Three-dimensional symmetry-breaking nontrivial topological states

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(Received 19 July 2013; revised manuscript received 3 February 2014; published 20 March 2014)

We discuss topological electronic states described by the Dirac Hamiltonian plus an additional one in three dimensions. When the additional Hamiltonian is an element of an Abelian group, electronic states become topologically nontrivial even in the absence of the fundamental symmetries such as the time-reversal symmetry and the particle-hole one. Such symmetry-breaking topological states are characterized by the Chern number defined in the two-dimensional partial Brillouin zone. The topological insulators in Zeeman fields are an example of the symmetry-breaking topological electric state. We show the crossover from the topological insulating phase to the topological semimetal one in strong Zeeman fields.

DOI: 10.1103/PhysRevB.89.115203 PACS number(s): 73.20.At, 73.20.Hb

Topological classification has successfully predicted a number of topologically nontrivial electronic states in the condensed matter. Each topological phase is characterized by a topological number defined in the presence of the fundamental symmetries preserved in the materials such as the time-reversal symmetry in topological insulators [1–4], the particle-hole symmetry in superfluids and topological superconductors [5,6], and the crystal symmetry in topological crystalline insulators [7,8]. The table of the topological classes [9,10] has suggested a close relationship between the appearance of the topological phase and the invariance of the Hamiltonian under the fundamental symmetries. However, the surface states, an evidence of the topological phase, often remain gapless even when the fundamental symmetries are broken by perturbations. For instance, Z₂ number in the presence of the time-reversal symmetry characterizes the topological state of the 3He-B phase belonging to class DIII. In the Zeeman field, however, 3He-B phase still hosts the gapless states on a surface parallel to the Zeeman field. Mizushima et al. [11] have explained the existence of the gapless surface states in terms of a topological number defined by using the remaining symmetry of the 3He-B phase under the Zeeman field. Finding a particular topological number for explaining a particular gapless surface states is a tool to search topologically nontrivial states in novel materials. On the basis of the prescription, we propose semimetal phases of a time-reversal invariant topological insulator under the strong Zeeman field. Such semimetals are an example of the symmetry-breaking topological materials because they are characterized only by the Chern number in the partial BZ.

We begin with the three-dimensional Dirac Hamiltonian which describes electronic structures of topological materials such as topological insulators, topological superconductors, and superfluids,

\[ H_0 = a \alpha^\mu \mathbf{p}_\mu + M \beta, \quad \mu = x, y, z, \]

\[ M = (m - b \mathbf{p}^2), \]

where \(a, b,\) and \(m\) are positive constants, \(\alpha^\mu\) and \(\beta\) are the \(4 \times 4\) Dirac matrices,

\[ \alpha^\mu = \sigma^\mu \tau^z = \begin{pmatrix} 0 & \sigma^\mu \\ \sigma^\mu & 0 \end{pmatrix}, \quad \beta = \sigma^0 \tau^z. \]

The diagonal \(2 \times 2\) blocked sectors describe the two orbital spaces in the topological insulators [12] or the particle-hole subspace in the topological superconductors. Here the Pauli matrices \(\sigma^\mu\) and \(\tau^0\) for \(\mu = x, y, z\) act on the spin and the orbital indices of an electron, respectively. The matrices \(\sigma^0\) and \(\tau^0\) are the \(2 \times 2\) identity matrix in the corresponding subspace. The index which appears twice in a single term means the summation for \(\mu = x, y, z\).

We first focus on a partial Brillouin zone specified by \(p_z = 0\). The Hamiltonian can be separated into two blocks as

\[ H_0^U = \begin{pmatrix} d(M) \cdot \sigma & 0 \\ 0 & d(-M) \cdot \sigma \end{pmatrix}, \]

\[ d(M) = (a \mathbf{p}_x, a \mathbf{p}_y, M_{p_z=0}), \]
by applying the unitary transformation $U H U^\dagger = U H U^\dagger$ with

$$U = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \quad (5)$$

The Hamiltonian of the blocked sector $h(\pm M) = d(\pm M) \cdot \sigma$ is a simple model of the quantum Hall systems \[13\] as shown in Fig. 1(b). The chiral edge modes of the two quantum Hall states (QHSs) with the opposite chiral edge mode as shown in (b), where the arrows denote the direction of the chiral edge current. The corresponding dispersion of the edge modes is shown in (c), (d) illustrates the dispersion of the edge modes under the antisymmetric Zeeman field which shifts the chemical potential of the two QHSs inversely. As a consequence, the Dirac point moves to another point in the BZ.

