Symmetry Protected Topological Semimetal in Topological Crystalline Insulator Thin Films with In-Plane Magnetic Field

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Weyl semimetal is a topologically protected semimetal in three dimensions. In this work we investigate a symmetry protected topological semimetal in two dimensions by taking an instance of a topological crystalline insulator (TCI) thin film. It is originally a mirror-symmetry protected topological insulator. It is demonstrated that the gap closes together with the emergence of two gapless cones carrying opposite chiralities, when the mirror symmetry is broken by applying in-plane magnetic field. This is a reminiscence of a pair creation of two Weyl cones in three dimensions. We also examine how robust it is. Perpendicular electric field is found to shift the gapless points and also renormalize the Fermi velocity in the direction of the in-plane magnetic field. On the other hand, the gap opens and the system becomes a quantum (anomalous) Hall insulator when the perpendicular Zeeman effect is applied. We argue that this two-dimensional topological semimetal is protected by the chiral symmetry.

Topologically protected states such as topological insulator are among the most exciting topics in modern condensed matter physics. Weyl semimetal has recently been found to be topologically protected in three-dimensional space. It has a non-degenerate linear dispersion and is described by $2 \times 2$ matrices. It can not be gapped by any perturbation, because any perturbation is also expanded in $2 \times 2$ matrices and only shifts the Weyl points. The emergence of Weyl semimetal is always accompanied by a pair of Weyl cones with opposite chiralities subject to the fermion doubling theorem. Each Weyl cone carries the opposite monopole charge. Topological protection is lost in two dimensions, where the semimetal is easily gapped and not stable. Nevertheless, we wish to argue that there exists a symmetry-protected topological semimetal in the two-dimensional space by taking an instance of topological crystalline insulator (TCI) thin film.

TCI is a topological insulator protected by the crystal symmetry. Its experimental realizations in Pb$_x$Sn$_{1-x}$Te excite studies of TCI. A thin film made of TCI provides us with a new platform of two dimensional electron system, where the mirror-symmetry about the two-dimensional plane plays a key role. When the film is thin enough, the gap opens due to hybridization between the front and back surfaces, and it turns the system into a topological insulator. The TCI thin film is a topological insulator protected by the mirror-symmetry. Accordingly the topological property of the mirror-Chern number. Very recently, TCI thin film made of SnTe was experimentally manufactured.

In this paper, we investigate the band structure and the topological property of TCI thin film in the presence of the Zeeman effect. First we introduce the mirror-symmetry breaking terms, which are the in-plane Zeeman terms and the perpendicular electric term. As they are increased, the gap reduces and closes, forming a gapless Dirac cone at a certain critical fields. Then the gapless Dirac cone splits into two gapless cones with opposite chiralities: Each gapless cone carries the opposite winding number. This is a reminiscence of a pair creation of two Weyl cones in three dimensions. We find the flat band emerges to connect the two gapless points in a nanoribbon. It is to be emphasized that the emergence of the two gapless points is solely due to the in-plane magnetic field, while electric field only shifts the position of the gapless points and renormalizes the Fermi velocity. By changing the direction of in-plane magnetic field, the positions of the gapless points rotate in parallel to the magnetic field direction. We next include the perpendicular Zeeman field additionally. It opens the gap and turns the system into a quantum (anomalous) Hall insulator. We also study the topological property of the gapless points in two dimensions. We show that they carry opposite winding numbers and that they may disappear only when they annihilate each other. The semimetal is topologically stable provided the spin lies within the plane. However, the topological stability is lost when the spin is allowed to have the out-of-plane component.

The Hamiltonian (1) is invariant under the mirror symmetry about the two-dimensional plane,

$$H_0 = \sigma_x k_x \sigma_x - v_y k_y \sigma_y, \quad m \tau_x, \quad (1)$$

where $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ and $\tau = (\tau_x, \tau_y, \tau_z)$ represent the spin and surface degrees of freedom; $v_i$ and $k_i$ are the Fermi velocity and the momentum into the $i$-direction; $m \tau_x$ represents the tunnelling term between the two surfaces. We have set $\hbar = 1$ for simplicity. The Hamiltonian (1) is invariant under the mirror symmetry about the two-dimensional plane,

$$MH(k)M^{-1} = H(k), \quad (2)$$

where the mirror operator is given by

$$M = -i \sigma_z \tau_x. \quad (3)$$

The Hilbert space is divided by the eigenvalues ($M = \pm i$) of the mirror operator. The mirror-Chern number $C_M$ is defined by the difference of the Chern numbers in these two
The gap closes when \( \mathcal{E}_{\text{ext}} = E_z \tau_z + B_x \sigma_x + B_y \sigma_y \). (4)

The first term is induced by applying electric field perpendicular to the TCI thin film. The other terms are the in-plane Zeeman terms. The in-plane Zeeman terms are induced by applying in-plane magnetic field.

