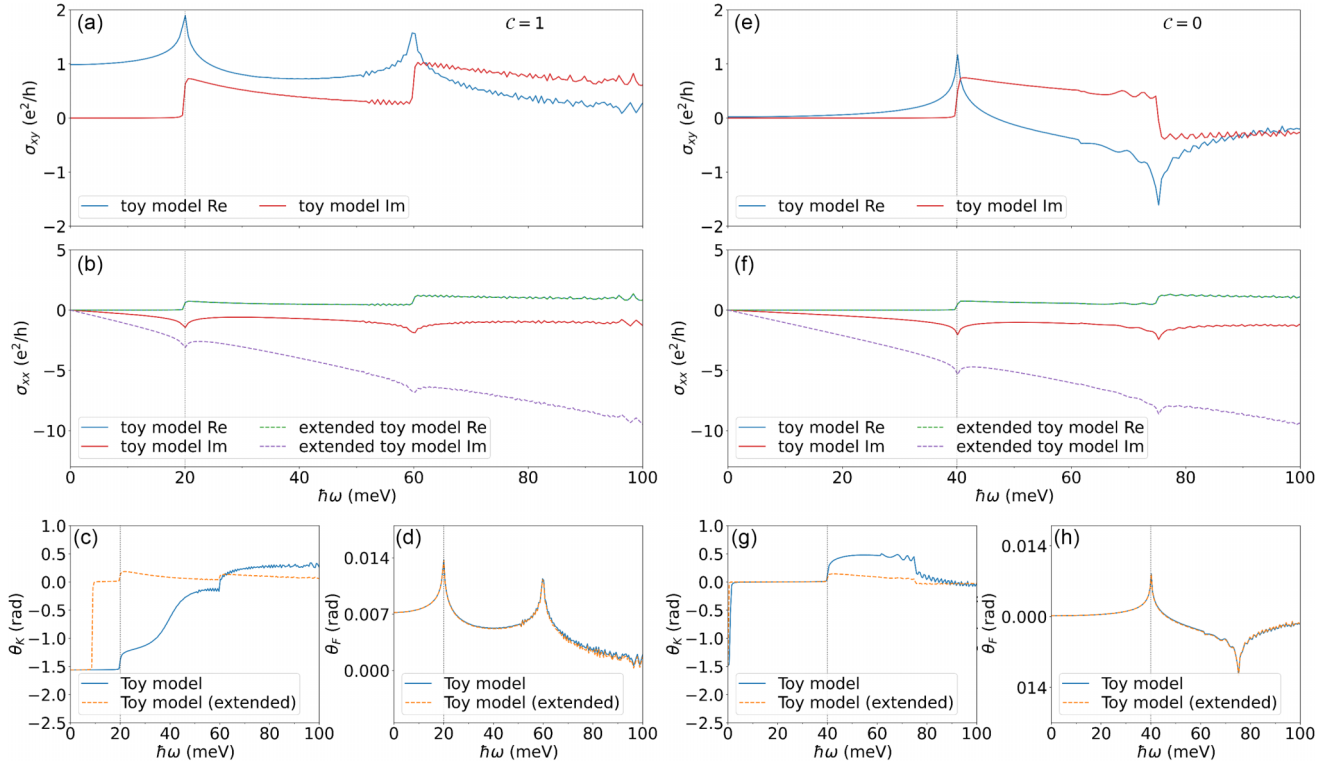


FIG. 6. Frequency-dependent optical and MO responses of the coupled Dirac cone model for our representative (a)–(d) $C = +1$ and (e)–(h) $C = 0$ cases. (a) and (e) Transverse (Hall) conductivity (σ_{xy}) and (b) and (f) longitudinal conductivity (σ_{xx} ; in units of e^2/h); real and imaginary parts are distinguished by different colors as indicated in the legends. Solid lines correspond to the coupled Dirac cone model (toy model), while dashed lines show the extended model including a phenomenological reactive correction $-i\kappa\omega$. (c) and (g) Kerr rotation $\theta_K(\omega)$ and (d) and (h) Faraday rotation $\theta_F(\omega)$ angles obtained from (σ_{xy}) and (σ_{xx}) . Vertical dotted lines mark the TSS energy gap value.

circular components changes rapidly. As a result, the value of the phase extracted via atan2 belonging to the first branch switches a branch earlier, and $\theta_K(\omega)$ exhibits an earlier and sharper steplike crossover toward values close to zero (see Figs. S3(b)–S3(d) in the Supplemental Material [54]). This

reduces the width of the ($\theta_K = -\pi/2$) plateau emanating from $\omega = 0$ and accounts for the steplike feature observed in the microscopic TB results. This also indicates that, outside the strictly low-frequency regime, the MO response cannot be inferred from the exchange gap alone and requires an explicit treatment of the multiband optical transitions.