FIG. 1. (Color online) In (a), a plane represents the two-dimensional partial Brillouin zone (BZ) embedded in the three-dimensional one. In the partial BZ, the two blocked Hamiltonians $h(M)$ and $h(-M)$ describe the two quantum Hall states (QHSs) with the opposite chiral edge mode as shown in (b), where the arrows denote the direction of the chiral edge current. The corresponding dispersion of the edge modes under the antisymmetric Zeeman field which shifts the chemical potential of the two QHSs inversely. As a consequence, the Dirac point moves to another point in the BZ.

operator is represented by

$$P_{\mu\nu} = \epsilon_{\mu
u\rho} \sigma^\rho \tau^z, \quad (6)$$

where $\epsilon_{\mu
u\rho}$ is antisymmetric symbol. Using the property of the Abelian group is a simple way to describe physics of the present issue. But it is not essential. To advance concrete discussions on $H_F$, we explicitly express an example of $H_F$,

$$\begin{pmatrix} a_0 + a_\mu \sigma^\mu & b_\mu \sigma^\mu + b_\nu \sigma^\nu \\ b^\mu \sigma^\mu + b^\nu \sigma^\nu & c_0 + c_\rho \sigma^\rho \end{pmatrix}, \quad (7)$$

where $\mu$, $\nu$, and $\rho$ represent $x$, $y$, and $z$, and they are not equal to one another. Coefficients $a_0$, $a_\mu$, $b_\mu$, and $c_\rho$ are real numbers but they are not necessary to be constants. The additional Hamiltonian contains the various effects: the intraband scattering without spin flip for $a_0$ and $c_\rho$, and with spin flip for $a_\mu$ and $b_\mu$, the modulation of spin-orbit interaction, e.g., anisotropy, for $b_\mu$, and etc.

The Abelian group $A_P$ has a subgroup of $A_{PQ}$. The perturbed Hamiltonian belonging to $A_{PQ}$ does not remove the gapless states on all the surfaces. To show this property, we consider the elements that commute with $P_{yz}$. The gapless states remain on the four surfaces perpendicular to the $yz$ plane under such perturbed Hamiltonian. Thus we show the gapless states on the remaining two surfaces parallel to the $yz$ plane. After applying the transformation by $U$ in Eq. (5), Eq. (1) with $p_y = p_z = 0$ becomes

$$H^W_{0} = W H_U^\dagger W = \begin{pmatrix} (d'(M) \cdot \sigma) & 0 \\ 0 & d'(M) \cdot \sigma \end{pmatrix}, \quad (8)$$

where $W$ is an unitary matrix of $W = \text{diag}[\sigma^0, -i\sigma^1]$. At the point of $p_x = p_z = 0$, the edge states on the $yz$ surface are degenerate at the zero energy. This is because the two blocked sectors are equivalent to each other in this representation and because each blocked sector preserves the “particle-hole symmetry” within the $2 \times 2$ space represented by a relation $\sigma^y (d' \cdot \sigma) \sigma^y = -d' \cdot \sigma$. Thus the degeneracy of the two edge states remains even when we add the “particle-hole” symmetrical Hamiltonian $H^W_Q$ to $H^W_{0}$. Such Hamiltonian $H^W_Q$ should satisfy the relation $Q_{yz}^W H^W_Q (Q_{yz}^W)^\dagger = -H^W_Q$ with $Q_{yz}^W = \sigma^y \tau^0$. The Hermitian matrices form the Abelian subgroup $A_{PQ}$ whose elements satisfy $Q_{yz} H^W_{PQ} Q_{yz}^\dagger = -H^W_{PQ}$ and $P_{yz} H^W_{PQ} P_{yz}^\dagger = H^W_{PQ}$ at the same time. In the original representation before applying the transformation of $W$ and $U$, the unitary matrix $Q_{yz}$ is given by

$$Q_{yz} = \sigma^x \tau^y. \quad (9)$$

When we consider elements invariant under $P_{\mu\nu}$, in general, the unitary matrix in Eq. (9) is represented as $Q_{\mu\nu} = \epsilon_{\mu\nu\rho} \sigma^\rho \tau^y$. In addition to the elements in $A_{PQ}$, the Hamiltonian proportional to the $4 \times 4$ identity matrix does not affect the gapless surface states at all.

