Boundary-obstructed topological phases of a Dirac fermion in a magnetic field

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It is known that in some higher-order topological (HOT) insulators, HOT phases are distinguished not by gap-closings of bulk states but by those of edge states, which are called boundary-obstructed topological phases (BOTP). In this paper, we investigate the BOTP of two-dimensional (2D) Su-Schrieffer-Heeger (SSH) model in a uniform magnetic field. At $\pi$-flux per plaquette, this model corresponds to the typical model of HOT insulators proposed by Benalcazar-Bernevig-Hughes (BBH). The BBH model can be approximated by Dirac fermions with two kinds of mass terms, which will be referred to as BBH Dirac fermion. To clarify the BOTP of the 2D SSH model around $\pi$ flux, we study the BBH Dirac model including a magnetic field. In continuum Dirac models, boundary conditions associated with the hermiticity of Hamiltonians are known to play a crucial role in determining the edge states. We first demonstrate that for the conventional Dirac fermion with a single mass term, such boundary conditions indeed determine the edge states even in the presence of a magnetic field. Next, imposing boundary conditions consistent to the lattice terminations, symmetries, and hermiticity of the Hamiltonian, we obtain the edge states of the BBH Dirac fermion in a magnetic field, and clarify its BOTP. In particular, we show that the unpaired Landau levels, which cause the spectral asymmetry, yield the edge states responsible for the BOTP.

I. INTRODUCTION

Higher-order topological (HOT) insulators [1–6] have been attracting much current interest [7–15]. While conventional (first-order) topological insulators (TI) accompany bulk gap-closings in their topological transitions, HOT insulators can change topological properties without bulk gap-closings: Instead, gap-closings of edge states induce HOT changes generically, implying that HOT insulating phases are distinguished by gap-closings of edge states. Such properties, called boundary-obstructed topological phases (BOTP), have been studied in Ref. [16].

One of typical examples for HOT insulators is the two dimensional (2D) second-order topological quadrupole model proposed by Benalcazar-Bernevig-Hughes (BBH) [1, 2]. This model is a kind of 2D generalization of the one-dimensional (1D) Su-Schrieffer-Heeger (SSH) model [17]. The BBH model has been further generalized by introducing locally oscillating flux of zero mean [18] or uniform flux [19], both of which interpolate the 2D SSH model with zero flux and the BBH model with $\pi$ flux per plaquette. It has been pointed out in Ref. [19] that as a function of the magnetic flux (Hofstadter butterfly), there appear many gapped regions at half-filling showing corner states. In particular, around $\pi$ flux, relatively a large gap is open, whose ground states are expected to belong to the BBH class. Thus, if anisotropic hoppings breaking $C_4$ symmetry are introduced, those ground states would reveal the BOTP.

In this paper, we investigate the BOTP [16] of the anisotropic BBH model [1, 2] in a magnetic field. To this end, we use the Dirac fermions in the continuum limit associated with high symmetry points of the BBH model [1, 20], which will be referred to as BBH Dirac fermion. We emphasize the importance of the boundary conditions of the Dirac fermions required 1) by the boundary termination on the lattice, 2) by symmetries of the lattice model, and 3) by the hermiticity of the Hamiltonians [5, 6, 21]. Based on exact and/or numerical solutions for edge states, we clarify the BOTP of the BBH Dirac fermion in a magnetic field.

This paper is organized as follows: The next Sec. II is devoted to the overview of the lattice BBH model and its continuum limit. First, we give a brief review of the BBH model in Sec. II A to fix our notational conventions, and second, taking the continuum limit of the lattice model, we derive the BBH Dirac fermion in a magnetic field in Sec. II B, including discussions of the boundary conditions in Sec. II B 2. As argued in [5, 6, 21], Hamiltonians of Dirac fermions are not necessarily hermitian if boundaries are introduced. Then, when we determine the edge states, boundary conditions which make the Hamiltonians hermitian play a crucial role. Generically, such boundary conditions allow various parameters. However, given a lattice model, lattice terminations would choose unique boundary conditions. We argue several aspects of the boundary conditions of the BBH model and BBH Dirac model.

Before discussing the BOTP of the BBH Dirac fermions, we discuss the conventional 2D Dirac fermion in Sec. III. In this case, we take account of generic boundary conditions. In the former part, Sec. III A, we give a brief review of edge states for the Dirac fermion in the absence of a magnetic field, and in the latter part, Sec III B, we show that among Landau levels of the Dirac fermion, the unpaired level, which causes the spectral asymmetry, is responsible for the edge states involved in topological properties of the model.

In Sec. IV, we switch to the BBH Dirac fermion. We first argue, in Sec. IV A 1, the BOTP of the BBH Dirac fermion in the absence of a magnetic field, although discussed already in Ref. [1], with particular emphasis on the boundary conditions. Next, in Sec. IV B, we dis-
unpaired Landau levels of the Dirac fermions are respon-

cuss the BOTP of the BBH Dirac fermion in a magnetic

II. BBH MODEL

In this section, we review basic properties of the BBH model in a uniform magnetic field. The BBH model, which is originally a 2D SSH model with \( \pi \) flux, has been generalized in Ref. [19], including arbitrary uniform flux. The model then interpolates a simple 2D SSH model with zero flux and the BBH model with \( \pi \) flux. It has been shown that around \( \pi \) flux, there appear relatively large