To elucidate further the origin of the discrepancy between the minimal coupled Dirac cone and the microscopic TB models, we introduce an extended coupled Dirac cone model. This extension does not add extra bands to the original 4N-band Hamiltonian. Instead, it phenomenologically accounts for the reactive longitudinal response of remote interband transitions and bulk/surface-hybridized states that are absent in the minimal low-energy model and is given below:

$$\sigma_{xx}^{\text{extd}}(\omega) = \sigma_{xx}(\omega) - i\kappa\omega. \quad (7)$$

Here, κ is a phenomenological parameter whose sign and magnitude are chosen to reproduce the linear low-frequency behavior of $\text{Im}\sigma_{xx}$ found in the TB calculation. As a result, for the conductivity component $\text{Im}\sigma_{xx}^{\text{extd}}$, the slope of the plot increases significantly [Figs. 6(b) and 6(f) (purple line)]. Using this extended model, the Kerr and Faraday angles were obtained for both cases $C = 0$ [Figs. 6(g) and 6(h)] and $C = 1$ [Figs. 6(c) and 6(d)]. In this case, we can see that the width of the plateau exactly matches the value of the energy gap, and the switch to zero is smoother than in the TB model.

The difference between the TB and toy model is directly related to how fast the complex quantity $z(\omega) =$

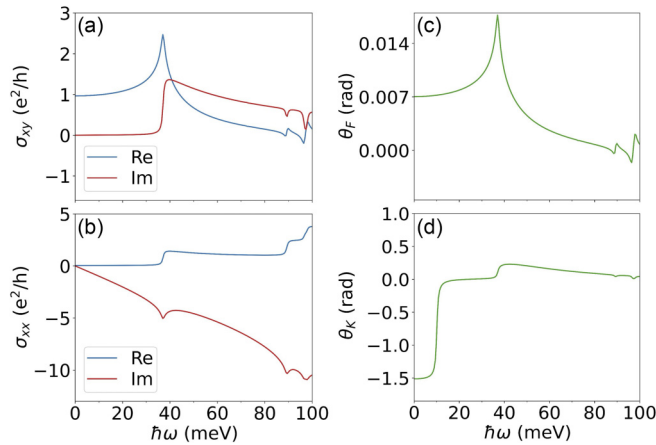


FIG. 7. Optical conductivity and MO response of the coupled Dirac cone model for an increased number of layers ($N = 31$). (a) Transverse (Hall) conductivity (σ_{xy}) and (b) longitudinal conductivity (σ_{xx} ; in units of e^2/h). Real and imaginary parts are shown in blue and red colors, respectively. (c) Faraday rotation $\theta_F(\omega)$ and (d) Kerr rotation $\theta_K(\omega)$ angles.

$E'_+(E'_-)^*$ reaches the branch-switching condition $\text{Re}z(\omega) = 0$ (see Figs. S2 and S3 in the Supplemental Material [54]). For finite κ , the crossing occurs within a narrow frequency interval, and the resulting step in θ_K appears almost discontinuous. In contrast, for $\kappa = 0$, the trajectory may first approach the real axis (i.e., $|\text{Im}z(\omega)|$ becomes small), leading to a smooth decay of θ_K before the final rapid collapse when the sign change of $\text{Re}z(\omega)$ is completed. Accordingly, increasing κ sharpens the crossover and reproduces the more abrupt step-like behavior seen in the TB results by effectively accelerating the evolution of $\text{Im}\sigma_{xx}$.

In evaluating MO responses, we used the frequency broadening value of $\eta = 0.08$ meV. This value is much smaller than the characteristic energy scale of the Kerr angle sharp step-like crossover. Thus, the rapid suppression of θ_K cannot be attributed to excessive numerical broadening (see Fig. S4 in the Supplemental Material [54]).

Moreover, in an experimental setup, the optical conductivity can be influenced by bulk carriers, an electric field, substrate, or by the dielectric environment. These factors may modify the reactive longitudinal response through additional optical channels, screening, and hybridization effects. Therefore, the phenomenological term introduced above should be understood as a minimal way to capture the functional trend of such multiband and environmental contributions within the low-energy model.

IV. CONCLUSIONS

In summary, we have studied the topology and MO response of various spin-flip states of a 5-SL MBT thin film by means of TB models obtained from first-principles calculations and a coupled Dirac cone model. We have shown that a nonzero net magnetization ($\sim 5 \mu_B$) does not guarantee the topological phase of 5-SL MBT. Instead, depending on the relative spin-orientation of the top and bottom SLs, a

5-SL can realize a Chern insulating phase with both $\mathcal{C} = +1$ and 0. The magnitude of the TSS gap is likewise controlled primarily by the local surface spin alignments rather than by a global magnetic order. We further demonstrated that these distinct topological phases are directly reflected in the MO response. In the low-frequency limit and within the TSS gap, the Faraday rotation exhibits a quantized response for the $\mathcal{C} = +1$ phase and vanishes for $\mathcal{C} = 0$, providing a robust probe of topology. In contrast, the Kerr rotation is found to be highly sensitive to the detailed frequency dependence of the longitudinal optical conductivity (σ_{xx}). By comparing realistic TB results with a coupled Dirac cone model, we clarified the limitations of the latter in describing Kerr rotation dynamics in spin-flip states and discussed the underlying mechanism responsible for rapid collapse of the Kerr plateau. Our results highlight the crucial role of surface-resolved magnetism in magnetic TIs and provide guidance for interpreting MO measurements on MBT thin films under different spin-flip configurations.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

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