A proposal of strong and weak phases in second-order topological insulators

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Abstract

Recently, it has been discovered theoretically that there exist novel types of 3-dimensional topological insulators (TIs) whose gapless states manifest themselves at 1-dimensional hinges. They are called second-order topological insulators (SOTIs). Most mathematical models of SOTIs compose of conventional strong topological insulators (STIs) and additional mass terms. In this paper, we investigate whether the models based on weak topological insulators (WTIs) can have hinge states as the same as those made based on the STIs. We found that the models based on WTIs have only trivial $\mathbb{Z}_2$ index determined by the Wilson loop formalism unlike the models based on STIs. However, they can be regarded as stacking of 2-dimensional SOTIs along the z direction. Thus, we propose that there are topologically three different phases in our considering system: ordinary insulator, strong SOTI, and weak SOTI phases. This classification suggests the existence of other topological invariants besides the $\mathbb{Z}_2$ index. Finally, we propose new indices which can distinguish weak SOTIs from ordinary insulators.

1. Introduction

A beautiful relation has attracted enormous research interest between the condensed matter physics and the mathematical concept ‘topology’ for the last several decades. Especially, topological insulators (TIs) have been investigated intensively [1–7]. Also, their application is studied extensively in the field of spintronics [8–13]. The $d$-dimensional TIs exhibit the gapless boundary states with the $(d - 1)$-dimension, which reflect the topology of the bulk states. In recent years, new types of topological phases, namely higher-order topological insulators (HOTIs), were proposed [14–17]. They exhibit the gapless boundary states whose dimension is lower than $(d - 1)$. Generally, $n$th-order TIs exhibit the gapless states at a $(d - n)$-dimensional boundary with codimension $d_c = n$ while they are gapped in the $d$-dimensional bulk states. In this scheme, the conventional TIs are classified as the first-order TIs. Hence, the higher-order topological phases are the generalization of the conventional ones and they have been recently paid much attention both theoretically [18–26] and experimentally [27–29].

In the 3-dimensional systems, there exist two main types of first-order TIs, namely strong topological insulators (STIs) and weak topological insulators (WTIs). The WTIs have gapless surface states at specific surfaces and can be regarded as stacked layers of 2-dimensional TIs while the STIs have gapless states at all surfaces. There is a question whether such two types also exist in second-order topological insulators (SOTIs) with gapless hinge states.

In this paper, we address this question. Typical mathematical models of 3-dimensional SOTIs are composed of the STIs and an additional mass term. The mass term eliminates the surface states of the STIs and induces the hinge states. The first model of SOTIs proposed by Schindler et al was an example in which this method is applied [17]. After that, this method have been widely applied to various topological crystalline insulators [18, 21–24]. However, to our knowledge, there are very few attempts introducing the mass term to the WTIs [21]. Ezawa has treated the hexagonal lattice models and investigated the weak phases of SOTIs of them. Moreover, a
few of studies of the weak phases of TIs do not provide the readers with concrete 3-dimensional plots of their electron densities. In this paper, we utilize the first-order TIs with a much simpler cubic lattice structure as the host materials for making the SOTIs in comparison to [21]. Therefore, it is easy to visualize the electron densities of TIs using this model. This results in that the readers can understand intuitively the distribution of the surface electron densities or the hinge electron densities of TIs. Especially, the visualization of the surface electron densities of the weak phases of TIs convinces the readers at a glance that the weak phases of TIs are made of the stacked layers of the 2-dimensional TIs along the specific direction. Also, at present, \( K \)-theory in mathematics is very successful in classifying the phase of TIs and topological superconductors [30–33]. However, \( K \)-theory cannot distinguish the strong phases of SOTIs from the weak phases of them. In this study, we propose the topological indices by which we can distinguish the strong phases of SOTIs from the weak phases of them. Using the indices, we can classify the strong phases and the weak phases of SOTIs systematically. As a result, the strong phases of SOTIs can be divided into two phases.

2. Theory

First of all, we explain a model Hamiltonian for describing SOTIs. The model is composed of the first-order TI and an additional mass term. In this model, the first-order TI being a host material can switch over from STIs to WTs by changing some parameters. In the rest part of this section, we explain how to determine topological invariants of the first-order TI and the SOTIs. In this paper, the Wilson loop formalism is utilized as a method of determining topological invariants.