A. Overview of the lattice model

The BBH Hamiltonian on the lattice in Fig. 1 is defined by

\[
H = \sum_j \left[ \gamma_1 (c_{1,j}^\dagger c_{3,j} + c_{2,j}^\dagger c_{4,j}) + \lambda_1 (c_{1,j}^\dagger c_{3,j+1} + c_{2,j+1}^\dagger c_{4,j}) \\
+ \gamma_2 (c_{1,j}^\dagger c_{4,j} - c_{2,j}^\dagger c_{3,j}) + \lambda_2 (c_{1,j}^\dagger c_{4,j+1} - c_{2,j+1}^\dagger c_{3,j}) \right] + \text{h.c} \\
= \sum_{i,j} c_i^{\dagger} \mathcal{H}_{ij} c_j,
\]

where \( \gamma_j \) denotes the hopping within a unit cell, whereas \( \lambda_j \) denotes the hopping between the unit cells in the \( j = 1, 2 \) direction, and simple \( c_j = (c_{1,j}, \ldots, c_{4,j})^T \) is the abbreviation of the multicomponent fermion annihi-

\[
\mathcal{H}(k) = \sum_{j=1}^{4} \Gamma_j g_j(k),
\]

where \( g_j(k) \) is given by \( g_j(k) = \lambda_j \sin k_j \) (\( j = 1, 2 \)) and \( g_{j+2}(k) = \gamma_j + \lambda_j \cos k_j \) (\( j = 1, 2 \)). The \( \Gamma \)-matrices are defined by \( \Gamma^1 = -\tau^2 \sigma^3, \Gamma^2 = -\tau^2 \sigma^1, \Gamma^3 = \tau^1 \sigma^0, \) and \( \Gamma^4 = -\tau^2 \sigma^2 \) as well as \( \Gamma_5 = -\tau^3 \sigma^0, \) where \( \sigma^\mu \) and \( \tau^\mu \) are conventional Pauli matrices with \( \sigma^0 = \tau^0 = 1 \).

They obey \( \{ \Gamma^j, \Gamma^k \} = 2\delta^{jk} (j, k = 1, \ldots, 4) \) and \( \Gamma_5 = (-i)^2 \Gamma^1 \Gamma^2 \Gamma^3 \Gamma^4 \), so that \( \text{tr} \Gamma_5 \Gamma^2 \Gamma^3 \Gamma^4 = (2i)^2 \).

For the BBH model, reflection symmetries play a crucial role:

\[
M_1 \mathcal{H}(k_1, k_2) M_1^{-1} = \mathcal{H}(-k_1, k_2), \\
M_2 \mathcal{H}(k_1, k_2) M_2^{-1} = \mathcal{H}(k_2, -k_1),
\]

where \( M_1 = i \Gamma^1 \Gamma_5, M_2 = i \Gamma^2 \Gamma_5 \).

Let us next consider the effect of a uniform magnetic field. In Ref. [19], the 2D SSH model in a generic magnetic field has been studied. This study was restricted to the model with \( C_4 \) symmetry, i.e., \( \gamma_1 = \gamma_2 = \gamma \) and \( \lambda_1 = \lambda_2 \). It has been shown that there appear several gapped regions in the Hofstadter butterfly whose half-filled ground states belong to the second-order topologi-

Now, let us relax the \( C_4 \) symmetry and compute the bulk energy gaps. In Fig. 2, we show gapless regions by black squares on the \( \gamma_1-\gamma_2 \) plane (0 \( \leq \gamma_i \leq 1.5 \)), where we have set \( \lambda = 1 \). Let \( \phi \) be a magnetic flux per plaquette. Then, the rightmost panel (\( \phi = \pi \)) corresponds to the BBH model. Indeed, one can find that the bulk gap closing occurs solely at \( \gamma_1 = \gamma_2 = 1 \). This is the BOTP: the ground state in the HOT insulating phase \( (\gamma_1, \gamma_2 < 1) \) can be deformed into the trivial insulating phase \( (\gamma_1 > 1 \) and/or \( \gamma_2 > 1) \) without bulk gap-closings. Such a feature is not restricted to \( \phi = \pi \): The second panel from the right, which is the case with \( \phi = \frac{3}{2} \pi \), is likewise, suggesting that the ground states belong to the same class of the BBH model.

The purpose of the present paper is to investigate such BOTP around the BBH model. Of course, one can do so using the lattice model. However, to clarify the universal feature of the BOTP, we use an effective Dirac fermion model in a magnetic field valid around \( \pi \)-flux region, and investigate its edge and corner states, instead of the di-

In passing, we mention that at \( \phi = \frac{3}{2} \pi \), as shown in the third panel from the right, gapped ground states in \( \gamma_1, \gamma_2 < 1 \) region always accompany bulk gap-closing across \( \gamma_1 = 1 \) or \( \gamma_2 = 1 \) lines. From the point of view of symmetries, entanglement polarizations, and computed corner states, ground states with \( \gamma_1, \gamma_2 < 1 \) in this panel belong to the HOT insulating phase, but the HOT change is distinguished by bulk-gap closings like first-order TI.
Although this phase is out of the scope of the present paper, it may be an interesting issue to clarify the nature of this phase.

**B. Continuum limit**

The lattice model (2) includes four Dirac fermions at high-symmetry points, \( k^* = (0, 0), (0, \pi), (\pi, 0), (\pi, \pi) \). In what follows, we set \( \lambda_\mu = \lambda \) for simplicity. Around these points, the Hamiltonian is approximated by

\[
\mathcal{H}_\alpha(k)/\lambda \equiv \mathcal{H}_\alpha(k) = \gamma^\mu k_\mu + \gamma^\mu + 2 m_\mu, \alpha. \tag{4}
\]

where \( \mu = 1, 2 \). The subscript \( \alpha \) of \( \gamma \) matrices means that not only the masses but also \( \gamma \)-matrices depend on the symmetry points: \( m_1 = 1 + \frac{\pi}{2} \lambda \) and \( \gamma^{1,3} = \pm \Gamma^{1,3} \) for \( k_1^* = 0, \pi \), and \( m_2 = 1 + \frac{\pi}{2} \lambda \) and \( \gamma^{2,4} = \pm \Gamma^{2,4} \) for \( k_2^* = 0, \pi \). As we can change the signs of any two of the \( \Gamma \) matrices by unitary transformations, we can redefine each fermion \( \mathcal{H}_\alpha \) with common \( \gamma^\mu (= \Gamma^\mu) \) matrices. We have to mention that the boundary matrices \( S_j \) (\( j = 1, 2 \)) introduced below are also independent of \( k^*_\alpha \). Thus, we will suppress \( \alpha \), but we should keep it in mind that the mass terms are dependent on \( k^*_\alpha \).

For the Dirac fermion (4), let us introduce a uniform magnetic field \( B \) (around \( \pi \) flux) in the \( z \)-direction (total magnetic flux per plaquette is \( \pi + Ba^2 \)). Then, the Hamiltonian becomes

\[
\mathcal{H} = -i\gamma^\mu D_\mu + \gamma^\mu + 2 m_\mu, \tag{5}
\]

where \( D_\mu = \partial_\mu - ieA_\mu \). We expect that this model is an effective model describing the HOT properties of the lattice model with a magnetic flux around \( \pi \) flux. In this paper, we choose the vector potentials in the Landau gauge such that

\[
A_1 = 0, \quad A_2 = B x_1, \tag{6}
\]

to obtain explicit wave functions in the next section.

1. **Symmetries of the model**

The Dirac fermion (5) obeys the following transformation laws,

\[
\begin{align*}
M_1 \mathcal{H}(x_1, x_2, B) M_1^{-1} &= \mathcal{H}(-x_1, x_2, -B), \\
M_2 \mathcal{H}(x_1, x_2, B) M_2^{-1} &= \mathcal{H}(x_1, -x_2, -B), \\
T \mathcal{H}(x_1, x_2, B) T^{-1} &= \mathcal{H}(x_1, x_2, -B),
\end{align*}
\tag{7}
\]

where \( M_1, M_2 \) are reflection matrices defined for the BBH model in Eq. (3), and \( T = K \) denotes the time reversal. Define \( \tilde{M}_j = M_j T \) (\( j = 1, 2 \)). Then, we have

\[
\begin{align*}
\tilde{M}_1 \mathcal{H}(x_1, x_2, B) \tilde{M}_1^{-1} &= \mathcal{H}(-x_1, x_2, B), \\
\tilde{M}_2 \mathcal{H}(x_1, x_2, B) \tilde{M}_2^{-1} &= \mathcal{H}(x_1, -x_2, B),
\end{align*}
\tag{8}
\]

The model in a magnetic field has also (antiunitary) reflection symmetries.

2. **Boundary conditions**

For the lattice BBH model in Fig. 1, we introduce a boundary between \( j_1 = 0 \) and \( j_1 = 1 \), and consider the system defined on the half-plane \( j_1 \geq 1 \). Let \( \psi_{jn}^{\ell} \) be the \( n \)th eigenstates of the Hamiltonian \( \mathcal{H}_{ij}^j \), such that \( \mathcal{H}_{ij}^j \psi_{jn}^{\ell} = \varepsilon_n \psi_{jn}^{\ell} \). Then, the boundary termination between \( j \) \( = 0, 1 \) is carried out by setting \( \psi_{1,j_1=0,j_2,j_3}^{\ell} = \lim_{j_1 \to 0} \varepsilon_n \psi_{jn}^{\ell} = 0 \). Thus, the boundary condition of the lattice model is specified by

\[
(S_1 - 1) \psi_{jn}^{\ell} \big|_{j_1=0} = 0, \quad S_1 = -i \gamma^3 \sigma^3 = i \Gamma^1 \Gamma^3. \tag{9}
\]

Correspondingly, the same boundary condition should be imposed on the eigenstates of the continuum models such that

\[
(S_1 - 1) \psi_n(x) \big|_{x_1=0} = 0, \quad S_1 = i \gamma^1 \gamma^3. \tag{10}
\]

Note here that \( S_1 \) does not depends on \( k^*_\alpha \), as already mentioned. Likewise, if one considers the system defined on \( j_2 \geq 1 \), one can impose the boundary condition

\[
(S_1 - 1) \psi_n(x) \big|_{x_1=0} = 0, \quad S_1 = i \gamma^1 \gamma^3. \tag{10}
\]
on \( j_2 = 0 \) using \( S_3 = -\tau^0 \sigma^3 = i\Gamma^2 \Gamma^4 \) for the lattice wave function \( \psi^j_{n} \), and correspondingly, for the continuum wave function,

\[
(S_2 - 1)\psi_n(x) \bigg|_{x_2=0} = 0, \quad S_2 = i\gamma^2 \gamma^4. \tag{11}
\]

3. Symmetries of the boundary matrices

So far we have considered the system defined on \( x_1 \geq 0 \) imposing the boundary condition (10). If the system is defined on the opposite side \( x_1 \leq 0 \), the boundary condition is

\[
(S_1 + 1)\psi_n(x) \bigg|_{x_1=0} = 0. \tag{12}
\]

If the bulk system has reflection symmetry along the \( x_1 \) direction, two systems with a boundary at \( x_1 = 0 \), one defined on \( x_1 \geq 0 \) and the other defined on \( x_1 \leq 0 \), should be switched by reflection. Here, note the following transformation laws of \( S_1 \):

\[
M_1 S_1 M_1^{-1} = -S_1, \quad M_2 S_1 M_2^{-1} = S_1. \tag{13}
\]

The former ensures that the boundary conditions Eqs. (10) and (12) are indeed switched by reflection \( M_1 \). The latter relation means that the boundary condition in the \( x_1 \) direction is not affected by reflection \( M_2 \) in the \( x_2 \) direction. Likewise, we have

\[
M_1 S_2 M_1^{-1} = S_2, \quad M_2 S_2 M_2^{-1} = -S_2, \tag{14}
\]

associated with reflection symmetry along the \( x_2 \) direction. Thus, the boundary conditions match the reflection symmetries. Finally,

\[
[S_1, S_2] = 0, \tag{15}
\]

implies that we can impose simultaneous boundaries both in the \( x_1 \) and \( x_2 \) directions. This enables us to observe the corner states.

4. Hermiticity of the Hamiltonian

The BBH Dirac Hamiltonian Eq. (5) should be hermitian even with a boundary [5, 6, 21], \( \langle \phi | \mathcal{H} | \psi \rangle = \langle \mathcal{H} | \phi | \psi \rangle \). Let us consider the system defined on the half-plane \( x_1 \geq 0 \). If we require

\[
(S_1 - 1)\psi_n(x) \bigg|_{x_1=0} = 0, \tag{16}
\]

the Hamiltonian becomes Hermitian, where \( \tilde{S}_1 \) is any matrix satisfying \( \{ \tilde{S}_1, \gamma_1 \} = 0 \) and \( \tilde{S}_1^2 = 1 \). See discussions in Refs. [5, 6, 21] and also in Sec. III A 2 in the present paper. Since \( S_1 \) defined in Eq. (10) belongs to \( \tilde{S}_1 \), the boundary condition (10) due to the boundary termination of the lattice model ensures the hermiticity of the continuum BBH Dirac Hamiltonian. The hermiticity in the \( x_2 \) direction is likewise.

III. CONVENTIONAL 2D DIRAC FERMION

As reviewed in the previous section, the BBH Dirac fermion has four components with two mass terms. Before discussing the edge states of the BBH Dirac model, we first derive those of the conventional minimal 2D Dirac fermion with one mass term whose Hamiltonian is given by

\[
\mathcal{H}_0 = -i\sigma^\mu D_\mu + m\sigma^3, \tag{17}
\]

where \( D_\mu = \partial_\mu - i e A_\mu \). As shown in Sec. IV, edge states of the BBH Dirac model can be derived by using those of Eq. (17).

A. In the absence of a magnetic field

1. Bulk states

The bulk Hamiltonian becomes

\[
\mathcal{H}_0 = \begin{pmatrix} m & k_1 - ik_2 \\ k_1 + ik_2 & -m \end{pmatrix}. \tag{18}
\]

Therefore, the spectrum is given by \( \epsilon_k(k) = \pm \sqrt{k^2 + m^2} \) with \( k^2 = k_1^2 + k_2^2 \).

2. Edge states

Assume that the system is defined on the half-plane \( x_1 \geq 0 \). The Hamiltonian should be hermitian, \( \langle \phi | \mathcal{H}_0 | \psi \rangle = \langle \mathcal{H}_0 | \phi | \psi \rangle \). Form the integration by parts,

\[
\int_0^\infty dx_1 \phi^\dagger(x)(-i\sigma^1 \partial_1)\psi(x) = -i\phi^\dagger(x)\sigma^1 \psi(x) \bigg|_{x_1=0}
\]

\[
+ \int_0^\infty dx_1 (-i\sigma^1 \partial_1 \phi^\dagger) (x)\psi(x), \tag{19}
\]

we see that the hermiticity of the Hamiltonian is ensured if the following condition is imposed:

\[
(S_1^0(\theta) - 1)\psi(x) \bigg|_{x_1=0} = 0, \quad S_1^0(\theta) = \cos \theta \sigma^2 + \sin \theta \sigma^3, \tag{20}
\]

where \( \theta \) is a fixed parameter, and \( S_1^0(\theta) \) is a generic matrix that is anticommutative with \( \sigma^1 \). Although \( \theta \) is a free parameter for the continuum model, lattice models and their boundaries would choose a specific value of \( \theta \), as discussed in Sec. II B 2. In the absence of a magnetic field, the Hamiltonian Eq. (17) becomes

\[
\mathcal{H}_0 = \begin{pmatrix} m & -i\partial_1 - ik_2 \\ -i\partial_1 + ik_2 & -m \end{pmatrix}. \tag{21}
\]
Let us solve $H_0\psi_0(x_1, k_2) = \varepsilon_0\psi_0(x_1, k_2)$ for edge states. Assume that
\[
\psi_0(x_1, k_2) = \frac{1}{\sqrt{N}} \psi_0 e^{iK x_1}, \quad K = k_1 + i\kappa, \quad (\kappa > 0),
\] (22)
where $N$ is the normalization factor toward the $x_1$ direction. In what follows, such a normalization factor for wave functions will be suppressed, for simplicity. Then, $\psi_0$ should be an eigenstate of $S_1^0(\theta)$: $S_1^0(\theta)\psi_0 = \psi_0$, and hence,
\[
\psi_0 = \begin{pmatrix} 1 \\ \chi \end{pmatrix}, \quad \chi = \frac{\sin \theta - 1}{i \cos \theta}.
\] (23)
The eigenvalue equation becomes
\[
\begin{pmatrix} m & K - ik_2 \\ K + ik_2 & -m \end{pmatrix} \begin{pmatrix} 1 \\ \chi \end{pmatrix} = \varepsilon_0 \begin{pmatrix} 1 \\ \chi \end{pmatrix}.
\] (24)
This equation leads to the following solutions for the edge state,
\[
\varepsilon_0 = k_2 \cos \theta + m \sin \theta, \\
k_1 = 0, \quad \kappa = -k_2 \sin \theta + m \cos \theta (> 0).
\] (25)
The condition $\kappa > 0$ ($e^{-\kappa} < 1$) restricts the range of $k_2$ such that
\[
k_2 < m \cot \theta \quad (\sin \theta > 0) \\
k_2 > m \cot \theta \quad (\sin \theta < 0).
\] (26)
In particular, when $\theta = 0, \pi$, we have
\[
\begin{cases}
\varepsilon_0 = k_2 & (m > 0) \\
\text{no edge states} & (m < 0)
\end{cases}
\text{ for } \theta = 0,
\begin{cases}
\text{no edge states} & (m > 0) \\
\varepsilon_0 = -k_2 & (m < 0)
\end{cases}
\text{ for } \theta = \pi.
\] (27)

Note that the edge states Eq. (22) satisfies the boundary condition (20) not only at $x_1 = 0$ but also all along $x_1 > 0$. On the other hand, as to the bulk states, not traveling waves $\psi_0 e^{\pm ik_1 x}$ but their linear combination, i.e., the standing wave, can satisfy the boundary condition (20) only at the boundary $x_1 = 0$. In Fig. 3, we show some examples of the edge states obtained above.

3. Effective Hamiltonian for the edge state

In the case with $\theta = 0$, the effective Hamiltonian of the edge state becomes very simple. The edge state obtained so far satisfies Eq. (20) all along $x_1 > 0$. Therefore, the edge state belongs to the subspace projected by $P = (1 + S_2^0)/2 = (1 + \sigma^2)/2$. Note that $P\sigma^1 P = P\sigma^3 P = 0$. Thus, the effective Hamiltonian of the edge state toward the $x_2$ direction is given by
\[
H_{0,1edge} = P H_0 P = P(-i\partial_2) P.
\] (28)
Since in this subspace, $\sigma^2$ can be set $\sigma^2 = 1$, we obtain
\[
H_{0,1edge} = \begin{cases}
-i\partial_2 & (m > 0) \\
\text{no edge states} & (m < 0)
\end{cases}.
\] (29)
This is of course consistent with the previous result in Eq. (27).

