Zeeman-field-induced valley-dependent topological phase transitions on the surface of a topological crystalline insulator SnTe

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Abstract

Mirror-symmetric (001) surfaces of a topological crystalline insulator SnTe host an even number of Dirac cone structures of surface states. A Zeeman field generically gaps the surface states, leading to a 2D topological insulator. By symmetry analysis and calculation of spin–Chern numbers, we show that with varying the direction of the Zeeman field, the system displays a rich phase diagram, consisting of a quantum anomalous Hall (QAH) phase with Chern number $C = 2$, a QAH phase with $C = 1$, a quantum pseudospin Hall phase, and an unusual insulator phase. In the QAH phase with $C = 1$ and the insulator phase, the two valleys $X$ and $Y$ are in different topological states. These valley-dependent topological phases provide a new pathway to potential applications of valleytronics.

1. Introduction

A topological insulator is one of the most fascinating concepts found in this decade [1, 2]. Recent flourish in the study of topological insulators is based on the finding of a time-reversal symmetry-protected topological insulator [3–5]. Most recently, a new class of topological insulator, a topological crystalline insulator (TCI) [6], has attracted much attention. Different from the $Z_2$ topological insulator, the metallic boundary states of a TCI are protected by crystal symmetry rather than time-reversal symmetry. This demonstrates the rich interplay between electronic topology and crystal symmetry in the TCI, and has advanced our understanding of the topological insulator.

Because the concept of TCI was proposed by Fu [6], on the theoretical frontier, intensive efforts have been devoted to classifying topological phases in different crystal symmetry classes [7–9]. On the other hand, there is great interest in seeking TCI materials both theoretically and experimentally. It has been predicted theoretically that a TCI state can be realized in the IV–VI semiconductor SnTe material class [10] and anti-perovskite material family $A_3BX$ [11]. The former has been confirmed experimentally by angle-resolved photoemission spectroscopy [12–14] and scanning tunneling microscopy measurements [15, 16].

The first material realization of TCI are the IV–VI semiconductors SnTe and related alloys $Pb_xSn_{1-x}Te(Se)$, in which there are three types of the surface states, the (001), (111) and (110) surfaces [10, 17], which have reflection symmetry with respect to the (110) plane. For the most interesting (001) surface, there exist four gapless Dirac cones [12–14], two of them, denoted by $\Lambda_{X,Y}^2$, are located along $\Gamma X$, close to and symmetric about $X$; two others, denoted by $\Lambda_{Y,Y}^2$, are located along $\Gamma Y$, close to and symmetric about $Y$, shown in figure 1(a). Because the gapless Dirac cones are protected by crystalline symmetry, it is proposed that they can be gapped through some symmetry-breaking perturbations such as Zeeman field and structure distortion [10, 18, 19]. It is predicted that each gapped Dirac cone contributes $\sigma_{ij} = \frac{e^2}{2\hbar}$ to the Hall conductance [19, 20]. However, in the previous paper [19], only a minimal model for each Dirac cone located at $\Lambda_{X,Y}^2$ is considered, which is a two-band $k \cdot p$ model and inevitably drops some information about spin or pseudospin. On the other hand, as pointed out in [21], although the low-energy band structures are largely determined by the gapless states at $\Lambda_{X,Y}^2$, the topological properties of the TCI surfaces are dictated by these gapped surface states at $X(Y)$. This prompts us to
consider a full four-band model containing the spin or pseudospin degree of freedom to investigate the topological property near $X(Y)$ point.