In a short summary, we have discussed the three-dimensional symmetry-breaking topological state whose electronic structures are represented by

$$H = H_0 + H_F, \quad (10)$$
where $H_P$ commutes with $\mathcal{P}_{x'y'} = e^{i\nu_0\sigma^y\tau^z}$. The set of such Hamiltonian forms the Abelian group $A_P$. The Chern number defined in the two-dimensional partial BZ specified by $p_x = 0$ characterizes the topologically nontrivial states. Generally speaking, the symmetry in a two-dimensional partial BZ is not necessary to be held in whole BZ in three dimensions. In addition, the gapped energy spectra in a two-dimensional partial BZ are not necessary to be held in whole BZ in three dimensions. The word “symmetry breaking” means that the symmetries preserved in $H_0$ are broken by $H_P$, and those preserved in $H_P$ are broken by $H_0$. In what follows, we discuss electronic states of the three-dimensional topological insulator under the Zeeman field as an example of the three-dimensional symmetry-breaking topological states.

The Zeeman field is represented by two vectors $\mathbf{B}$ and $\tilde{\mathbf{B}}$ as
\begin{equation}
H_1 = B_0 \sigma^x t^0 + \tilde{B}_0 \sigma^x t^z, \tag{11}
\end{equation}
where $B_0 \sigma^x t^0$ and $\tilde{B}_0 \sigma^x t^z$ are the symmetric and the antisymmetric parts of the Zeeman field with respect to the two orbitals, respectively. The antisymmetric part of $\tilde{B}_0 \sigma^x t^z$ is attributed to the difference of the coupling constants to the Zeeman field in the two orbitals and is dominant in $\text{Bi}_2\text{Se}_3$ [12]. We consider the subgap states on the $yz$ surface for a while. When the weak Zeeman field of $B, \tilde{B} < m$ is applied along the $z$ axis parallel to the $yz$ surface, the two QHSs in the two-dimensional partial BZ on the $p_x, p_z$ plane still remain decoupled from each other because the $H_1$ commutes with $\mathcal{P}_{xy}$. Applying the unitary transformation of $U$, the Hamiltonian becomes
\begin{equation}
H_1^U = B_0 \sigma^x t^0 + \tilde{B}_0 \sigma^0 t^z. \tag{12}
\end{equation}
The symmetric Zeeman field $B_0$ gives a constant correction to $M$ in Eq. (3) and does not affect the Dirac point in two-dimensional BZ at all. On the other hand, the antisymmetric Zeeman field $\tilde{B}_0$ shifts the chemical potential of the two QHSs inversely. As a result, the Dirac point moves from the $\Gamma$ point $(p_y, p_z) = 0$ as shown in Fig. 1(d). The situation is similar to the shift of the Dirac point at the interface facing to a ferromagnetic insulator [14–17].

Next we consider the Zeeman field in the direction perpendicular to the $yz$ surface. We conclude that the symmetric Zeeman field would remove the gapless states from the $yz$ surface because it does not belong to the Abelian subgroup $A_{PQ}$. On the other hand, the antisymmetric Zeeman field leaves the gapless states because it belongs to the Abelian subgroup $A_{PQ}$. It is easy to confirm these conclusions by the argument below. Both the symmetric $B_0 \sigma^x t^0$ and the antisymmetric $\tilde{B}_0 \sigma^x t^z$ Zeeman field commute with $\mathcal{P}_{x'y'} = \sigma^y t^z$ but do not commute with either $\mathcal{P}_{xy} = \sigma^z t^x$ or $\mathcal{P}_{xz} = -\sigma^y t^z$. The symmetric Zeeman field does not anticommute with $Q_{yz}$ in Eq. (9), which indicates the gapless states are no longer guaranteed on the $yz$ surface. On the other hand, the antisymmetric Zeeman field anticommutes with $Q_{yz}$, which means the antisymmetric Zeeman field belongs to $A_{PQ}$. This is because the antisymmetric Zeeman field preserves the “particle-hole symmetry” in each QHS. As a result, the symmetric (antisymmetric) Zeeman field removes (leaves) the gapless energy spectra on the surface perpendicular to the Zeeman field. So far we have considered the weak Zeeman field of $m < |B|$ and $m < |\tilde{B}|$, another topological phases would be also expected because the two QHSs still remain decoupled from each other. We will confirm the last statement by numerical calculation.