2.1. Model Hamiltonian

We start by introducing a Bloch Hamiltonian of SOTIs. The Bloch Hamiltonian used in this paper is as follows:

\[
\mathcal{H}(\mathbf{k}) = \mathcal{H}_{\text{host}}(\mathbf{k}) + \mathcal{H}_{\text{mass}}(\mathbf{k}),
\]

with

\[
\mathcal{H}_{\text{host}}(\mathbf{k}) = \left( M + \sum_{i=x,y,z} t_i \cos k_i \right) \tau_z \otimes \sigma_0 + \Delta_1 \sum_{i=x,y,z} \sin k_i \tau_z \otimes \sigma_i,
\]

and

\[
\mathcal{H}_{\text{mass}}(\mathbf{k}) = \Delta_2 (\cos k_x - \cos k_y) \tau_y \otimes \sigma_0.
\]

In the above formulation, \( \sigma_i \) and \( \tau_i \) are the Pauli matrices for the spin and orbital degrees of freedom, respectively. We regard \( M \) as a kind of tuning parameter. While \( t_i \) indicates the nearest neighbor hopping strength between the same orbitals, \( \Delta_i \) represents the nearest neighbor hopping strength between different orbitals. When the parameters \( t_i \) are isotropic such as \( t_x = t_y = t_z = t \), the total Hamiltonian \( \mathcal{H} \) corresponds to the very model proposed by Schindler et al [17]. Unless otherwise specifically noted, we set the lattice constants to unity in all the directions for simplicity. The host Hamiltonian \( \mathcal{H}_{\text{host}} \) represents the Wilson–Dirac type (first-order) TIs and plays a role as host materials for making SOTIs. Then, the host Hamiltonian preserves time-reversal symmetry \( T \mathcal{H}_{\text{host}}(\mathbf{k}) T^{-1} = \mathcal{H}_{\text{host}}(-\mathbf{k}) \), where \( T = \tau_0 \otimes \sigma_z \), \( K \) and \( K \) stands for the complex conjugation. We can switch over from the STIs to the WTs by adjusting the parameters \( M \) and \( t_i \). In addition, when \( t_x = t_y = t \), the host Hamiltonian has also a 90°-rotational symmetry around the \( z \) axis \( C_4^x \mathcal{H}_{\text{host}}(\mathbf{k}) (C_4^x)^{-1} = \mathcal{H}_{\text{host}}(D_{C_4^x} \mathbf{k}) \), where \( C_4^x = \tau_0 \otimes e^{-i\pi/2} \) and \( D_{C_4^x} \mathbf{k} = (-k_y, k_x, -k_z) \). On the other hand, the mass term \( \mathcal{H}_{\text{mass}} \) indicates orbital currents whose strength is denoted by \( \Delta_2 \). This term breaks both \( T \) and \( C_4^x \) symmetry, individually. However, the antiunitary combination \( C_4^x T \) is always preserved even when \( \Delta_2 \) takes finite values. Thus, the total Hamiltonian \( \mathcal{H} \) respects \( C_4^x T \) symmetry as follows:

\[
(C_4^x T) \mathcal{H}(C_4^x T)^{-1} = \mathcal{H}(D_{C_4^x} T \mathbf{k}),
\]

where \( D_{C_4^x} \mathbf{k} = (k_y, -k_x, -k_z) \). In order to examine systems made based on the WTs, we assume that the parameters \( t_i \) are uniaxially anisotropic in the \( z \) direction such as \( t_x = t_y = t = t_z \). Note that this assumption does not affect the \( C_4^x T \) symmetry of the system.