It is interesting to note that the Dirac cones near $X$ and $Y$ points are protected by different reflection mirrors, thus applying different symmetry-breaking perturbations can open gaps at the Dirac cones near $X$ and $Y$ points separately, which opens up the possibility of the valley-dependent topological phase transitions [22, 23]. In this paper, we investigate how to use a Zeeman field to achieve the valley-dependent topological phase transitions, as the Zeeman field orienting in different directions corresponds to different symmetry-breaking perturbations. We find that when the direction of a Zeeman field with a fixed magnitude $B$ varies in space, a rich topological phase transition can occur. Using the pseudospin Chern numbers to classify the topological phases, we obtain a phase diagram on a sphere of radius $B$, consisting of a quantum anomalous Hall (QAH) phase with Chern number $C = 2$, a QAH phase with $C = 1$, a quantum pseudospin Hall (QPSH) phase, and an insulator phase. Among these phases, the QAH phase with Chern number $C = 1$ and the insulator phase are very interesting, as the $X$ and $Y$ points are in different topological states. For the QAH phase with Chern number $C = 1$, one valley is in the QAH phase, while the other is in the QPSH phase. The insulator phase is unusual in that both valleys are in the QPSH phase, but their pseudospin Chern numbers have opposite signs, although the total Chern number and total pseudospin Chern number of the two valleys are zero. These valley-dependent topological phases provide a new pathway to potential application of the TCI in valley-based electronics.

2. Model Hamiltonian

We adopt the four-band $k \cdot p$ model for the (001) surface states of the TCI near $X$ point derived in [17]:

$$ H_X = v_1 k_x \sigma_y - v_2 k_y \sigma_x + m \tau_x + \delta \sigma_\alpha \tau_\alpha, $$

where $k$ is the momentum with respect to $X$ point, $v_1, v_2$ are the velocities along $x$ and $y$ direction, $\sigma_\alpha$ and $\tau_\alpha$ ($\alpha = x, y, z$) are the Pauli matrices for the spin and pseudospin, respectively. The pseudospin represents the cation–anion degree of freedom, and $m$ and $\delta$ describe the pseudospin mixing. The first two terms describe two degenerate Dirac cones. The Dirac points of these cones are located precisely at $X$ and $Y$ points. The first pseudospin mixing term $m \tau_x$ shifts the energy of the two Dirac cones from zero to positive and negative energies $m$ and $-m$. The second pseudospin mixing term $\delta \sigma_\alpha \tau_\alpha$ lifts this degeneracy everywhere except for two points on the axis $k_x = 0$, where two bands with opposite mirror eigenvalues $\pm i$ (associated with the reflection $M_\alpha$) cross each other. The band hybridization generates a pair of Dirac points at energy $E = 0$ located on opposite sides of $X$ at momenta $k_{X} = \pm \frac{\sqrt{m^2 + \delta^2}}{v_2}$, as illustrated in figure 1(b).

The $X$ point is invariant under three point group symmetry operations $C_2$, $M_x$, and $M_y$, which represent the two-fold rotation around surface normal, and mirror symmetry with respect to reflections of $x$ and $y$ axes, $M_x : x \rightarrow -x$ and $M_y : y \rightarrow -y$. In addition, the time-reversal symmetry $\Theta$ is present. The Hamiltonian is
invariant under the corresponding symmetry operations. When various perturbations are added, they have to satisfy a certain symmetry constraint, which has been summarized in [18]. Here, we only consider the effect of a Zeeman field on the surface of the TCI. It is apparent that the out-of-plane field $B_z$ breaks both mirror symmetries, while an in-plane field $B_x$ parallel to the $x$ axis preserves the mirror symmetry $M_y$ but breaks the mirror symmetry $M_x$, and vice versa for $B_y$. According to symmetry analysis, the allowable coupling terms for the three components of the Zeeman field are given by [18]

\[
\begin{align*}
V_{B_x} &= \mu_x B_x \sigma_x + \eta_x B_x \tau_y + \lambda_x B_x \sigma_6 \tau_x, \\
V_{B_y} &= \mu_y B_y \sigma_y + \eta_y B_y \sigma_3 \tau_z + \lambda_y B_y \sigma_5 \tau_z, \\
V_{B_z} &= \mu_z B_z \sigma_z + \eta_z B_z \sigma_3 \tau_z + \lambda_z B_z \sigma_5 \tau_z.
\end{align*}
\]

(2)

In the next section, we study the topological phase transitions with varying the directions of the Zeeman field.

