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Title(English)	Bulk-boundary correspondence of first- and second-order topological insulators and their effects on the crystal shapes
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Type(English)	Outline

Outline of thesis

Topological phases of matter have come to occupy a central place in condensed matter physics. There are various topological phases in solids, *e.g.*, topological insulators, Weyl semimetals, Dirac semimetals, and so on. In terms of a geometric phase of the wave function in the bulk, we define topological invariants to capture the topological phases. When a topological invariant is nontrivial in a given system, the system has topological gapless states at the boundaries. The correspondence between the topology in the bulk and the boundary states is called bulk-boundary correspondence.

Among various topological phases of matter, a topological insulator is one of the most fundamental topological phases. Topological insulators are classified in terms of a $\mathbb{Z}_2$ topological invariant, and their gapless boundary states are protected by time-reversal symmetry. As long as the $\mathbb{Z}_2$ topological invariant does not change and time-reversal symmetry is preserved, the surface states are stable against perturbations. Two- and three-dimensional topological insulators have one-dimensional and two-dimensional topological gapless states, respectively. These topological phases have the correspondence between the topological invariants in the n-dimensional bulk and the $(n-1)$-dimensional gapless states. We refer to such topological phases as first-order topological insulators. Then an interplay between crystal symmetry and topology leads to topological crystalline insulators (TCIs), which are topological insulators protected by crystal symmetries. The three-dimensional TCIs have gapless surface states protected by crystal symmetries, such as mirror symmetry and glide symmetry. The TCI with the surface states is also classified as a first-order topological insulator. In recent years, the concept of first-order topological insulators has been extended to second-order topological insulators (SOTIs). The three-dimensional SOTIs are materials with gapped bulk and surfaces, but with topologically protected gapless states at the intersection of two surfaces. These gapless states are called hinge states. In the SOTIs, the topological nature of n-dimensional bulk manifests itself not as $(n-1)$- but as $(n-2)$-dimensional gapless states.

Although we need to calculate the topological invariant in a given material for diagnosing whether the material is topological or trivial, it is not easy to calculate the topological invariant directly from the definition of the topological invariant. This difficulty is one obstacle to the search for topological materials. On the other hand, by using information on crystal symmetries, we can simplify calculations of the topological invariants. For example, in the presence of inversion symmetry, the $\mathbb{Z}_2$ topological invariant can be obtained from the parity eigenvalues of occupied states at the high symmetry points. Because the energy levels and their wave functions at any k points in a given material can be obtained from modern implementations of the density functional theory, we can easily find the symmetry eigenvalues the high-symmetry points. Thus, it is important to construct a theory of topological phases in terms of only the symmetry eigenvalues. According to the previous works, it is known that SOTIs with inversion symmetry are characterized by a $\mathbb{Z}_4$ topological invariant, which can be calculated from the symmetry eigenvalues of occupied states at high-symmetry points. Although the connection between the $\mathbb{Z}_4$ topological invariant and hinge states has been discussed in previous works, these works are based on the $\boldsymbol{k} \cdot \boldsymbol{p}$ Dirac Hamiltonian or specific models. Therefore, this approach cannot be applied to systems whose surfaces are not described by the Dirac model. In order to complete the proof, it is necessary to establish a theory on the connection between the $\mathbb{Z}_4$ invariant and hinge states for general systems.

We will also discuss surface energies of the TCI and the SOTI in the latter half of this thesis. The surface energies and the crystal facets affect morphologies of materials, and therefore they are vital factors in controlling the properties of nanomaterials and in applications to the material design. In particular, the surface energies determine equilibrium crystal shapes, which can be realized in nanocrystals, and the surface energies are mainly determined by chemical bondings in crystals. Although the crystal shapes of TCIs have been observed, it is not well understood how the topological boundary states affect the crystal shapes. In addition, it is still unknown whether the surface energies of the TCIs and the SOTIs can be understood only from the chemical bondings.

Given that the topological materials possess gapless states at their boundaries, we need to consider a system with boundaries in order to study the topological boundary states. On the other hand, the topological invariant of the topological material is defined by the wave functions in the bulk without boundaries. Thus, in order to comprehend the relationship between the topology in the bulk and the topological boundary states, it is helpful to study the process of changing boundary conditions from periodic boundary conditions to open boundary conditions. We refer to this process as the "cutting procedure".

The purpose of this thesis is to discover and understand novel phenomena brought about by the topological phases via the cutting procedure. This procedure gives us two crucial pieces of information on topological phases of matter: (i) spectral flow and (ii) surface energy. The spectral flow is a flow of energy bands through the cutting procedure. Through an analysis of the spectral flows, we can show the bulk-boundary correspondence of the TCI and the SOTI, as we will discuss in the first half of this thesis. In addition, we can also obtain the surface energy via the cutting procedure. We apply the cutting procedure in one direction and get how much the energy changes through the cutting procedure, which gives us the surface energy. As we will discuss in the latter half of this thesis, we discover that the topological boundary states affect the surface energy, resulting in unique equilibrium crystal shapes. This thesis is organized to show the bulk-boundary correspondence of the TCI and the SOTI and to explore novel phenomena induced by topological phenomena via the cutting procedure as mentioned above. This thesis is organized as follows.