2.2. Wilson loop formalism

The topological phases of 3-dimensional first-order TIs are determined by a set of \( \mathbb{Z}_2 \) indices, namely \((i_0; i_1, i_2, i_3)\). The first one is called strong index while the others are called weak indices. In order to investigate each index of the first-order host-TIs for making the SOTIs, we utilize a hybrid Wannier center [34, 35]. The \( \mathbb{Z}_2 \) index has the value of 1 when the trajectory of the hybrid Wannier center winds around a cylinder odd times. Hybrid Wannier center sheets along the \( x \) direction \( \hat{x}(k_y, k_z) \) are given by
\[ \tilde{x}(k_y, k_z) = \frac{a_z}{2\pi} \int_{BZ} A_z(k) \, dk_z \mod a_x, \]
with the non-Abelian Berry connection
\[ A_{\mu \nu}(k) = -i \langle u_m(k) | \partial_{\nu} | u_0(k) \rangle, \]
where \( | u_m(k) \rangle \) represents the eigenstate of an occupied band \( m = 1, \cdots, N_{\text{occ}} \) and \( a_x \) denotes the lattice constant of the \( x \) direction. Considering the case of half filling, the number of occupied bands \( N_{\text{occ}} \) is equal to half the number of all bands. Since crystals have the translational symmetry, the polarization in the crystals cannot be determined uniquely. Therefore, we define the polarization by introducing the \( \text{mod} \, a_x \) in order to eliminate the ambiguity. Henceforth, the lattice constants are set to unity again. It is obvious that the hybrid Wannier center sheets do not satisfy the gauge invariance when we consider that the eigenstates \( | u(k) \rangle \) are transformed by unitary matrix \( U(N_{\text{occ}}) \), which is gauge transformation itself. Topological invariants have to be determined uniquely regardless of a specific gauge. In order to avoid this obstacle, we calculate the hybrid Wannier center sheets by utilizing the Wilson loop operator which is gauge invariant. Wilson loop operator with respect to a closed path \( p \) in the Brillouin zone (BZ) is defined as follows:
\[ \mathcal{W}(k) = \text{P} \left[ \exp \left( \int_{C_p} i \mathbf{A}(k) \cdot dp \right) \right], \]
where \( \text{P}[.] \) denotes the path-ordered product and \( k_\perp \) represents the wavevector perpendicular to the closed path \( p \). From the above definition, we can obtain the Wilson loop \( \mathcal{W}(k) \) on a path along \( k_x \), where \( dp = (dk_x, 0, 0) \) and \( k_\perp = (k_y, k_z) \). Diagonalizing the Wilson loop operator,
\[ \mathcal{W}(k_y, k_z) \theta_j^x(k_y, k_z) = \exp[i\theta_j^x(k_y, k_z)], \]
we obtain eigenstates \( | \theta_j^x(k_y, k_z) \rangle \) with eigenphases \( \theta_j^x(k_y, k_z) \), where \( j = 1, \cdots, N_{\text{occ}} \). Since the hybrid Wannier center sheets correspond to the eigenstates of the Wilson loop,
\[ \tilde{x}^j(k_y, k_z) = \frac{\theta_j^x(k_y, k_z)}{2\pi}, \]
where \( \tilde{x}^j(k_y, k_z) \) represents the polarization of the \( j \)th occupied band. Therefore, we do not need to distinguish the hybrid Wannier center sheets \( \tilde{x} \) from the Wilson loop eigenphases \( \theta_x \). When we fix one parameter among \( (k_y, k_z) \) to one of time-reversal invariant momenta (TRIM), the trajectory of the hybrid Wannier center is obtained. For instance, if we set \( k_y = \pi \) in equation (9), we get the trajectory of the hybrid Wannier center \( \tilde{x}(\pi, k_z) \) with respect to \( k_z \). This leads to the weak index \( \nu_2 \) on the basis of the notation in [3]. Hybrid Wannier center sheets \( \nu(k_y, k_z) \) and \( \tilde{x}(k_y, k_z) \) are also obtained in the same way. Numerical implementation of Wilson loop formalism is explained in detail in [36].

In the case of SOTIs having \( C^T \) symmetry, the topological invariant is proven to be a \( \mathbb{Z}_2 \) index, which we designate as \( \xi_{C^T} \) [17] in this paper. It is confirmed that the \( \mathbb{Z}_2 \) index \( \xi_{C^T} \) can also be determined by the Wilson loop \( \mathcal{W}(k) \) on a path along \( k_x \) [17, 37]. The \( C^T \) invariant momenta, namely \( (k_x, k_z) \in \{(0, 0), (\pi, \pi)\} \), are important. This is because these \( C^T \) invariant momenta correspond to the TRIM in the first-order TI s due to \( (C^T)^4 = -1 \). Thus, we need to investigate the trajectory of the hybrid Wannier center sheet \( \tilde{x}(k_y, k_z) \) along a closed path including the \( C^T \) invariant momenta in order to evaluate the \( \mathbb{Z}_2 \) index of the SOTIs.

