論文の内容の要旨

Study of diagnostic methods of nodal line semimetals and an intrinsic link to topological crystalline insulators

（ノーダルライン半金属の判別手法とトポロジカル結晶絶縁体への接続に関する研究）

氏名　　立石　幾真

In this dissertation, we enhance the diagnostic method for nodal line semimetals in the case where spin-orbit coupling is negligible. We also show that the nodal line semimetals diagnosed by the present enhanced method ("δ indices") are linked to topological crystalline insulators when the spin-orbit coupling is introduced. This link reveals a clear difference between the topological crystalline insulator classes that have not been distinguished by the previous methods. Our result suggests that the obtained link can lead to the enhancement of the diagnostic methods for topological insulators and topological crystalline insulators.

In the derivation of the δ indices, we assume not only time-reversal and space inversion symmetries, which guarantee the stability of nodal lines, but also a four-fold rotation or four-fold screw symmetry. The δ indices are derived by considering a subgroup reduction of space groups and by applying the "symmetry-based indicator" defined in the space group with lower symmetry. With this approach, we give calculation formulas of the δ indices based on symmetry eigenvalues for each of the five Bravais lattices with a four-fold rotation or screw symmetry (i) primitive tetragonal lattice, (ii) body-centered tetragonal lattice, (iii) primitive cubic lattice, (iv) face-centered cubic lattice, and (v) body-centered

cubic lattice. By using the δ indices, we give three kinds of nodal line semimetals that are newly diagnosed by the δ indices: (a) face-centered cubic lattice (Ca, Ba, and SnSe), (b) body-centered square lattice (Ca_2As), and (c) nonsymmorphic tetragonal lattice (tight-binding model in the space group 127).

Based on the above examples of nodal line semimetals, we discuss to what kind of topological insulator class these nodal line semimetals are linked when spin-orbit coupling is introduced. By using k・p perturbation models, we show that these nodal line semimetals are linked to topological crystalline insulators by introducing spin-orbit coupling. In the examples (a) and (b), we show that a nontrivial mirror Chern number emerges on the mirror-invariant plane that is penetrated by the nodal lines before introducing spin-orbit coupling. It is also proved that the value of mirror Chern number corresponds to how many times the mirror-invariant plane is penetrated by the nodal lines. In particular, in the example (a), two types of nodal line configurations are realized depending on a parameter. We show that, by checking the differences in the nodal line configurations, it is possible to diagnose two different topological crystalline insulators classes that have not been diagnosed by the previous methods. This link between the nodal lines and the mirror Chern numbers is also confirmed in real materials, by comparing the results of first-principles calculations for Ca and Ba. In the example (c), on the other hand, we show that a characteristic configuration of nodal lines (concentric intersecting coplanar ellipses, CICE nodal lines), which appear due to the nature of the nonsymmorphic space group, is linked to a glide-protected topological crystalline insulator. In this case, we show that the CICE nodal lines correspond to the nontrivial glide topological invariants. This result suggests that by finding a nodal line semimetal with CICE nodal lines, we can find a topological crystalline insulator protected by the glide symmetry, which has not been diagnosed by the previous methods.