3. Phase diagram

As mentioned above, the gapless Dirac cones located at $\pm q$ are protected by mirror symmetry $M_\sigma$, so the terms in $V_{B_x}$, which are invariant under $M_\sigma$, do not open up an energy gap, but just shift the positions of degenerate points. To our surprise, although all the terms in $V_{B_y}$ and $V_{B_z}$ break the mirror symmetry $M_\sigma$, not every one of them can open up a gap. Our calculation shows that among the mirror symmetry $M_\sigma$ breaking perturbations, only $\sigma_x, \sigma_z, \sigma_3 \tau_z, \sigma_5 \tau_z$ could open up a gap. From figure 2(a), one can see that among the four gap-opening terms, an infinitesimal $\sigma_x$ term or $\sigma_z \tau_z$ term is sufficient to open up a gap. The $\sigma_z \tau_z$ and $\sigma_3 \tau_z$ terms open up a gap only when they reach certain critical values. The $\sigma_x$ and $\sigma_5 \tau_z$ terms cannot open up a gap. They just shift the positions of the degenerate points, the same as $V_{B_y}$, and their respective influences on the band structures are shown in figures 2(b) and (c).

In general, in two dimensions the band degeneracy is protected by certain symmetry [24], e.g., the point group or time-reversal symmetry. Sometimes the symmetry is not so apparent, as it may consist of a translation, a complex conjugation and a gauge transformation. Owing to the difficulty to find it, such a symmetry may be called a hidden symmetry [25, 26]. Different from the point group and time-reversal symmetry, the hidden-symmetry-invariant points are not always at the high-symmetry points in the Brillouin zone, and their positions may also depend on the parameters [26]. In the present system, we conjecture that while $\sigma_x$ and $\sigma_z \tau_z$ break the mirror symmetry $M_\sigma$, a hidden symmetry still exists in the system. Similarly, for the terms $\sigma_y \tau_z$ and $\sigma_3 \tau_z$ when their strengths are smaller than the corresponding critical values, the hidden symmetry keeps protecting the band degeneracy. When their strengths exceed the critical values, the hidden symmetry is broken, leading to the gap opening.

Due to the presence of a pseudospin degree of freedom, the pseudospin Chern numbers can be defined when the energy gap is opened. Applying the standard method to calculate the pseudospin Chern numbers [27–29], we can derive the pseudospin Chern numbers $C_{X \pm}$ for the $X$ valley. The values of the pseudospin Chern numbers characterize the topological phases of the X valley. If $C_{X+} + C_{X-} \neq 0$, $X$ is in the QAH phase. Among the four gap-opening terms, $\sigma_z$ and $\sigma_y \tau_z$ will induce the QAH phase. If $C_{X+} = -C_{X-} = 0$, $X$ is in the QPSH phase. When $\sigma_z \tau_z$ and $\sigma_y \tau_z$ exceed the critical values and open an energy gap, the system enters the QPSH phase. If $C_{X+} = C_{X-} = 0$, $X$ is in the topologically trivial phase, but none of the terms in equation (2) could induce this phase.
When the terms inducing the QPSH effect and inducing the QAH effect coexist, along with the change in the strengths of the terms, the energy gap may close and then reopen. Accompanied with the energy gap closing, topological phase transitions occur. The terms $\sigma_z \tau_x$ and $\sigma_x \tau_z$ have a similar effect, favoring the QPSH phase, and $\sigma_z \tau_z$ and $\sigma_x \tau_x$ have a similar effect, favoring the QAH phase. For example, we may consider first that the two terms $\sigma_z \tau_z$ and $\sigma_x \tau_x$ coexist, which favor the QPSH and QAH effect, respectively, to study the topological phase transitions. In other words, we assume that the perpendicular Zeeman field only induces the coupling term $\sigma_z \tau_z$ and the in-plane Zeeman field only induces $\sigma_x \tau_x$. For definitiveness and without loss of generality, we fix the amplitude of $\sigma_z \tau_z$ and then increase the strength of $\sigma_x \tau_x$ from zero. It is found that along with increasing the strength of $\sigma_x \tau_x$, the gap first reduces, and closes at a critical value, then reopens. After the gap reopens, the pseudospin Chern numbers change from $C_{x+z} = C_{x-} = C_{y-} = C_{y+} = \pm \frac{1}{2}$ to $C_{x+z} = -C_{x-} = C_{y-} = C_{y+} = \pm \frac{1}{2}$. This means that a topological phase transition from the QAH phase to QPSH phase occurs for the $X$ valley. Because the amplitudes of $\sigma_z \tau_z$ and $\sigma_x \tau_x$ depend on the strengths of the $y$ and $z$ components of the Zeeman field, the above result indicates that the topological property of $X$ is actually determined by $B_y$ and $B_z$. For a fixed $B_x$, there exists a critical value $B_{yc}$ that closes the energy gap. If $B_y$ is bigger than $B_{yc}$, the $X$ point is in the QPSH phase. Otherwise, it is in the QAH phase.