When we would like to know what the topological index of the hinge states is, we must use the nest-version of Wilson loop. From the definition (7), it is obvious that the Wilson loop operator is unitary. Thus, we can express the operator as the exponential of a Hermitian matrix,
\[ \mathcal{W}(k_x) = \exp[i\mathcal{H}(\mathcal{W}(k_x))], \]
where \( \mathcal{H}(\mathcal{W}) \) is called Wannier Hamiltonian and \( k_\perp \) represents the momentum perpendicular to the path \( p \) of the Wilson loop as in equation (7). As you can see, the eigenphases \( \theta_m(k_x) \) of the Wilson loop are eigenvalues themselves of the Wannier Hamiltonian. Therefore, the eigenvalues \( \theta_m(k_x) \) can be regarded as some kind of energy bands when we regard Wannier Hamiltonian as a Hamiltonian of some system. They are called Wannier bands. The above identification leads to a notion that when the Wannier bands are gapped for all \( k_\perp \), the Wannier bands themselves can be classified from the viewpoint of topology. In the same way as the determination of the topology of the ordinary energy bands, the hybrid Wannier center of the Wannier bands determines the topological index of the Wannier bands which show whether the gapless hinge states exist or not [15, 16]. Two sectors of the Wannier bands are defined as follows:
\[ \theta^-_p = \{ \theta_j^x(k_x) \text{ s.t. } \theta_j^x(k_x) < 0 \}, \]
\[ \theta^+_p = \{ \theta_j^x(k_x) \text{ s.t. } \theta_j^x(k_x) > 0 \}. \]
They are referred to as occupied bands and unoccupied bands, respectively. The eigenstates \( | \theta^{\pm, j}_p(k_x) \rangle \) (where \( j = 1, \cdots, N_{\text{occ}}/2 \)) of these sectors can be used for making the following Wannier states:
is perpendicular to the closed path host. First of all, we focus on the host

In this section, we discuss the numerical calculation results of the host

3. Results and discussion

In order to investigate the differences between the STIs and the WTIs, we choose the parameters of the first-order TIs described by the host Hamiltonian $H_{\text{host}}$. We obtain STIs when $M = 2.0$ and $t_z = 1.0$ are chosen while we obtain WTIs when $M = 1.0$ and $t_z = 0.5$ are chosen.

Figures 1(a) and (b) exhibit the energy dispersions of the first-order TIs in the case of the STIs and the WTIs, respectively. Here, we impose the open boundary condition (OBC) with $N_x = 15$ sites in the x direction and the periodic boundary condition (PBC) in the other directions. For simplicity, we set the parameters to be $t = 0.5$. There exist linear dispersions detached from bulk bands. We set $t = \Delta_t = 1.0$ in both the cases.

$|w_p^{\pm,i}(\mathbf{k})\rangle = \sum_{n=1}^{N_{\text{occ}}} |u_n(\mathbf{k}_0)\rangle |\theta_p^{\pm,i}(\mathbf{k})\rangle^+,$

where $|u_n(\mathbf{k}_0)\rangle$ are eigenstates at the base point $\mathbf{k}_0$ of Wilson loop and the superscript $j$ ($= 1, \cdots, N_{\text{occ}}/2$) labels the Wannier bands. Therefore, the hybrid Wannier centers $\theta_p^{\pm,j} / 2\pi$ of the Wannier bands $\theta_p^{\pm,j}$ are calculated from the Wilson loop of the Wannier states $|w_p^{\pm,i}(\mathbf{k})\rangle$ as follows:

$\mathcal{W}_{\theta_p^{\pm,j}}(\mathbf{k}) = P \left\{ \exp \left( \oint_{\mathbf{p}} \mathbf{i} \mathbf{A}_{\theta_p^{\pm,j}}(\mathbf{k}) \cdot d\mathbf{p} \right) \right\},$

$\mathcal{W}_{\theta_p^{\pm,j}}(\mathbf{k}) |\theta_p^{\pm,j}(\mathbf{k})\rangle = e^{i\theta_p^{\pm,j}(\mathbf{k})} |\theta_p^{\pm,j}(\mathbf{k})\rangle,$

where the Berry connections of the occupied and unoccupied Wannier bands are given by

$[\mathbf{A}_{\theta_p^{\pm,j}}(\mathbf{k})]_{\alpha\alpha'} = -i \langle w_p^{\pm,j}(\mathbf{k}) | \partial_{\mathbf{k}_i} |w_p^{\pm,j}(\mathbf{k})\rangle,$

and $|\theta_p^{\pm,j}(\mathbf{k})\rangle$ are the eigenstates of the Wilson loop of the Wannier states with the eigenphases $\theta_p^{\pm,j}(\mathbf{k})$. Here, the momentum $\mathbf{k}$ is perpendicular to the closed path $\mathbf{p}$. This Berry connection is a scalar since we use the four band model ($N_{\text{occ}} = 2$).

3. Results and discussion

In this section, we discuss the numerical calculation results of the host first-order TIs and the SOTIs made on the host. First of all, we focus on the host first-order TIs in the case of $\Delta_t = 0$ for two main purposes. The first purpose is to investigate the differences between the STIs and the WTIs. For this purpose, we examine their energy dispersions and electron densities, respectively. The other one is to make topological phase diagram of the host first-order TIs.