In what follows, we confirm the analysis above by the numerical calculation for the combined Hamiltonian $H = H_0 + H_1$ on the tight-binding lattice,
\begin{equation}
H = \sum_p c(p)^\dagger \left[ \left( m - b \sum_{y,z} (1 - \cos p_x) \sigma^0 t^z \right. \right.
\end{equation}
\begin{equation}
+ a \sin p_\nu \sigma^\nu t^x + \sigma^\nu (B_0 t^0 + \tilde{B}_0 t^z) \right] c(p), \tag{13}
\end{equation}
with the parameters $m, a$, and $b$ used in Ref. [17]. Here $c(p) = (c_1^\dagger, c_2^\dagger, c_3^\dagger, c_4^\dagger)^T$ is the annihilation operator with four components corresponding to spin $\uparrow, \downarrow$ and orbital 1,2 subspaces. To calculate the energy spectra of the surface state on the $yz$ plane, we consider the lattice along $x$ axis with
\begin{equation}
\sum_{p_x} \cos p_x c_1^\dagger(p_x) c(p_x) \rightarrow \frac{1}{2} \sum_j (c_1^\dagger(j + 1)c_1(j) + \text{H.c.}),
\end{equation}
\begin{equation}
\sum_{p_x} \sin p_x c_1^\dagger(p_x) c(p_x) \rightarrow \frac{1}{2l} \sum_j (c_1^\dagger(j + 1)c_1(j) - \text{H.c.}),
\end{equation}
where we utilize $j$ as the position on the $x$ axis and employ the hard-wall boundary condition in the $x$ axis.

At first, we consider the weak Zeeman field. The topological phases can be confirmed by the appearance of the gapless surface states. In Fig. 2, we show the energy spectra of the surface states on the $yz$ plane under the symmetric Zeeman field with $|B| = m/2$ and $|\tilde{B}| = 0$ in (a) and (c), and those
FIG. 3. (Color online) The energy spectra on the \(yz\) surface under the large Zeeman field applied in the \(y\) direction. The results are plotted along the \(p_y\) axis with \(p_z = 0\) (upper figures) and along the \(p_z\) axis with \(p_y = 0\) (lower figures). The left figures of (a) and (c) are the results for the symmetric Zeeman field at \(B_y = 1.5m\). The right figures of (b) and (d) are calculated under the antisymmetric Zeeman field at \(\tilde{B}_y = 1.5m\).

In Figs. 3(a) and 3(c), we show the energy spectra on the \(yz\) surface under the strong symmetric Zeeman field in the \(y\) axis with \(B_y = 1.5m\). The semimetal hosts the chiral surface modes, so-called the Fermi arc as shown by a pair of linear dispersion in (c). The spectra in Fig. 3 include the contribution from the two \(yz\) planes parallel to the Zeeman field. When one \(yz\) surface hosts a chiral mode with the positive velocity, the other \(yz\) surface hosts a chiral mode with the negative velocity. The results are consistent with a study of the large Zeeman field in Ref. [22]. In the purely two-dimensional system, the semimetallic states are realized in the junction between a TI and a ferromagnetic insulator [23]. On the other hand, the antisymmetric Zeeman field biases the two QHSs reversely but holds the Chern number unchanged. As a result, the topological insulator qualitatively changes into the nodal semimetal as shown in Figs. 3(b) and 3(d), where we show the excitation spectra of bulk states under the strong antisymmetric Zeeman field in the \(y\) axis with \(B_y = 1.5m\). We have confirmed that the semimetallic states always appear even when the two types of Zeeman components coexist. The characteristic feature of the resulting semimetallic state is dominated by the larger component. The numerical results in Fig. 3 might imply the applicability of our approach to metallic materials.

Finally, we show the numerical results for the large Zeeman field \(m < |B|\) and \(m < |\tilde{B}|\). According to Eqs. (3) and (12), the large enough symmetric Zeeman field equalizes two of the Chern numbers of the two QHSs because \(\text{sgn}[M + B] = \text{sgn}[-M + B]\). Therefore, the net Chern number becomes nontrivial in the two-dimensional BZ. The electronic states of the topological insulator under the large symmetric Zeeman field consist of a number of QHSs with the same Chern number stacking in momentum space. As a consequence, electronic states become the Weyl semimetal phase [18–21].

The authors are grateful to K. Nomura for useful comments on our manuscript. This work was supported by the “Topological Quantum Phenomena” (Grant No. 22103002) Grant-in Aid for Scientific Research on Innovative Areas from the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan.