

Report of MERIT internship (domestic)

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Hirayama group, D1

MERIT 12-th

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1. Internship Overview

【Period】

1 November 2024 - 29 November 2024

【Host organization】

RIKEN Center for Emergent Matter Science (CEMS)

Quantum Matter Theory Research Group

Group Director: Akira Furusaki

【Research theme】

Topological phase transitions and Wilson loops in $C_{2z}T$ -symmetric insulators

2. Research Background

In recent years, research aimed at classifying electronic states in materials and describing their physical properties using the concept of topology in mathematics has garnered significant attention. A general classification theory based solely on the symmetry of the system has led to the discovery of numerous topological phases and their material realizations. However, the study of topological phases in spinless systems remains in its developmental stages. In particular, spinless topological insulators have been experimentally realized in artificial quantum systems such as photonic crystals, drawing attention as an unexplored frontier of topological phases. Nevertheless, no candidates for their material realization have yet been discovered.

A topological invariant that characterizes a spinless topological insulator is not universally defined for all insulators. Rather, it is defined only for systems that satisfy specific conditions related to the number of bands and their representations. These conditions vary depending on the type of topological invariant. For instance, the Euler class is defined exclusively for systems with two bands that respect $C_{2z}T$ symmetry as

$$e_2 = \frac{1}{2\pi} \int_{\text{BZ}} d\mathbf{S} \cdot \tilde{\mathbf{F}}_{12}$$

where $\tilde{\mathbf{F}}$ denotes the real antisymmetric Berry curvature. Spinless topological insulators characterized by the Euler class have received considerable attention due to phenomena arising from their inherent fragility and the unique behavior exhibited by band crossings protected by winding numbers. These distinctive features have prompted extensive theoretical studies to explore their fundamental properties, as well as experimental efforts to realize them in photonic lattices, metamaterials, and other artificial quantum systems.

To accelerate research on the Euler class, including the exploration of its material realization, this internship focused on developing a more efficient method for calculating the Euler class than

conventional approaches, which are typically based on Wilson loops. In addition, to deepen the general understanding of spinless topological insulators, we investigated systems in which multiple spinless topological invariants can be defined. Our efforts were directed toward deriving equations that relate these topological invariants and achieving a detailed understanding of the topological phase transitions that occur between trivial insulators and spinless topological insulators.

3. Research Content

The transformation properties of the real Berry curvature, which is used to define the Euler class, under symmetry operations such as rotations and mirror reflections in momentum space were analytically investigated. Based on this analysis, the conditions under which the Euler class is necessarily trivial and those under which it can become nontrivial were identified. For cases where the Euler class can be nontrivial, an analytical formula was derived that allows the Euler class to be calculated solely from the information of the occupied bands at high-symmetry points in most cases. While there are certain conditions under which this formula is not applicable, the topological and symmetry-related implications of these conditions were examined. Additional calculations were performed to extract as much topological information as possible from the information of the occupied bands at high-symmetry points.

For systems in which multiple topological invariants characterizing spinless insulating phases can be simultaneously defined, we derived analytical expressions for the relationships among these topological invariants. The derived equations were found to be consistent with the results of numerical calculations for previously established theoretical models. Furthermore, for new topological phases that had not been investigated in prior studies but were suggested by the present analytical results, two- and three-dimensional tight-binding models that realize these phases were constructed. The band structure and bulk topology of these models were numerically calculated. For the three-dimensional tight-binding models, gapless surface bands reflecting the nontrivial topology of the bulk were also numerically computed. Notably, some of the constructed three-dimensional models can be regarded as counterexamples to claims made in previous studies, and the implications of these results were discussed in detail. Through this investigation, we achieved a more detailed understanding of how individual topological invariants characterizing spinless insulating phases correspond to gapless surface states. In addition, we demonstrated that the process of topological phase transitions, which had previously been discussed separately for each topological invariant, can be understood in a consistent manner through relational equations that link these topological invariants.

4. Acknowledgements

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