Then, we set $\Delta_t$ to be finite and discuss the cases of the SOTIs. From the viewpoint of the energy dispersions and the electron densities, we are going to investigate whether the systems made based on the WTIs can have gapless hinge states in the same way as the systems made based on the STIs.

3.1. First-order topological insulator as a host material

In order to investigate the differences between the STIs and the WTIs, we choose the parameters of the first-order TIs described by the host Hamiltonian $H_{\text{host}}$. We obtain STIs when $M = 2.0$ and $t_z = 1.0$ are chosen while we obtain WTIs when $M = 1.0$ and $t_z = 0.5$ are chosen.

Figures 1(a) and (b) exhibit the energy dispersions of the first-order TIs in the case of the STIs and the WTIs, respectively. Here, we impose the open boundary condition (OBC) with $N_x = 15$ sites in the x direction and the periodic boundary condition (PBC) in the other directions. For simplicity, we set the parameters to be $t = \Delta_t = 1.0$. As shown in figure 1, there exist gapless surface states which appear as linear dispersions in both the cases. However, investigating the surface states carefully, it is found that there is a crucial difference between the STIs and the WTIs. The surface states of the STIs are connecting the valence bands to the conduction bands as shown in figure 1(a). On the other hand, the surface states of the WTIs are detached from the both bulk bands as shown in figure 1(b). This is one of the features which distinguishes the WTIs from the STIs.
SOTIs and the OIs from the calculation of both the energy dispersions and the electron densities. For simplicity, henceforth, we discuss numerical calculation results in the cases of the SOTIs. First, we review the features of the 3.2. Second-order topological insulator

These phase-boundary conditions are illustrated by black dashed lines shown in Figure 2. We impose the OBC with $N_x = N_y = N_z = 15$ sites in all the directions. From the figure 2(a), it is confirmed that the case of the SOTIs all the almost electrons spread over the surfaces widely. On the other hand, figure 2(b) shows that the electron densities of the WTIs exhibit periodic patterns along z direction although the electrons exist on the surfaces. The texture of the electron densities leads to the finding that the system is made of stacked 2-dimensional first-order TIs with 1-dimensional gapless edge states along the z direction. The finding is consistent with the statement in [3].

In order to investigate the set of $Z_2$ indices of the host first-order TIs, we calculate the hybrid Wannier center sheets for the STIs and the WTIs and obtain them in figures 3(a) and (b) for the STIs and them in figures 3(c) and (d) for the WTIs, respectively. From the information of the hybrid Wannier center sheets shown in figures 3(a) and (b), the four $Z_2$ indices are obtained such as $\nu_1 = \nu_2 = \nu_3 = 1$ and $\nu_0 = 1$. As a result, the set of $Z_2$ indices of the STIs with $M = 2.0$ and $t_z = 1.0$ is determined to be (1;111). Similarly, the hybrid Wannier center sheets shown in figures 3(c) and (d) inform us of $\nu_1 = \nu_2 = 0$, $\nu_3 = 1$, and $\nu_0 = 0$ for the WTIs with $M = 1.0$ and $t_z = 0.5$. Therefore, the WTIs considered here have the set of $Z_2$ indices (0;001). From the electron densities shown in figure 2(b), it is verified that the set of weak indices of (001) corresponds to the reciprocal vector $G_0 = (0, 0, 1)$ reflecting which direction the 2-dimensional TIs are stacking in.

Using the Wilson loop formalism, we have obtained the topological phase diagram of the host first-order TIs described by the Hamiltonian $\mathcal{H}_{\text{host}}$ as shown in figure 4. A Dirac cone appears in the bulk energy structure when the values of energies are equal to zero at the eight TRIM, namely $\Gamma = (0, 0, 0)$, $X = (\pi, 0, 0)$, $Y = (0, \pi, 0)$, $Z = (0, 0, \pi)$, $P = (0, 0, \pi)$, $Q = (\pi, 0, \pi)$, $R = (\pi, \pi, 0)$, and $M = (\pi, \pi, \pi)$. At the very momenta, the system undergoes the topological phase transition. The energies at these momenta are analytically obtained by

$$
E(\Gamma) = \pm (t_z + M + 2t),
$$

$$
E(X) = E(Y) = \pm (t_z + M),
$$

$$
E(Z) = \pm (t_z - M - 2t),
$$

$$
E(P) = E(Q) = \pm (t_z - M),
$$

$$
E(R) = \pm (t_z + M - 2t),
$$

$$
E(M) = \pm (t_z - M + 2t).
$$

These phase-boundary conditions are illustrated by black dashed lines shown in figure 4.