B. In the presence of a magnetic field

In this section, we derive edge states of the model (17) in the presence of a uniform magnetic field. We will show that the boundary condition (20) also plays a crucial role.
The Hamiltonian (17) becomes

\[ H_0 = \begin{pmatrix} m & -iD_1 - D_2 \\ -iD_1 + D_2 & -m \end{pmatrix}. \] (30)

It follows from \([D_1, D_2] = -ieB\) that the following commutation relation holds,

\[ [-iD_1 + D_2, -iD_1 - D_2] = 2i[D_1, D_2] = 2eB. \] (31)

To obtain explicit wave functions, we choose the gauge potential given in Eq. (6). Then, since the Hamiltonian does not depend on \(x_2\), \(-i\partial_2\) can be Fourier-transformed such that \(-i\partial_2 \to k_2\). Therefore, we can define the creation and annihilation operators

\[ a = \frac{-iD_1 + sD_2}{\sqrt{2|eB|}}, \quad \frac{d}{dz} + \frac{z - sz_0}{2}, \]

\[ a^\dagger = \frac{-iD_1 - sD_2}{\sqrt{2|eB|}}, \quad \frac{d}{dz} - \frac{z - sz_0}{2}, \] (32)

where \(s = \text{sgn} eB\), \(z = \sqrt{2|eB|x_1}\) and \(z_0 = \sqrt{2|eB|k_2}\).

Using these operators, the Hamiltonian can be written as

\[ H_0 = \begin{cases} \begin{pmatrix} m & \sqrt{2eBa} \\ \sqrt{2eBa} & -m \end{pmatrix} & (s = 1) \\ \begin{pmatrix} m & -m \\ \sqrt{2eBa} & -m \end{pmatrix} & (s = -1) \end{cases} \] (33)

Now we assume \(eB > 0\) \((s = 1)\), and solve the eigenvalue equation,

\[ \begin{pmatrix} m & \sqrt{2eBa} \\ \sqrt{2eBa} & -m \end{pmatrix} \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \varepsilon_0 \begin{pmatrix} \varphi \\ \chi \end{pmatrix}. \] (34)

The upper component \(\varphi(z)\) obeys \((2eBa^\dagger a + m^2)\varphi(z) = \varepsilon_0^2\varphi(z)\), which can be written as,

\[ \left( \frac{d^2}{dz^2} + \nu + \frac{1}{4}(z - z_0)^2 \right)\varphi(z) = 0, \]

\[ \nu = \frac{\varepsilon_0^2 - m^2}{2eB}, \] (35)

using Eq. (32). It is known that the solution of Eq. (35) is given by \(\varphi(z) = D_\nu(z - z_0)\), where \(D_\nu(z)\) is the parabolic cylinder function [22]. Although this function is divergent at \(z \to -\infty\) for generic \(\nu\), as in Eq. (A5), it is convergent at \(z \to \infty\) and normalizable on the semi-infinite line \(0 < z < \infty\), as in Eq. (A4). For several useful formulae of the parabolic cylinder functions, see Appendix A.

Note that the lower component satisfies \(\chi(z) = \sqrt{2eBa}\varphi(z)/\varepsilon_0 + m\). Thus, the eigenfunction is given by

\[ \psi_{0,\nu}(x_1, k_2) = \begin{cases} \varepsilon_0^2 \begin{pmatrix} 1 \\ \varepsilon_0 + m \end{pmatrix} & (s = 1) \\ \frac{-\varepsilon_0 - m}{\sqrt{2eB}}D_{\nu-1}(z - z_0) & (s = -1) \end{cases}, \] (36)

where we have used Eq. (A2) and the normalization factor has been suppressed. It follows from Eq. (35) that generically two paired eigenstates with opposite energies appear for a fixed \(\nu\). Likewise, in the case of \(s = -1\), we obtain

\[ \psi_{0,\nu}(x_1, k_2) = \begin{cases} \frac{\varepsilon_0 - m}{\sqrt{2eB}}D_{\nu}(z + z_0) & (s = 1) \\ \varepsilon_0 + m \begin{pmatrix} 1 \\ \varepsilon_0 - m \end{pmatrix} & (s = -1) \end{cases}. \] (37)
In what follows, we restrict our discussions to the case of 

\( s = 1 \).

1. Bulk states

The bulk wave function should be normalized on the infinite line, \(-\infty < z < \infty\). Therefore, \( \nu \) is restricted to non-negative integers, \( \nu = 0, 1, 2, \cdots \equiv n \), and eigenvalues and eigenfunctions are obtained, in the case of \( s = 1 \), such that

\[
\varepsilon_{0,0} = m, \\
\psi_{0,0}(x_1, k_2) = \begin{pmatrix} D_0(z - z_0) \\ 0 \end{pmatrix}, \\
\varepsilon_{0,n}^{\pm} = \pm \sqrt{2eBn + m^2}, \\
\psi_{0,n}^{\pm}(x_1, k_2) = \begin{pmatrix} D_n(z - z_0) \\ \pm \sqrt{2eB} D_{n-1}(z - z_0) \end{pmatrix}.
\]

(38)

These are famous Landau levels of a massive Dirac fermion [23]. When \( m = 0 \), chiral symmetry ensures that the positive and negative levels are always paired except for zero energy. In the present model, there appear one zero energy state. When the mass becomes finite, the nonzero energy Landau levels are shifted in such a way that they are still paired in positive and negative energies. The zero energy Landau level moves to energy \( m \), and has no partner. This level causes the spectral asymmetry, which has intimate relationship with the parity anomaly [24–28] and is responsible for the bulk topological invariant [23].