We now consider the effect of the Zeeman field on the $Y$ point. In the absence of the Zeeman field, the Hamiltonian near the $Y$ point is given below

$$H_Y = \nu_2 k_y \sigma_y - \nu_1 k_y \sigma_x + m \tau_z + \delta \sigma_z \tau_y.$$  \hspace{1cm} (3)

Similar to $X$, for $Y$ point we could obtain the Hamiltonian of the Zeeman field based on symmetry analysis. For simplicity, we also just consider two terms $\sigma_z \tau_z$ and $\sigma_y \tau_y$ the same as $X$ point. A difference is that now the term $\sigma_z \tau_z$ is induced by $x$ component $B_x$, rather than $y$ component $B_y$. Indeed, we can deduce the effect of the Zeeman field on $Y$ point from that on $X$ point by symmetry considerations. Because $X$ and $Y$ are related to each other by a rotation of $\frac{\pi}{2}$, the band structure near $X$ has a symmetry-related copy near $Y$. For example, Zeeman field $B_y$ breaking both symmetries $M_4$ and $M_2$ has the same effect on $X$ and $Y$, while the effect of Zeeman field $B_x (B_z)$ on $Y$ can be deduced from the effect of Zeeman field $B_y (B_x)$ on $X$. Therefore, the topological property of the $Y$ point is determined by $B_y$ and $B_z$.

After the effect of Zeeman field $B$ on the $X$ and $Y$ points has been understood, we can investigate the topological phase transitions of the TCI surface containing both $X$ and $Y$ valleys in the presence of the Zeeman field. Before studying the phase diagram, we first briefly compare our results with a previous work about the QAH effect, and analyze the QPSH effect in our four-band model. Take the perpendicular Zeeman field as an instance. In the two-band model [19], when a perpendicular Zeeman field is applied, every gapped Dirac cone contributes a quantized Hall conductance $\pm \frac{e^2}{2h}$, so that the total Hall conductance is $\sigma_H = \pm \frac{e^2}{2h}$, with $\pm$ determined by the direction of the Zeeman field. In the four-band model under consideration, as shown above, when only a perpendicular Zeeman field is applied, $C_{x+z} = C_{x-} = C_{y+} = C_{y-} = \pm \frac{1}{2}$, with $\pm$ determined by the direction of the Zeeman field, so the total Chern number, defined as $C = C_{x+z} + C_{x-} + C_{y+} + C_{y-}$, equals to $\pm 2$. This indicates that the Hall conductance is $\sigma_H = \pm \frac{2e^2}{h}$, which is consistent with the two-band model.