3.2. Second-order topological insulator

Henceforth, we discuss numerical calculation results in the cases of the SOTIs. First, we review the features of the SOTIs and the OIs from the calculation of both the energy dispersions and the electron densities. For simplicity, we set $t = \Delta_1 = \Delta_2 = 1.0$ in the same way as the previous session. When $M = 2.0$ and $t_z = 1.0$, the systems described by total Hamiltonian $\mathcal{H}$ become SOTIs. The SOTIs are constructed by adding the additional mass term to the STIs whose sets of $Z_2$ indices are (1;111). Alternatively, OIs are obtained when $M = 3.5$ and $t_z = 1.0$. Figure 5 shows the energy dispersions calculated under the OBC with $N_x = N_y = 15$ sites in the $x$ and $y$ directions but the PBC in the $z$ direction. As the same as the case of the STIs, there exist crossing linear dispersions which are connecting the valence bands to the conduction bands as shown in figure 5(a). Each linear

![Figure 2. Electron densities of the host first-order TIs under the OBC with $N_x = N_y = N_z = 15$ sites in all the directions. (a) Electron densities of the STIs with $M = 2.0$ and $t_z = 1.0$. All the almost electrons spread over the all surfaces. (b) Electron densities of the WTIs with $M = 1.0$ and $t_z = 0.5$. The periodic pattern of the intensity appears along the z direction. We set $t = \Delta_1 = \Delta_2 = 1.0$ in both the cases.](image-url)
dispersion is double degenerate and corresponds to localized states at the 1-dimensional hinges. Since the bulk states of the OIs are topologically trivial, the linear dispersions does not appear as shown in figure 5 (b).

From the electron densities calculated under the OBP with \( N_x = N_y = N_z = 15 \) sites in all the directions of figure 6, it is confirmed that almost all the electrons in the SOTIs with \( M = 2.0 \) and \( t_z = 1.0 \) concentrate at the hinges. In addition to the four hinges, the electrons seem to spread over the top and bottom surfaces normal to the \( z \) direction. This is because those surfaces are not affected by the additional mass term. Thus, it is considered as the vestiges of the gapless surface states of the host STIs.

In order to investigate the topological invariant \( \xi_0 \) which distinguishes the SOTIs from the OIs, we calculate the trajectories of the hybrid Wannier center sheets by using the Wilson loop, as shown in figure 7. We take a closed path through \( C_4^T \) invariant momenta such as \((k_x, k_y) = (0, 0) \rightarrow (0, \pi) \rightarrow (\pi, \pi) \rightarrow (0, 0)\). Note that the hybrid Wannier centers are not quantized at the momentum \((k_x, k_y) = (0, \pi)\) because this point does not hold the \( C_4^T \) symmetry. Figure 7(a) shows the trajectories of the hybrid Wannier center sheets of the SOTIs with \( M = 2.0 \) and \( t_z = 1.0 \). Since the trajectories wind around the cylinder only one time, the systems are characterized by the topologically non-trivial \( \mathbb{Z}_2 \) index, namely \( \xi_0 = 1 \). This result is consistent with the existence of the linear dispersions as shown in figure 5(a). Figure 7(b) shows the trajectories of the hybrid Wannier center sheets of the OIs with \( M = 3.5 \) and \( t_z = 1.0 \). Since the trajectory does not wind around the cylinder, the systems have the topologically trivial \( \mathbb{Z}_2 \) index, namely \( \xi_0 = 0 \).

Next, we are going to tackle the question whether the systems composed of both the WTIs and the additional mass term have the gapless hinge states as the same as the systems made based on the STIs. Figures 8(a) and (b) show the energy dispersions and the electron densities of the systems composed of both the WTIs and the mass term in the case of \( M = 1.0 \), \( t_z = 0.5 \), and \( t = \Delta_1 = \Delta_2 = 1.0 \), respectively. If \( \Delta_2 = 0.0 \), the systems become the WTIs whose sets of \( \mathbb{Z}_2 \) indices are \( (0; 001) \) as mentioned in the previous section. Although there exist gapless
linear dispersions as shown in figure 8(a), they are apart from both the valence and conduction bands unlike the linear dispersions connecting those bands as shown in figure 5(a). From the figure 8(b), it is found that all the almost electrons seem to exist at the hinges. However, the intensities of the electron densities have periodic patterns along the $z$ direction in contrast to the electron densities of the SOTIs in figure 6. The texture of the electron densities forces us to consider that the system can be regarded as being made of stacked layer of 2-dimensional SOTIs with 0-dimensional gapless corner states.