2. Edge states

When the system is defined on \( x_1 \geq 0 \), the wave functions Eqs. (36) or (37) are always normalizable. Instead of the normalizability, the boundary condition (20) imposed on these wave functions determines the eigenvalues and eigenstates. To be concrete, the boundary condition on the wave function (36) is given by

\[
\sin \theta D_{\nu}(z_0) - \cos \theta \frac{\varepsilon_{0,n} - m}{\sqrt{2eB}} D_{\nu-1}(z_0) = D_{\nu}(-z_0),
\]

(39)

where \( \varepsilon_0 \) and \( z_0 \) are defined, respectively, in Eq. (35) and below Eq. (32). This is a nonlinear equation which determines \( \varepsilon_0 \) as a function of \( k_2 \). It is not difficult to solve this equation using, e.g., Mathematica which includes parabolic cylinder functions as built-in functions.

We show in Fig. 4, numerical solutions of Eq. (39) in the case of \( eB > 0 \). The eight panels in Fig. 4 correspond to those in Fig. 3 in the absence of a magnetic field. For large \( k_2 \), the spectra of Eq. (39) converge to those of the bulk Landau levels (38). This is natural, since the center of the harmonic potential in Eq. (35), \( x_1 = k_2/(eB) \), is located far from the boundary at \( x_1 = 0 \) in the case of \( s = 1 \). However, when \( k_2 \) becomes smaller, and at a certain value, \( k_2 \sim 0 \), boundary effects become larger and the states gradually change their characters. In this region, the spectra move away from those of the bulk Landau levels: Basically, the positive and negative Landau levels go towards more positive and negative energies, respectively, when \( k_2 \) decreases from positive to negative values. This is of course due to the boundary effects: Since Eq. (35) is the Schrödinger equation for the 1D harmonic oscillator, one can expect that the boundary makes \( \varepsilon_0^2 \) larger if \( \varepsilon_0^2 > m^2 \). However, the exception is the unpaired Landau level with energy \( m \). As can be seen from the leftmost upper panel, Fig. 4 (a), \( (m > 0 \) and \( \theta = 0 \)), the \( \varepsilon_0 = m > 0 \) Landau level causes the spectral flow across zero energy. This level passes through the energies prohibited for the bulk system. This is the edge state corresponding to the case in Sec. III A 2 in the absence of a magnetic field. Indeed, the behavior of this edge state depends on \( \theta \), and it resembles that in Fig. 3 as a function of \( \theta \). In particular, \( k_2 \ll 0 \), they asymptotically become the same linear dispersions.

As shown in III A 2, the wave function \( \psi_0(x_1, k_2) \) in Eq. (22) in the absence of a magnetic field satisfies the boundary condition (20) not only at \( x_1 = 0 \), but everywhere on \( x_1 \geq 0 \). This enables us to obtain the effective Hamiltonian for the edge state in Sec. III A 3. Unfortunately, the wave functions in Eqs. (36) or (37) satisfy the boundary condition only at the boundary, \( x_1 = 0 \), in the presence of a magnetic field.

Therefore, to check the properties of the edge state in the presence of a magnetic field, we compare the wave functions associated with the states of the unpaired Landau level \( \psi_{0,n=0}(x_1, k_2) \) with that of the exact wave function for the edge state \( \psi_0(x_1, k_2) \) given by Eqs. (22), (23), and (26) in the absence of a magnetic field. In Fig. 5, we show the local density profile for several \( k_2 \). Figure 5 (a)
is the case of the unpaired Landau level in Fig. 4 (a). In this panel, we find that when \( k_2 \) varies from positive to negative values, the wave function \( \psi_{0,0}(x_1, k_2) \) changes its character from the bulk state in Eq. (38) to the edge state in Eq. (22).

On the other hand, in the case of \( \theta = \pi \) in Fig. 5 (b), the local density has different profile from the edge state in (a) even for negative \( k_2 \). The density profile is for bulk states rather than edge states. Indeed, in this case, there are no edge states in the absence of magnetic field, as shown in Eq. (27) as well as in Fig. 3 (d). Note that this case, \( m > 0 \) and \( \theta = \pi \) with spectrum \( \varepsilon_0 \), is equivalent to the case of \( -m(< 0) \) and \( \theta = 0 \) with the spectrum \( -\varepsilon_0 \).

Therefore, when we restrict our discussions to the case of \( \theta = 0 \), we conclude that the system with \( m > 0 \) shows the edge state, as in Fig. 4 (a), which can be approximated, for \( k_2 < 0 \), by the edge state in the absence of a magnetic field in Fig. 3 (a), whereas the system with \( m < 0 \) shows no edge state, as in Fig. 4 (c), which corresponds to Fig. 3 (e). Therefore, effective Hamiltonian of the edge state in \( k_2 < 0 \) in the presence of a magnetic field is basically given by Eq. (29) in the absence of a magnetic field.

### IV. BBH Dirac Model

Based on the edge states derived so far, we discuss those of the BBH Dirac fermion in Eq. (5). To this end, the following \( \gamma \)-matrices are convenient:

\[
\gamma^j = \tau^1 \sigma^j, \quad (j = 1, 2, 3), \quad \gamma^4 = \tau^2 \sigma^0, \quad \gamma_5 = \tau^3 \sigma^0.
\]

Then, the Hamiltonian becomes

\[
H = \left( H_0 + i m_2 \right) \left( H_0 - i m_2 \right),
\]

where \( H_0 \) is given by Eq. (17) with \( m = m_1 \). The boundary matrix \( S_1 \) in Eq. (10) is \( S_1 = i \gamma^1 \gamma^3 = \tau^0 \sigma^2 \) in the present basis. This can be written as

\[
S_1 = \begin{pmatrix}
S_1^0(0) \\
S_1^1(0)
\end{pmatrix},
\]

where \( S_1^0(0) \) is defined in Eq. (20) with \( \theta = 0 \). In what follows, we solve edge states for a half plane \( x_1 \geq 0 \) satisfying

\[
H \psi(x) = \varepsilon \psi(x), \quad (S_1 - 1) \psi(x)|_{x_1=0} = 0. \quad (43)
\]

#### A. In the absence of a magnetic field

1. Bulk states

The Hamiltonian in the momentum representation is

\[
H(k) = \gamma^\mu k_\mu + \gamma^\mu k_\mu m_\mu.
\]

Therefore, the bulk spectrum is

\[
\varepsilon(k) = \pm \sqrt{k^2 + m^2},
\]

where \( k^2 = k_1^2 + k_2^2 \) and \( m^2 = m_1^2 + m_2^2 \). Each state above is doubly-degenerate. The bulk gap-closing occurs at \( m_1 = m_2 = 0 \) only.