The system is described by \( H = H_0 + H_{\text{ext}} \). The band structure changes as a function of the external fields. The band gap is located at \( k_x = k_y = 0 \), where the energy spectrum reads

\[ E = \pm \sqrt{B_x^2 + B_y^2 \pm \sqrt{m^2 + E_z^2}}. \]  (5)

The gap closes when

\[ B_x^2 + B_y^2 = m^2 + E_z^2, \]  (6)

where a topological phase transition occurs.

Before the topological phase transition the system is an insulator. It is a mirror-Chern insulator without the external fields, as we have stated. When we analyze a nanoribbon based on the tight-binding model, gapless edge modes appear, as signals the topological nature of the bulk [Fig. 1(a)]. However, edge modes are gapped in the presence of the mirror-symmetry breaking terms, where the edge gap becomes a continuous function of \( E_z, B_x \) and \( B_y \). The mirror-Chern number \( C_M \) becomes also a continuous function of \( E_z, B_x \) and \( B_y \) and is no longer quantized. For instance, we find

\[ C_M = \frac{m}{2\sqrt{m^2 + E_z^2}}, \]  (7)

when we apply only \( E_z \). It is reduced to the quantized value, \( C_M = \frac{1}{2} \text{sign}(m) \), in the limit \( E_z = 0 \).

**Topological Semimetal:** We investigate the TCI thin film after the phase transition point, where the gap closes [Fig. 1(b)]. We may choose the direction of the in-plane magnetic field as the \( x \)-axis without loss of generality. It is found that a gapless Dirac cone is decomposed into two gapless cones and that flat edge modes appear connecting the two gapless points in a nanoribbon solely due to the effect of the in-plane magnetic field [Fig. 1(c)]. The emergence of the flat band corresponds to the Fermi arc connecting the two Weyl points in the surface of a Weyl semimetal in three dimensions.

To study the phenomenon analytically we examine the energy spectrum of the Dirac theory,

\[ E = \pm \sqrt{v_x^2 k_x^2 + \left( \sqrt{v_x^2 k_x^2 + m^2 + E_z^2} \pm B_x \right)^2}. \]  (8)

We show the band structure in Fig. 2. The phase transition point (c) becomes \( M_z^2 = m^2 + E_z^2 \). Beyond the point, a gapless Dirac cone is decomposed into two gapless cones located at \((k_x, k_y) = (\pm k_x^N, 0)\) with

\[ k_x^N = \frac{1}{v_x} \sqrt{B_z^2 - m^2 - E_z^2}. \]  (9)

We also refer to these gapless points as the \( X_\pm \) points.

It is convenient to employ the effective 2 \( \times \) 2 Hamiltonian by taking only two bands nearest to the Fermi energy. We may derive it in the second order perturbation theory around the \( X \) point. The effective Hamiltonian reads

\[ H_{\text{eff}} = (B_x - m - \frac{v_x^2 k_x^2 + E_z^2}{m + B_z}) \sigma_x - v_y k_y \sigma_y. \]  (10)
The energy spectrum is given by

\[ E = \pm \sqrt{\left(\frac{v_x^2 k_x^2 + m^2 + E_z^2 - B_x^2}{m + B_x}\right)^2 + v_y^2 k_y^2}, \tag{11} \]

which agrees with [8] up to the order of \(k_x^4\).

At the transition point \(B_x^2 = m^2 + E_z^2\) [Fig.2(b)], the energy spectrum is highly anisotropic,

\[ E = \pm \sqrt{\frac{1}{m + B_x} v_x^2 k_x^4 + v_y^2 k_y^2}. \tag{12} \]

The energy dispersion is Schrödinger-like in the \(k_x\) direction, while it is Dirac-like in the \(k_y\) direction.