Nevertheless, the trajectories of the hybrid Wannier center sheets do not wind around the cylinder as shown in figure 9. This means $\xi_0 = 0$ and results in that the systems composed of the WTI and the mass term are
classified into the OIs. Therefore, it is considered that the gapless hinge states of the systems made based on the WTIs are different from those of the systems made based on the STIs. However, the existence of the gapless linear dispersions seems to contradict the topological triviality of the system made based on the WTIs. In addition, a separation of the linear dispersions and the bulk bands is the feature of the energy dispersions in the case of the WTIs as shown in figure 1(b). Moreover, the periodic patterns of the electron densities also resemble
those of the host WTIs which are characterized by the index set \((0;001)\). From the above speculations, we claim that the systems considered here can be classified into topologically protected new phase i.e. ‘weak SOTI phase’ although the systems have only the trivial index of \(\xi_0 = 0\). In the above scheme, we call a topological phase with \(\xi_0 = 1\) ’strong SOTI phase’. This classification gives a conjecture that the topological invariant \(\xi_0\) corresponds to the strong index \(\nu_0\) which distinguishes the topological phases of the 3-dimensional first-order TIs.

We would like to characterize the weak SOTIs using the hybrid Wannier centers shown in figure 10. The trajectories of the hybrid Wannier centers are calculated by the ‘nested’ Wilson loop and originate from the occupied Wannier band defined in section 2.2. Figure 10(a) shows the trajectories of the hybrid Wannier centers of the strong SOTIs with \(M = 2.0\) and \(t_z = 1.0\). It is obvious that the Wannier bands \(\theta^\nu_z\) corresponding to the strong SOTIs are topologically nontrivial since the trajectories wind around the cylinder only once in the same way as the ordinary hybrid Wannier centers. This reflects the fact that in the strong SOTIs the topological invariant of the hinge states is nontrivial. Figures 10(b) and (c) show the trajectories of the hybrid Wannier centers of the OIs with \(M = 3.5\) and \(t_z = 1.0\) and the weak SOTIs with \(M = 1.0\) and \(t_z = 0.5\), respectively. If we follow the conventional criterion based on the number of windings of the hybrid Wannier centers, the topological phases which we do call ‘the weak SOTIs’ are also classified into just OIs. This is because both the trajectories of the hybrid Wannier centers shown in figures 10(b) and (c) do not wind around the cylinder. However, there are crucial differences between the hybrid Wannier centers of the weak SOTIs and those of the OIs. The crucial differences are the values which the hybrid Wannier centers take at the CTz invariant momenta \(k_z \in [0, \pi]\). If the hybrid Wannier centers take the values of \(\pm 1.0\) (in units of \(\pi\)) in this system, that means that quadrupole moments \(Q_{xy}\) exist in the \(xy\) planes in the weak SOTIs but quadrupole moments do not exist in the OIs. This is because the quadrupole moments are composed of the hybrid Wannier centers of the Wannier bands [15, 16] as follows:

\[
Q_{xy}(k_z) = 2\frac{\theta^\nu_y(k_z)}{2\pi} \frac{\theta^\nu_z(k_z)}{2\pi}.
\]
Although we do not show explicitly here, \( \theta^q_{yz}(k) \) holds at all over the momentum of \( k \). Thus, we can obtain the same graphs as figure 10 for \( \theta^q_{yz}(k) \). Using both the values of \( \theta^q_{yz}(k) \) and \( \theta^q_{xy}(k) \), we can obtain the value of \( Q_{xy}(k) \). Here, we change the interpretation of the hybrid Wannier centers of the Wannier bands and abandon the thought that we need to count the number of winding to determine the topological indices of the system. Now, we propose that the weak SOTIs can be classified by the 'new indices' defined below from the quadrupole moments at the \( \mathbb{C}_2^4 \) invariant momenta.