In our four-band model, if the total pseudospin Chern numbers $C_x = -C_y = 1$, where $C_{x\pm}$ and $C_{y\pm}$, the system is in the QPSH phase. Similar to the quantum spin Hall effect, according to bulk–edge correspondence, the pseudospin Chern numbers $C_e = -C_e = 1$ indicate that there is a pair of pseudospin-polarized edge modes counterpropagating at the open boundary of the surface of the TCI. To study the edge states directly, it is necessary to find an equivalent tight-binding Hamiltonian for the TCI surface. This is generally difficult due to the complexity of Hamiltonian equations (1)–(3). However, in the special case of $B_y = B_y$, such an equivalent tight-binding Hamiltonian can be constructed on a square lattice with two spins and two orbits on each site. The model Hamiltonian is given by $H = H_0 + H'$, where

$$H_0 = i \sum_{i \tau} \lambda_{i \tau} c_i^{\dagger} \left[ \hat{d}_{\tau} \times d_{\tau} \right] c_{i \tau} + m \sum_{i \tau} c_i^{\dagger} \tau_x c_{i \tau} + \sum_{\langle \langle \rangle \rangle \tau} \lambda_{i \tau} c_i^\dagger \tau_x c_{i \tau},$$  \hspace{1cm} (4)

$$H' = -t_2 \sum_{\langle \langle \rangle \rangle \tau} \tau_x c_{i \tau}^\dagger \tau_z c_{j \tau}.$$  \hspace{1cm} (5)

Here, $c_i^{\dagger}$ ($c_i$, $c_i^\dagger$) is the creation operator on site $i$ with $\tau = \pm 1$ standing for two orbits, namely, $s$ and $p$ orbits. The first term of $H_0$ is the Rashba spin–orbit coupling, $\hat{d}_{\tau} = (\sigma_x, \sigma_y, \sigma_z)$ represents the Pauli matrix for spin, and $d_{\tau}^\dagger = n - r_{\tau}$ connects a pair of the $l$th nearest neighbor sites $i$ and $j$ in the lattice with $\lambda_{l \tau}$ the coupling strength. Here, we only consider the contribution from the nearest and next nearest neighbor sites ($l = 1, 2$) with $\lambda_1 = \frac{\tau + \tau}{4}$, $\lambda_2 = -\frac{\tau - \tau}{4}$. The second term is the $s$–$p$-orbit coupling with amplitude $m$ and $\tau$ the orbit different from $\tau$. The third term is the nearest neighbor hopping term, which can open up gaps at $\langle \langle \rangle \rangle = (0, 0)$ and $(\tau, \tau)$. It can be easily shown that the lattice Hamiltonian $H_0$ can be reduced to the first three terms of $H_0$ and $H_0$ near $(\tau, 0)$ and $(0, \tau)$ except the forth term. This is not an important issue as the forth term does not qualitatively influence the topology of the system. $H'$ stands for the spin– and orbit–dependent next nearest neighbor hopping term with $t_2 = \lambda_y B_y / 4$, where we have set $B_x = B_y = B_0$. This term can open gaps at the $X$ and $Y$ points, and drive
the system into the QPSH phase. To study the edge states, we calculate the energy spectrum of a long ribbon with 60 chains. The calculated energy spectrum is shown in figure 3(a). It is clear that there exist four different edge states at a given Fermi energy in the bulk band gap. Through the analysis of the spatial distribution of the wave functions, as shown in figure 3(b), one can find that the edge states represented by solid lines localize near one boundary of the ribbon, while the other two edge states represented by dashed lines localize near the other boundary. Take the edge states indicated by solid lines on one boundary as an example. From the slopes of the red and green lines, it is easy to determine that the two edge states are counterpropagating. We also examine the pseudospin polarizations of their wave functions, the red line being almost fully $s$-orbit polarized and the green line $p$-orbit polarized. Therefore, there exist two counterpropagating edge states with opposite pseudospin polarizations on a sample edge in the case $C_+ = -C_- = 1$, which give rise to no net charge transfer, but can contribute to a net transport of pseudospin. In general, adding terms to the Hamiltonian, which do not close the bulk gap and mix the pseudospin, can gap out the edge states. From the viewpoint of edge states, the QPSH phase will no longer be well defined. However, the nontrivial bulk band topology characterized by the pseudospin Chern numbers will remain intact [29], and can have some observable effects, such as topological pseudospin pumping directly from the bulk of the system, as proposed recently [30].