Beyond the transition point \(B_x^2 > m^2 + E_z^2\) [Fig.2(c)], we rewrite the Hamiltonian (10) as

\[ H_{\text{eff}} = -\frac{v_x^2}{m + B_x} (k_x - k^X) (k_x + k^X) \sigma_x - v_y k_y \sigma_y. \tag{13} \]

In the vicinity of \(X_{\pm}\) point, we can approximate \(k \pm k^X = \pm 2k^X\) and obtain

\[ H_{\text{eff}}^{X_{\pm}} = \mp \tilde{v}_x (k_x \mp k^X) \sigma_x - v_y k_y \sigma_y, \tag{14} \]

where \(\tilde{v}_x\) is the renormalized velocity,

\[ \tilde{v}_x = \frac{2v_x^2 k^X}{m + B_x}. \tag{15} \]

The energy spectrum in the vicinity of the \(X_{\pm}\) points is

\[ E_{\pm} = \pm \sqrt{\frac{v_x^2 k_x^2}{m + B_x} + v_y^2 k_y^2}. \tag{16} \]

The role of \(E_z\) is to shift the position of the gapless points and renormalize the Fermi velocity.

For general in-plane field \(B_x \neq 0\) and \(B_y \neq 0\), we obtain the effective 2-band Hamiltonian

\[ H_{\text{eff}} = (B || - m - \frac{(v_x k_x B_x - v_y k_y B_y)^2}{B_x^2 (m + B_x)}) \sigma_x - \frac{v_x k_x B_x + v_y k_y M_y}{B m ||} \sigma_y, \tag{17} \]

with

\[ B_x^2 = m^2 + E_z^2. \tag{18} \]

By setting the both coefficients of \(\sigma_x\) and \(\sigma_y\) zero, we find that the gap closes at \((k^X_x, k^X_y)\) and \((-k^X_x, -k^X_y)\) with

\[ k^X_x = \frac{1}{v_x} |B_x| \sqrt{1 - m^2 / B_x^2}, \quad k^X_y = \frac{1}{v_y} |B_y| \sqrt{1 - m^2 / B_y^2}. \tag{19} \]

It is parallel to the direction of magnetic field. We can control the position of Weyl cones by changing the direction of magnetic field.

We proceed to discuss the topological stability of the \(X_{\pm}\) points. The Hamiltonian is of the form

\[ H_{\text{eff}} = R(n_x \sigma_x + n_y \sigma_y), \tag{20} \]

where \(n_x\) and \(n_y\) are normalized fields subject to \(n_x^2 + n_y^2 = 1\). It has two eigen-spinors with the eigen-energy \(E_{\pm} = \pm |R|\). The state corresponding to the filled band is given by the spinor

\[ |S\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi/2} \\ -e^{i\phi/2} \end{pmatrix}, \tag{21} \]

when we parametrize \((n_x, n_y) = (\cos \phi, \sin \phi)\). The spin of the state is given by \(s_i = \langle S | \sigma_i | S \rangle\), which we show in Fig.4. We note that \(s_i = -n_i\). The spin direction forms a hedgehog structure in the vicinity of the \(X_{\pm}\) point, while it forms an anti-hedgehog structure in the vicinity of the \(X_{\pm}\) point. There are a source and a sink of the spin flow at these points. They are described by a topological charge.

We may defined a winding number for the spin configuration \((s_x, s_y)\) by

\[ Q = \frac{1}{2\pi} \int dk \langle s_x(k) \partial_{k_x} s_y(k) - s_y(k) \partial_{k_y} s_x(k) \rangle, \tag{22} \]

where the integration is carried out along the boundary of the Brillouin zone. It is trivial to see

\[ Q = \frac{1}{2\pi} \int dk \partial_{k_x} \phi. \tag{23} \]

In general, it yields \(Q = 0, \pm 1, \pm 2, \cdots\), because \(\phi\) is defined only modulo \(2\pi\). For the specific field configuration given in [13], we find \(Q = \pm 1\) for the gapless cones at \(X_{\pm}\). These values are topologically protected because any perturbation cannot change the quantized value of the topological charge.
is a topological insulator. Indeed, it is a quantum anomalous
edge modes persist though they are no longer flat [Fig.1(d)].

Precisely the same analysis is carried out for the Dirac cone at the
Y point, from which a pair of gapless cones emerge located at the
Y± point under in-plane magnetic field.

**Breaking Topological Semimetal:** We include the perp-
endicular Zeeman effect to the semimetallic state. The per-
pendicular Zeeman effect may be introduced either by intro-
ducing the perpendicular magnetic field or the proximity ef-
flect with attachment of ferromagnets. The introduction of the
magnetic field turns the system into a quantum Hall insula-
ator while the ferromagnets turns the system into a quantum
anomalous Hall insulator. The difference is whether electrons
perform cyclotron motion and form Landau levels. For sim-
plicity we only introduce the Zeeman term.

Our external Hamiltonian now is

\[ H_{\text{ext}} = E_z \tau_z + B_y \sigma_x + B_y \sigma_y + B_z \sigma_z. \]  

(24)

By setting \( B_y = 0 \) for simplicity, the effective Hamiltonian
(13) is modified as

\[ H_{\text{eff}}^{X \pm} = -\tilde{v}_x (k_x \mp k^X) \sigma_x - v_y k_y \sigma_y \mp \sqrt{1 - \frac{m^2}{B_z^2}} B_z \sigma_z. \]  

(25)

The gap opens at the \( X \pm \) points \((\pm k^X, 0)\), which never occurs
in the three dimensions but is allowed in the two dimensions.
The band gap \( \Delta \) is given by

\[ \Delta = 2 \sqrt{1 - \frac{m^2}{B_z^2}|B_z|}. \]  

(26)

The Chern number is calculated for each cone as

\[ C = \frac{1}{2} \text{sgn}(B_z). \]  

(27)

Since there are four cones at the \( X \pm \) and \( Y \pm \) points, the total
Chern number is \( C = 2 \text{sgn}(B_z) \). The non-zero Chern number
manifests the system shows quantum anomalous Hall effects.

We show the band structure of bulk and nanoribbon calcul-
ated based on the tight-binding model in Fig.1. The flat bands
are canted by increasing \( B_z \) and form chiral edges. Gapless
edge modes persist though they are no longer flat [Fig.1(d)].

The emergence of gapless edge modes signals that the system is
a topological insulator. Indeed, it is a quantum anomalous
Hall insulator.

We examine the winding number. The Hamiltonian is now of the form

\[ H_{\text{eff}} = R(n_x \sigma_x + n_y \sigma_y + n_z \sigma_z). \]  

(28)

With the parametrization \( (n_x, n_y, n_z) = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \), the state corresponding to
the filled band is given by the spinor

\[ |S\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi/2} \sin \frac{\theta}{2} \\ -e^{i\phi/2} \cos \frac{\theta}{2} \end{pmatrix}. \]  

(29)

The spin direction is given by \( s_i = \langle S | \sigma_i | S \rangle \). We define the vortex number still by (22) with the use of \( (s_x, s_y) \). It be-
comes a continuous function of \( B_z \),

\[ Q = \frac{\sin \theta}{2\pi} \int dk_x \partial_{k_x} \phi, \]  

(30)

and quantized only when \( B_z = 0 \), or \( \sin \theta = \pm 1 \).

We would like to argue what types of perturbation may
open the gap. Obviously they are those which appear in the
coefficient of \( \sigma_z \) in the effective \( 2 \times 2 \) Hamiltonian (13). As far
as we keep \( B_z = 0 \), any quantum perturbation cannot change
the topological number which is an integration over the clas-
sical field. It can change only when we change the external
field \( B_z \). Namely we are able to control the band gap by the
Zeeman field \( B_z \).

The condition of the breaking term is that the term is propor-
tional to \( \sigma_z \) in the \( 2 \times 2 \) theory. It is represented by the
chiral symmetry, that is, the Hamiltonian anticommutes with
the generator \( \sigma_z \), \( \{ H, \sigma_z \} = 0 \). The semimetal is stable when
there exists the chiral symmetry, while it is gapped when the chiral
symmetry is broken. In the original \( 4 \times 4 \) Hamiltonian,
the terms \( \sigma_z, \tau_x \sigma_z, \sigma_y \tau_z \) and \( \sigma_z \tau_x \) produce such a term and
give a gap. It is also described by the chiral symmetry for
\( 4 \times 4 \) Hamiltonian, \( \{ H, \sigma_z \} = 0 \).

**Discussions:** We have shown that a semimetal emerges
in a TCI thin film by applying in-plane magnetic field. This
semimetal contains a pair of gapless cones with the oppo-
site chirality to each cone, as is a reminiscence of a pair of
Weyl cones in three dimensions. This semimetal is topologi-
ically robust as long as the magnetic field direction is in-plane.
The transition between the insulator phase and the semimetal-
lic phase will be experimentally detectable by electric transport
measurement.

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