From the viewpoint of the above reinterpretation, we propose that 'new indices' \( \xi_i \) defined here are the 'weak indices' for SOTIs in order to distinguish the weak SOTIs from the OIs. They are defined as follows:

\[
\xi_i = \begin{cases} 
1 & (Q_{xy}(k)|_{k_z=0,\pi} = \frac{1}{2} \text{ mod } 1) \\
0 & (Q_{xy}(k)|_{k_z=0,\pi} = 0 \text{ mod } 1)
\end{cases}
\]  

where subscript \( i \) takes the values of 1 and 2 depending on whether \( k_z = 0 \) or \( k_z = \pi \), respectively. From the above definition, each weak index is obviously a \( \mathbb{Z}_2 \) index. On the other hand, the strong index \( \xi_0 \) can be obtained by the ordinary Wilson loop using Bloch states. Thus, in this scheme, the topological phases of the model which we consider are classified by the set of \( \mathbb{Z}_2 \) indices, namely \( (\xi_0; \xi_1; \xi_2) \), and the weak SOTIs considered here have the set of \( \mathbb{Z}_2 \) indices \( (0;11) \).

In addition to the speculations that the systems made based on the WTIs must be in a new topological phase from both the energy dispersions and the electron densities, also on the basis of the above discussion from the nested Wilson loop of the Wannier bands, we have derived the topological phase diagram of the system described by the total Hamiltonian \( H \) shown in figure 11. A Dirac cone appears in the bulk energy structure when the values of energies are equal to zero at the \( \mathbb{C}_2^4 \)\( T \) invariant momenta, namely \( \Gamma = (0, 0, 0), Z = (0, 0, \pi), R = (\pi, \pi, 0), \) and \( M = (\pi, \pi, \pi) \). At the very momenta, the system undergoes the topological phase transition between different topological phases. The energies at these momenta are

![Figure 11. Topological phase diagram of the SOTIs which we consider. Yellow and purple regions exhibit the 'strong SOTIs' and 'weak SOTIs', respectively.](image-url)
analytically obtained by
\[
E(\Gamma) = \pm(t_z + M + 2t), \\
E(Z) = \pm(t_z - M - 2t), \\
E(R) = \pm(t_z + M - 2t), \\
E(M) = \pm(t_z - M + 2t). \tag{18}
\]

These phase-boundary conditions are illustrated by black dashed lines shown in figure 11. It is noticed that the topological phase diagram of the host TI and that of the SOTI resemble each other. This similarity claims that the each topological phases of the SOTI inherit those of the host first-order TIs. The topological phase diagram is expected to use as one of guidelines for searching novel higher-order topological materials described by our using Hamiltonian.

Finally, we consider whether the bulk-corner correspondence exists. From the figure 11, we can speculate that the following equation holds:
\[
\xi_0 = \xi_1 + \xi_2 \mod 2. \tag{19}
\]

This means that the bulk-corner correspondence in the narrow sense does not hold since the bulk-corner correspondence states that the topological invariant of the bulk equals that of the corner. However, we have found that there is the above relation between the topological invariant of the bulk and that of the corner.

4. Conclusion

We have studied whether or not the systems composed of both the WTIs and the additional mass term have the gapless hinge states as the same as the systems composed of both the STIs and the additional mass term. The numerical calculation results of the energy dispersions have shown that the gapless dispersions in the systems do exist but that they are different from those of the SOTIs since they are detached from the bulk bands. Moreover, when observing the existence of the hinges obviously from the calculation results of the electron densities, we are enforced to consider that the systems can be regarded as stacked layer of the 2-dimensional SOTIs. Those features of the systems resemble that of the WTIs. As a result, it is natural to consider that the systems composed of the WTIs are in a new topological phase. Thus, we have regarded the systems made based on the WTIs as systems called 'weak SOTIs'. This scheme is a generalization of the concept of the WTIs to the SOTIs. We call the ordinary SOTIs to the 'strong SOTIs' in this scheme.

However, the bulk \( \mathbb{Z}_2 \) index \( \xi_0 \) determined by the hybrid Wannier center sheets calculated using the Wilson loop cannot distinguish the system made based on the WTIs from the OIs. In order to overcome this problem, we have reinterpreted the hybrid Wannier centers, which are calculated using nested Wilson loop, of Wannier bands and proposed new indices, namely \( \xi_1 \) and \( \xi_2 \). Each new index is a \( \mathbb{Z}_2 \) index and characterizes the weak SOTIs. Hence, the topological phases of the model which we consider are classified by the set of \( \mathbb{Z}_2 \) indices \( (\xi_0, \xi_1, \xi_2) \). On the basis of the set of \( \mathbb{Z}_2 \) indices, we have obtained the topological phase diagram of the model which we consider. Therefore, we have discovered that the topological phases of the SOTIs inherit that of the host first-order TIs. Moreover, we have speculated the relation between the topological invariant of the bulk and that of the corner from the topological phase diagram.

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