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Outline of thesis

Over the decades, important roles of the relations between topology and symmetry in modern condensed matter physics have been recognized by the tour de force works. The importance of topology in condensed matter physics is recognized by the discovery of quantum Hall effect. Energy levels in the quantum Hall systems form quantized Landau levels and the systems insulating in bulk, but they host gapless conducting states localized at edges under a strong magnetic field in two-dimensional systems. Since these robust gapless edge states are protected by topology, unless the topological invariant known as the Chern number characterizing the quantum Hall states changes, we cannot adiabatically deform them to conventional quantum states for electrons in solids. Namely, topological invariants which are integrals of wavefunctions encode topology of a given system, and two systems with a different value of topological invariants cannot be continuously deformed to each other. The trigger to encourage researches on topological phases is the discovery of a Z_2 topological insulator. The Z_2 topological insulators which appear in the presence of time-reversal symmetry have attracted tremendous attention because of their unique and robust surface properties, and they are characterized by the Z_2 topological invariant, where anti-unitariness of time-reversal symmetry plays a key role. Realistic materials for the Z_2 topological insulator are shortly established by experiments in two-dimensional and three-dimensional systems. Physicists have focused on the relations between topology and symmetry, and they have classified various topological phases ensured by combinations of internal symmetries, such as time-reversal symmetry, particle-hole symmetry, and chiral symmetry.

Beyond internal symmetries, crystal symmetries of crystalline materials, such as spatial inversion, reflection, and rotational symmetries, play a fundamental role to understand such topological phases. An introduction of crystal symmetries has enriched our knowledge for topological invariants. For instance, the Z_2 topological invariant for the Z_2 topological insulator has a complicated expression when inversion symmetry is absent, while it is expressed as a simple formula as a product of parity eigenvalues at time-reversal invariant momenta when inversion symmetry is preserved. In addition, since the seminal proposal of a topological crystalline insulator, whose topological phase is ensured by crystal symmetries, various combinations of internal symmetry and crystal symmetries have turned out to give an immense list of new topological phases. In particular, the materials of the SnTe class are revealed to be mirror-symmetric topological crystalline insulators, and they are the first material realization for the topological crystalline insulators protected by crystal symmetries. Besides symmorphic symmetries, topological phases with nonsymmorphic symmetries have been vigorously discussed. Due to the nonsymmorphic nature, they host exotic surface states, such as Möbius or hourglass type. Furthermore, a new class of topological crystalline insulators, dubbed higher-order topological insulators, hosting gapless boundary states emerging in less than $d-1$ dimension for a d-dimensional bulk insulating system, has also been revealed.

The concept of topology was extended from gapped (insulating) states to gapless (metal or semimetal) states, so-called topological semimetal phases hosting gapless points or line nodes at generic momentum ensured by topological reasons. Studies on topological semimetal phases not only enriches our understanding for bulk topology but led us to new concepts of several exotic particles, such as Weyl (Dirac) fermions in a Weyl (Dirac) semimetal phase. Even though most of topological gapless points appear at a generic mometum, symmetry helps us realizing materials for topological semimetal phases. Moreover, topological nodal-line semimetals are closely associated with symmetries; mirror or glide symmetry, or inversion and time-reversal symmetries without spin-orbit couplings.

Superconductivity is also an ideal field to study topological phases since the band structures of superconductors have a gap or gapless nodes naturally, and some topological superconducting phases are predicted to exhibit Majorana fermions. Furthermore, there is no reason to restrict ourselves to electronic systems. A photonic crystal is one of the best playgrounds to investigate physics of topological materials. Because of exotic properties of bosonic systems, they have much potential for realizations and applications. In the similar context, we can also expand our arguments to magnons, phonons, and so on.

For comprehensive classifications of these topological phases, an approach based on the K-theory, which is a mathematical approach for gapped systems, has been adopted. By narrowing down our interest to space-group symmetry which crystalline systems belong to, a general formalism to determine whether a given crystallographic system is topologically trivial or nontrivial only from information of symmetry have been attracting research interest, such as topological quantum chemistry and symmetry-based indicators; in these approaches, topology of the bands and their compatibility relations are studied in the context of topological phases protected by space-group symmetries. Topological quantum chemistry gives minimal band connections from representation theory which an atomic insulator satisfies, and it has led us to a catalogue having all the topologically different connections. Symmetry-based indicators are particularly useful in diagnosing topologically distinct band structures from the combinations of irreducible representations at high-symmetry momenta. These approaches focus on different aspects of topological phases. In the K-theory approach, one can comprehensively classify nontrivial phases, whereas an explicit formula for a topological invariant does not follow immediately from the theory. On the other hand, the symmetry-based indicator can reveal only the topological phases characterized by combinations of irreducible representations. Thus, this theory cannot capture topological phases which cannot be known only from the irreducible representations. Thus even with these powerful tools, one cannot reach a full understanding of nontrivial topological phases protected by space-group symmetry, and there is much room for further investigation.

In the present thesis, we focus on the glide-Z_2 topological crystalline insulator without time-reversal symmetry. A glide operation is a product of a reflection and a fractional translational operations, and it is nonsymmorphic. Such topological phases are characterized by the Z_2 topological invariant and the Chern number associated with the normal vector of the glide plane. The nature of a Z_2 topology for the magnetic glide-symmetric systems is very different from that for the time-reversal-symmetric Z_2 topological insulators, ensured by the antiunitary property of the time-reversal operation, because of an absence of antiunitary symmetry in magnetic glide-symmetric systems. The reason we have been interested in this topological phase is as follows. First, glide symmetry yields Z_2 topological phases in systems with no internal symmetry whereas other symmetries can have (mirror) Chern insulating phases characterized by an integer topological invariant. Second, even though the first topological phenomenon in condensed matter physics was discovered in magnetic systems, namely the quantum Hall effect, there is still few proposals for magnetic topological materials because it is challenging to break time-reversal symmetry in electronic systems without significant spin-orbit coupling or by strong magnetic fields. Therefore, the more we understand this Z_2 topological phase with glide symmetry, the more we can deepen our knowledge for topological phases in magnetic systems and nonsymmorphic symmetry. Since the glide symmetry is contained in many space groups, this glide-symmetric topological crystalline insulator phase, ensured by the Z_2 topological invariant, can exist in many space groups as well.

To reach our goal, we first study phase transitions between the glide-Z_2 magnetic topological crystalline insulator and the normal insulator phases in spinless systems when glide symmetry is preserved in the phase transition. In general cases in such a phase transition, we find that a spinless Weyl semimetal phase should appear between two distinct topological phases, and the behavior of Weyl nodes is associated with the change of the glide-Z_2 topological invariant. We construct a general theory describing such a phase transition based on an effective model, and then support our scenario by performing numerical calculations. Next, we study topological phases when inversion symmetry is introduced in magnetic systems with glide symmetry, to see an intriguing interplay between topology and glide symmetry. If we add inversion symmetry, we show that the Z_2 topological invariant characterizing glide-symmetric systems can be solely expressed in terms of the irreducible representations at high-symmetry points in momentum space. In particular, we find that the glide-symmetric Z_2 magnetic topological crystalline insulator is directly related to a higher-order topological insulator ensured by inversion symmetry. We also construct all invariants which characterize topology of layer constructions for the systems with glide and inversion symmetries. This construction is solely based on real-space geometries of layers. We then show that these invariants completely agree with the set of topological invariants constructed from the topology in momentum space. Finally, we give a strategy for manipulation of the glide-Z_2 topological phase based on the relationship between space-group representations and band structures, and discuss its consequences in photonic crystals. We find that the irreducible representations at the particular high-symmetry point determine whether a given photonic crystal is topological or not, and by putting dielectrics at some of Wyckoff positions we can realize the band structure with a set of corresponding irreducible representations.

The organization in this thesis is the following. In Chapter 2, we warm up by reviewing the physics of Berry phase, connection, and curvature, band theory, symmetry and representations theory, and several topological phases of matter. Basically we focus on how the band structure can be affected by topology and symmetry, what makes topological phases different from trivial phases, how we can distinguish them, and what properties emerge. Chapter 3 is devoted to a theory for phase transitions that the Weyl semimetal phase emerges between the topologically trivial and nontrivial phases in spinless glide-symmetric magnetic systems. In Chapter 4, we study the fate of the glide-Z_2 invariant when inversion symmetry is added. We find that with this additional inversion symmetry, topological invariants are solely expressed from the irreducible representations at high-symmetry points in momentum space, both for a primitive lattice and a nonprimitive lattice. In Chapter 5, we construct real-space topological invariants by a layer construction in magnetic systems to support our results in Chapter 4, and we also construct simple tight-binding models exhibiting the glide-Z_2 topological phase and the Chern insulator phase. In Chapter 6, we argue topological photonic crystals ensured by glide symmetry and we propose a way to realize such a photonic crystal in the context of Wyckoff positions. We summarize our conclusions of the previous chapters in Chapter 7.

Publication List

1. Heejae Kim, Ken Shiozaki, and Shuichi Murakami
   Glide-symmetric magnetic topological crystalline insulators with inversion symmetry,
   Physical Review B **100**, 165202 (2019).

2. Heejae Kim and Shuichi Murakami
   Emergent spinless Weyl semimetals between the topological crystalline insulator and normal insulator phases with glide symmetry,
   Physical Review B **93**, 195138 (2016).