2. Edge states

Let us consider the system defined on \( x_1 \geq 0 \). Let \( \psi_0(x_1, k_2) \) be the edge state wave function (22) of \( H_0 \) in Eq. (21), i.e., \( H_0 \psi_0(x_1, k_2) = \varepsilon_0 \psi_0(x_1, k_2) \) satisfying the boundary condition Eq. (20) with \( \theta = 0 \). Then, for \( m_1 > 0 \)

\[
\psi(x_1, k_2) = \left( \varepsilon \psi_0(x_1, k_2) \right) \left( \varepsilon_0 + i m_2 \right) \psi_0(x_1, k_2),
\]

is the wave function satisfying Eq. (43). Here, \( \varepsilon = \pm \sqrt{\varepsilon_0^2 + m_2^2} = \pm \sqrt{k_2^2 + m_2^2} \) is the dispersion of the edge states. The gap-closing of these edge states occur at \( m_2 = 0 \) regardless of \( m_1(> 0) \). On the other hand, when \( m_1 < 0 \), there are no edge states. Taking account of the discussions in Sec. III A 3, an effective Hamiltonian of the 1D edge state localized along \( x_1 \sim 0 \) is given by

\[
m_1 > 0, \quad H_{\text{edge}} = \left( -i \partial_2 + i m_2 \right) \left( -i \partial_2 - i m_2 \right),
\]

\[
m_1 < 0, \quad \text{no edge states}.
\]

The above Hamiltonian \( H_{\text{edge}} \) is nothing but the 1D massive Dirac fermion. It should be noted that \( \sigma^2 \) of \( S_1 = \tau^0 \sigma^2 \) acts as 1 in this subspace.

In addition to the boundary along \( x_1 = 0 \), let us introduce another boundary along \( x_2 = 0 \) and consider the above edge state (47) in the region \( x_2 \geq 0 \). As discussed in Sec. II, the boundary condition toward \( x_2 \) for the BBH Dirac fermion is given by \( S_2 = i \gamma^2 \gamma^4 = -\gamma^3 \sigma^2 \) in the present basis (40). In the subspace of Eq. (47), we can set \( \sigma^2 = 1 \), so that \( S_2 \) acts as \( S_2 = -\gamma^3 \) in the space of Eq. (47). Thus, the zero-dimensional edge state of \( H_{\text{edge}} \)

\[
H_{\text{edge}} \psi'(x_2) = \varepsilon' \psi'(x_2),
\]

\[
(S_2 - 1) \psi'(x_2)|_{x_2=0} = 0, \quad S_2 = -\gamma^3,
\]

is obtained as follows:

\[
m_2 > 0, \quad \varepsilon' = 0, \quad \psi'(x_2) = \sqrt{2m_2} \left( \begin{pmatrix} 0 \\ e^{-m_2 x_2} \end{pmatrix} \right),
\]

\[
m_2 < 0, \quad \text{no edge states}.
\]

The above transition at \( m_2 = 0 \) with keeping \( m_1 > 0 \) is the boundary obstruction of the edge states mentioned below Eq. (46).
B. In the presence of a magnetic field

Finally, we consider the BBH Dirac model in a magnetic field in Eq. (41). In this section, we restrict our discussions to the case of $eB > 0$. Even in the presence of a magnetic field, completely the same discussions in Sec. IV A 2 are applied to this case.

![Graph of BBH Dirac model](image)

FIG. 6: Edge (and bulk) states of the BBH Dirac model with (a) $m_1 = 1$ and (b) $m_1 = -1$. Other parameters used are $m_2 = 0.1$ and $B = 1.5$. The dashed lines are the bulk spectrum of the BBH Dirac model in a magnetic field, $\pm m_1$ and $\pm \sqrt{(\epsilon_{0,n})^2 + m_2^2}$.

We first mention that considering Eq. (41), the bulk spectrum is given by $\pm \sqrt{2eBn + m^2}$ ($n = 0, 1, \cdots$), where $m^2 = m_1^2 + m_2^2$. Therefore, the bulk gap at zero energy is given by $2m$.

Next, let us consider the system defined in the region $x_1 \geq 0$. Let $\psi_{0,\nu}(x_1, k_2)$ be the wave function (36) of $H_0$, on which the boundary condition (20) (i.e., (39)) with $\theta = 0$ is imposed. Then,

$$\psi_{\nu \pm}(x_1, k_2) = \left( \frac{\varepsilon \psi_{0,\nu}(x_1, k_2)}{(\varepsilon_{0,\nu} + im_2)\psi_{0,\nu}(x_1, k_2)} \right), \quad (50)$$

is the wave function of (41) with energy $\varepsilon = \pm \sqrt{\varepsilon_{0,\nu}^2 + m_2^2}$ satisfying Eq. (43).

In Fig. 6, we show an example of the spectrum of the BBH Dirac model in a magnetic field. The case with small $m_2 > 0$ is shown in Fig. 6 (a), in which the gap-closing of the edge spectrum, i.e., the boundary-obstruction at $m_2 = 0$ is manifest. As discussed in Sec. III B 2, the edge state of $H_0$ can be basically given by Eq. (29), implying that an effective Hamiltonian for the edge state at $k_2 < 0$ of the present BBH Dirac model is also given by Eq. (47). Thus, even in a magnetic field, the gap-closing of the edge state induces the HOT change associated with a corner state. This boundary-obstruction occurs with keeping the bulk gap $2m$ open. On the other hand, in the case of $m_3 < 0$, no gap-closing is observed, as is expected in Fig. 6 (b). Therefore, we conclude that the ground states of the BBH model in a magnetic field show the same BOTP as the BBH model, as far as the Dirac fermion description is valid around $\pi$ flux.