Besides the pseudospin degree of freedom, there exists the valley degree of freedom in the TCI surface due to the two cones or valleys $X$ and $Y$. This provides us with a new platform for valleytronics. Valleytronics [31–34], a technology of manipulating the degree of freedom, to which an inequivalent degenerate state electron near the Fermi level belongs, is a promising candidate for the next generation electronics. The main target of valleytronics is the honeycomb lattice systems. Indeed, various valley-dependent topological phases have been proposed theoretically in honeycomb lattices, such as the quantum valley Hall phase [32–35], valley-polarized QAH phase [22], spin-valley Hall phase [36], and quantum spin-QAH phase [23]. It is expected that these topological phases can also be achieved on the TCI surface. As shown above, the effects of a Zeeman field on the $X$ and $Y$ valleys of the TCI surface are different, such that valley-dependent topological phase transitions may happen with varying the Zeeman field.

In the above discussions, we show that the topological property of $X(Y)$ is determined by $B_x(B_y)$ and $B_z$. This indicates that it is possible to induce topological phase transitions through controlling the orientation of the Zeeman field. Therefore, we fix the magnitude $B$ of the Zeeman field, and change its direction alone to study the topological phase transitions. Specifically, we consider a sphere with radius $B$, on which each point denotes a unique direction of the Zeeman field. The calculated phase diagram on the sphere is plotted in figure 4, in which different colors represent different topological phases. Yellow, blue, green and brown represent the QAH phase with total Chern number $C = 2$, QAH phase with total Chern number $C = 1$, QPSH phase, and insulator phase, respectively. We take figure 4(a) as an instance to illustrate these phases. In the yellow area I, owing to the strong $B_x$ and $B_y$ fields, the pseudospin Chern numbers are $(G_{\chi^+}, G_{\chi^-}) = \left(\frac{1}{2}, \frac{1}{2}\right)$, $(G_{\gamma^+}, G_{\gamma^-}) = \left(\frac{1}{2}, \frac{1}{2}\right)$, for the $X$ and $Y$ points, respectively. The system is in the QAH phase, with the total Chern number $C = 2$. In the blue area II, the $x$ component $B_x$ of the Zeeman field is bigger than the critical value $B_{x_{cr}}$ determined by corresponding $B_y$ and the pseudospin Chern numbers for the $Y$ point change to $(G_{\gamma^+}, G_{\gamma^-}) = \left(\frac{1}{2}, -\frac{1}{2}\right)$. For the $X$ point, the pseudospin Chern numbers are still $(G_{\chi^+}, G_{\chi^-}) = \left(\frac{1}{2}, \frac{1}{2}\right)$, as the $y$ component of $B_y$ is small. As a result, the total Chern number is $C = 1$, and the system is in a QAH phase. In the green area III, $B_x$ and $B_y$ are bigger than the critical values $B_{x_{cr}}$ and $B_{y_{cr}}$, as determined by the corresponding small $B_z$, so the pseudospin Chern numbers for

![Figure 3](image-url)