Chapter 1 provides the background of our works, the purpose of this thesis, and the outline of this thesis, as an introduction to this thesis. Chapter 2 provides an introduction to the geometric phase in quantum mechanics and the basics of topological phases of matter as a preliminary part toward the main part of this thesis. In addition, we discuss the basic properties of tight-binding models and the role of crystal symmetries in the tight-binding model in this chapter.

In Chapter 3, we show the bulk-boundary correspondence of the TCIs and the SOTIs only from information on the symmetry eigenvalues of occupied states. To show the bulk-boundary correspondence, we study changes in the band structures in the process of changing the boundary condition from the periodic boundary condition to the anti-periodic boundary condition. We study behaviors of gapless states through the cutting procedure in one direction, and thereby we show that the surface states appear in terms of parity eigenvalues satisfying certain conditions. In addition, by applying the cutting procedures in two directions, we give a proof that the hinge states appear only from the parity eigenvalues.

In Chapter 4, we also find all the possible configurations of chiral hinge states in SOTIs with inversion symmetry through an analysis of the sign of the surface Dirac mass. The configurations are uniquely determined from each magnetic space group as a massless line of the surface Dirac mass, and then we exhaust all possible configurations of the hinge states in the SOTIs in all type-I magnetic space groups with inversion symmetry. In particular, in the presence of glide symmetry, for particular surface orientations, the surface Dirac mass changes sign by changing the surface terminations. By applying this result to a layered antiferromagnet, we find a difference in the hinge states between the cases with an even and odd number of layers.

In Chapter 5, we extend the bulk-boundary correspondence of the SOTI protected by inversion symmetry to those protected by rotoinversion symmetry. Then, based on the bulk-boundary correspondence, we propose a class of Weyl semimetals having the chiral hinge states protected by rotoinversion symmetry.

In Chapter 6, we show that topological surface states affect surface energies and crystal facets in an unconventional way. By adding a magnetic field to a topological insulator, we can realize a TCI phase protected by mirror symmetry. In the TCI protected by mirror symmetry, the gapless states appear only on the surfaces which are invariant under the mirror operation. By studying changes in the crystal shapes through this process, we unveil that the anisotropy of the surface states affects the surface energy and the crystal shape. We also calculate the crystal shape of the SOTI and discover that the positions of the hinge states affect the crystal shape of the SOTI.

In Chapter 7, in addition to the TCI protected by mirror symmetry, we focus on the TCI protected by nonsymmorphic symmetries. The TCI with nonsymmorphic symmetries is particularly interesting because of the presence of fractional translations, such as glide mirror and screw rotations. We show that the surface energy of glide-symmetric TCIs depends on the surface orientation in a singular way via the parity of the Miller index. This singular surface energy of the TCI affects equilibrium crystal shapes, resulting in emergence of unique crystal facets of the TCI. This singular dependence of the topological surface states is unique to the TCI protected by the glide symmetry in contrast to a TCI protected by mirror symmetry.

In Chapter 8, we summarize this thesis and give an outlook of our theories of the bulk-boundary correspondence and the crystal shapes of the TCIs and the SOTIs.

List of Publications and Preprints

List of publications

5. **Yutaro Tanaka**, Tiantian Zhang, Makio Uwaha, and Shuichi Murakami,
"Anomalous Crystal Shapes of Topological Crystalline Insulators,"
Physical Review Letters **129**, 046802 (2022) (**Editors' Suggestion**).

4. **Yutaro Tanaka**, Ryo Takahashi, Ryo Okugawa, and Shuichi Murakami,
"Rotoinversion-symmetric bulk-hinge correspondence and its applications to higher-order Weyl semimetals,"
Physical Review B **105**, 115119 (2022).

3. **Yutaro Tanaka**, Ryo Takahashi, Tiantian Zhang, and Shuichi Murakami,
"Theory of inversion-$\mathbb{Z}_4$ protected topological chiral hinge states and its applications to layered antiferromagnets,"
Physical Review Research **2**, 043274 (2020).

2. **Yutaro Tanaka**, Ryo Takahashi, and Shuichi Murakami,
"Appearance of hinge states in second-order topological insulators via the cutting procedure," Physical Review B **101**, 115120, (2020).

1. Ryo Takahashi, **Yutaro Tanaka**, and Shuichi Murakami,
"Bulk-edge and bulk-hinge correspondence in inversion-symmetric insulators,"
Physical Review Research **2**, 013300, (2020).

Chapters 3, 4, 5, and 7 of this thesis are based on the author's publications 2, 3, 4, and 5, respectively.

List of preprints

1. Ren Sasaki, **Yutaro Tanaka**, and Shuichi Murakami,
"Systematic study for two-dimensional Z2 topological phase transitions at high-symmetry points in all layer groups,"
arxiv:2210.15974 (2022).