V. SUMMARY AND DISCUSSION

To clarify the BOTP, we investigated the 2D BBH model in a uniform magnetic field using an effective Dirac fermion model in the continuum limit. We emphasized the importance of the boundary condition for the Dirac fermion to obtain the edge states: We argued the boundary condition from the point of view of the lattice termination, symmetry, and the hermiticity condition. We firstly solved the edge states for the conventional 2D Dirac fermion in the absence/presence of a magnetic field imposing a generic boundary condition. Using these, we next derive the edge states of the BBH Dirac fermion. The gapped edge states of the BBH Dirac fermion show the gap-closing when the HOT insulating phase changes, which is nothing but the BOTP. This occurs even in the presence of a magnetic field, in which the edge states associated with the unpaired Landau level causes the BOTP.

The result in the present paper may be limited within small magnetic fields around $\pi$ flux, since we use the linear dispersion approximation of the BBH model. Indeed, as discussed in Sec. II A, Fig. 2 shows at least in $5\pi/6 \leq \phi(\leq 7\pi/6)$, the BOTP exists, but in $\phi \leq 2\pi/3$, the HOT phase transitions accompany bulk gap-closings. It then follows that the Dirac fermion description around $\pi$ flux cannot be extended into such a region. It may be an interesting future problem to clarify the nature of this phase.

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Appendix A: Parabolic cylinder functions $D_{\nu}(z)$

The solutions $D_{\nu}(z)$ of the equation

$$\left( \frac{d^2}{dz^2} + \nu + \frac{1}{2} - \frac{1}{4} z^2 \right) D_{\nu}(z) = 0, \quad (A1)$$

are called parabolic cylinder functions [22]. These functions obey

$$\left( \frac{d}{dz} + \frac{z}{2} \right) D_{\nu}(z) = \nu D_{\nu-1}(z),$$

$$\left( \frac{d}{dz} - \frac{z}{2} \right) D_{\nu}(z) = -D_{\nu+1}(z). \quad (A2)$$

Other linearly independent solution of Eq. (A1) is $D_{\nu}(-z)$ if $\nu$ is not an integer, or $D_{-\nu-1}(iz)$ for any $\nu$. When $\nu$ is a non-negative integer, $\nu = n \equiv 0, 1, \cdots$, $D_{n}(z)$ corresponds to the familiar wave function of the
1D harmonic oscillator,

\[ D_n(z) = 2^{-\frac{n}{2}} e^{-\frac{1}{2}z^2} H_n(2^{-\frac{1}{2}} z), \quad (A3) \]

where \( H_n(z) \) is the Hermite polynomial of degree \( n \). The asymptotic behavior of \( D_\nu(z) \) for large values of \(|z|\) and a fixed value of \( \nu (\neq n) \) is

\[ D_\nu(z) = z^\nu e^{-\frac{1}{2}z^2} (1 + O(|z|^{-2})) \]
\[ \left( |\arg z| < 3\pi/4 \right), \quad (A4) \]

whereas

\[ D_\nu(z) = z^\nu e^{-\frac{1}{2}z^2} \left( 1 + O(|z|^{-2}) \right) \]
\[ - \frac{(2\pi)^{\frac{1}{2}}}{\Gamma(-\nu)} e^{i\nu\pi} z^{-\nu-1} e^{\frac{1}{4}z^2} \left( 1 + O(|z|^{-2}) \right), \quad \left( \pi/4 < \arg z < 5\pi/4 \right). \quad (A5) \]

Therefore, Eq. (A5) tells that \( D_\nu(z) \) diverges as \( z^{-\nu-1} e^{\frac{1}{4}z^2} \) for real negative \( z, z \to -\infty \), if \( \nu (\neq n) \).

[1] W. A. Benalcazar, B. A. Bernevig, and T. L. Hughes, Physical Review B 96, 245115 (2017).
[2] W. A. Benalcazar, B. A. Bernevig, and T. L. Hughes, Science 357, 61 (2017).
[3] F. Schindler, A. M. Cook, M. G. Vergniory, Z. Wang, S. S. P. Parkin, B. A. Bernevig, and T. Neupert, Science Advances 4, eaat0346 (2018).
[4] S. Hayashi, Communications in Mathematical Physics 364, 343 (2018).
[5] K. Hashimoto and T. Kimura, Physical Review B 93, 195166 (2016).
[6] K. Hashimoto, X. Wu, and T. Kimura, Physical Review B 95, 165443 (2017).
[7] J. Langbehn, Y. Peng, L. Trifunovic, F. von Oppen, and P. W. Brouwer, Physical Review Letters 119, 246401 (2017).
[8] Z. Song, Z. Fang, and C. Fang, Physical Review Letters 119, 246402 (2017).
[9] M. Ezawa, Physical Review Letters 120, 026801 (2018).
[10] M. Ezawa, Physical Review B 98, 045125 (2018).
[11] F. Liu and K. Wakabayashi, Physical Review Letters 118, 076803 (2017).
[12] E. Khalaf, Physical Review B 97, 205136 (2018).
[13] A. Matsugatani and H. Watanabe, Physical Review B 98, 205129 (2018).
[14] T. Fukui and Y. Hatsugai, Physical Review B 98, 035147 (2018).
[15] D. Călugăru, V. Juričić, and B. Roy, Physical Review B 99, 041301 (2019).
[16] E. Khalaf, W. A. Benalcazar, T. L. Hughes, and R. Queiroz (2019), arXiv:1908.00011.
[17] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Physical Review Letters 42, 1698 (1979).
[18] W. A. Wheeler, L. K. Wagner, and T. L. Hughes, Physical Review B 100, 245135 (2019).
[19] Y. Otaki and T. Fukui, Physical Review B 100, 245108 (2019).
[20] T. Fukui, Physical Review B 99, 165129 (2019).
[21] E. Witten (2015), arXiv:1510.07698.
[22] H. Bateman, Higher transcendental functions, vol. II (McGraw-Hill Book Company, 1953).
[23] K. Ishikawa, Physical Review D 31, 1432 (1985).
[24] G. M. L. Alvarez-Gaumé, S. Della, Annals of Physics 163, 288 (1984).
[25] K. Ishikawa, Physical Review Letters 53, 1615 (1984).
[26] G. W. Semenoff, Physical Review Letters 53, 2449 (1984).
[27] A. N. Redlich, Physical Review Letters 52 (1984).
[28] A. N. Redlich, Physical Review D 29 (1984).