**Figure 3.** (a) Energy spectrum versus wave vector $k_y$ for a ribbon. (b) The real space probability distribution of the edge states. The red circles and green triangles represent two pseudospin-polarized states, respectively.
Therefore, the conductivity. For the insulator phase, owning to different signs of Chern number are zero, the system is in an insulator phase. The two phases, i.e., the QAH phase, with pseudospin Chern numbers are different between the two regions are in different topological phases, because the pseudospin Chern numbers in the two regions are different. In the upper area, the pseudospin Chern numbers for phase with pseudospin Chern numbers ±1, one can see that the point is in the QPSH phase with pseudospin Chern numbers (C_{X^+}, C_{X^-}) = \left( \frac{1}{2}, -\frac{1}{2} \right), (C_{Y^+}, C_{Y^-}) = \left( -\frac{1}{2}, \frac{1}{2} \right). This means that when an electric field is applied, electrons with opposite pseudospins in the X valley flow in the same direction transverse to the electric field. However, in the Y valley, electrons with opposite pseudospins flow in the opposite direction transverse to the electric field. Therefore, the X valley gives rise to a net Hall conductivity, while the Y valley contributes to a pseudospin Hall conductivity. For the insulator phase, owning to different signs of B_x and B_y, the X and Y valleys have opposite pseudospin Chern numbers (C_{X^+}, C_{X^-}) = \left( \frac{1}{2}, -\frac{1}{2} \right), (C_{Y^+}, C_{Y^-}) = \left( -\frac{1}{2}, \frac{1}{2} \right). Therefore, X and Y are in the QPSH states, but contribute to opposite pseudospin Hall conductivities. This phase is very similar to the valley Hall effect, in which upon the application of an electric field, electrons in different valleys will flow to opposite directions transverse to the electric field, giving rise to a net valley Hall current in the bulk [32–35]. In the present case, the two valleys give rise to opposite pseudospin Hall currents, leading to a net valley-pseudospin Hall current. The two phases, i.e., the QAH phase, with C = 1, and the unusual insulator phase, can be used to generate valley polarization and valley-pseudospin polarization by the Zeeman field, forming the basis for valleytronics.

It is worth noting that the regions with the same color are not always in the same topological phase. They are only in the same kind of topological phase. For example, both the green regions in figure 4(a) are in the QPSH phase, but they are in different topological phases, because the pseudospin Chern numbers in the two regions are different. In the upper area, the pseudospin Chern numbers for phase are C_{X(Y)^\pm} = \pm \frac{1}{2}. While in the lower area, where B_x and B_y are negative, the pseudospin Chern numbers are C_{X(Y)^\pm} = \mp \frac{1}{2}.

Figure 4. The z and x direction views of the phase spheres determined by the pseudospin Chern numbers. Each point on the sphere denotes a unique direction of the Zeeman field. Gray lines represent phase boundaries where the band gap closes. The amplitude of the Zeeman field is taken to be B = 0.4 eV. In (a) and (b), only two terms \sigma_x and \sigma_y are considered, and we set \mu_x = \lambda_x = 1. The inset illustrates the effect of a nonzero \sigma_z term on the phase boundaries. In (c) and (d), all terms that could be induced by the Zeeman field are considered, and we set \mu_x = \mu_y = \mu_z = 1, \lambda_x = \lambda_y = \lambda_z = 0.8, \eta_x = \eta_y = \eta_z = 0.5.

Both X and Y change to (C_{X(Y)^+}, C_{X(Y)^-}) = \left( \frac{1}{2}, -\frac{1}{2} \right). Now, the total Chern number is 0, but the total pseudospin Chern number is C_{X^\pm} = \pm 1, and the system is in the QPSH phase. Finally, in the brown area IV, similar to the case in the green area III, the amplitudes of B_x and B_y are bigger than the critical values determined by the corresponding B_z, but B_y is negative, so the pseudospin Chern numbers for X and Y are (C_{X^+}, C_{X^-}) = \left( \frac{1}{2}, -\frac{1}{2} \right), (C_{Y^+}, C_{Y^-}) = \left( -\frac{1}{2}, \frac{1}{2} \right). Since now both total Chern number and total pseudospin Chern number are zero, the system is in an insulator phase.

It is interesting to examine more closely the topological properties of the QAH phase with Chern number C = 1 in the blue area II, and the insulator phase in the brown area IV. Because in the two phases, the pseudospin Chern numbers are different between X and Y. They are valley-dependent topological phases, and may have potential application in valleytronics. For the QAH phase with C = 1, one can see that the point is in the QAH phase with pseudospin Chern numbers (C_{X^+}, C_{X^-}) = \left( \frac{1}{2}, -\frac{1}{2} \right), (C_{Y^+}, C_{Y^-}) = \left( -\frac{1}{2}, \frac{1}{2} \right). Since now both total Chern number and total pseudospin Chern number are zero, the system is in an insulator phase.
So far we only consider the effect of the terms $\sigma_2$, inducing the QAH phase, and $\sigma_5\tau_5$, inducing the QPSH phase. However, when a Zeeman field is applied, every term in equation (2) is allowable. It is necessary to consider the influence of the other terms in equation (2) on the phase diagram. For example, for the X point, we consider the term $\sigma_2\tau_2$ in $V_{Bx}$. Its effect is similar to the term $\sigma_2\tau_5$ in Hamiltonian (1), whose strength determines the critical value for $\sigma_2\tau_5$ to open up a gap. In the presence of the term $\sigma_2\tau_2$ in $V_{Bx}$, a larger Zeeman field $B_x$ is needed to open up a gap and induce a topological phase transition. In the inset, the blue line represents the correction of the term $\sigma_2\tau_2$ to the phase diagram, in which only the X point is considered. In comparison with the gray line, where the term $\sigma_2\tau_2$ is neglected, we can clearly see that when $B_x = 0$, $\sigma_2\tau_5$ increases the critical value for $B_x$ to drive the X point to the QPSH phase. Similarly, other terms in equation (2) would rectify the phase diagram in various ways. The phase diagrams are plotted in figures 4(c) and (d) taking into account all the terms induced by the Zeeman field. In the above, we have chosen to focus on a particular parameter set for clarity of presentation. However, we need to point out that there exists a parameter regime, where only the QAH phase can occur in the system. This is because the terms, $\sigma_2\tau_2$ and $\sigma_5\tau_5$, which favor the QPSH phase, can open up an energy gap only when their strengths exceed certain critical values. Only under this condition, all the four phases shown in figure 4 are possible. Otherwise, the QAH phase will dominate the phase diagram with the absence of the QPSH phase.

In the above discussion, we only consider a surface of the TCI. This is different from strong topological insulators, in which the Hall conductance of a single surface is half-quantized. Resolving this anomaly in strong topological insulators requires combining the two Dirac surface states in a two-surface geometry, such that the sum of their Hall conductivities is an integer. However, this anomaly is automatically resolved for the interesting insulators, in which the Hall conductance of a single surface is half-quantized. Resolving this anomaly in strong transport as it can be isolated. We can further consider thin-film geometries. First, we assume that the thin film is thick enough such that the hybridization between the two surfaces could be neglected. When the top and bottom surfaces share the same Zeeman field, their contributions to pseudospin Chern numbers are the same in the local frame of one of the two surfaces. The pseudospin Chern numbers in the thin-film phase sphere will be doubled compared with those shown in figure 4 for a single surface. If the field direction on either surface can be independently controlled, the total Chern number from $-2$ to $2$ can be realized. In addition, when the thickness is comparable to the decay length of the surface states, the hybridization between the two surfaces becomes significant, and could lead to a richer phase diagram [19, 20].

4. Summary

In this paper, we have investigated topological properties of the surface states of the TCI in the presence of a Zeeman field, which breaks the time-reversal and mirror symmetries with respect to reflection of the $x$ and $y$ axes. It is found that changing the direction of the Zeeman field can achieve valley-dependent topological phase transitions. By symmetry analysis and using the pseudospin Chern numbers to characterize the topological quantum phase, we obtain a phase sphere with radius $B$, consisting of a QAH phase with Chern number $C = 2$, a QAH phase with Chern number $C = 1$, a QPSH phase, and an unusual insulator phase. In the $C = 1$ QAH phase and the insulator phase, the two valleys $X$ and $Y$ are in different topological phases. The valley-dependent topological phases provide a platform to design low-power electronics and advance the application of TCI-based valleytronics.

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