High-throughput screening for Weyl semimetals with S4 symmetry

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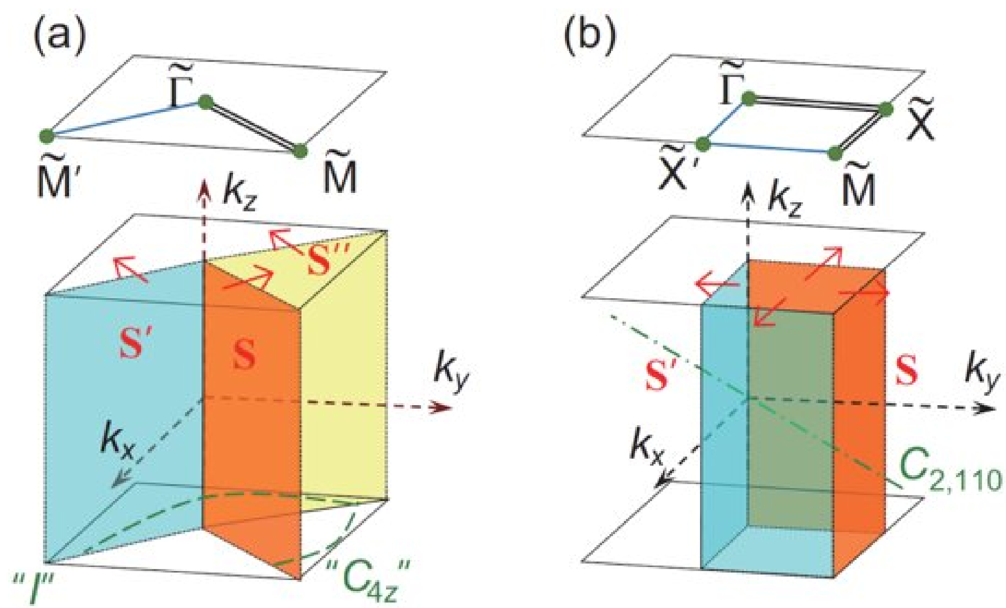

The definition of χ in systems with S4 symmetry on the orange surface S. The system in (b) has C2,110 symmetry. Credit: Science China Press

A new topological invariant χ is defined in systems with S_4 symmetry to diagnose the existence of Weyl fermions. By calculating χ, the computational cost for searching Weyl semimetals is greatly reduced. Recently, Gao et al. implemented this method in the high-throughput screening and found a lot of new Weyl semimetal candidates with exotic properties, providing realistic platforms for future experimental study of the interplay between Weyl fermions and other exotic states.

Using the symmetries of the systems, people can define various topological invariants to describe different topological states. The topological materials can be accurately discovered by calculating the topological invariants. Recently, researchers found that irreducible representations and compatibility relationships can be used to determine whether a material is topological nontrivial/trivial insulator (satisfying the compatibility relations) or topological semimetal (violating the compatibility relations), which leads to a large number of topological materials predicted by theoretical calculations.

However, Weyl semimetals go beyond this paradigm because the existence of Weyl fermions does not need any symmetry protections (except for lattice translation symmetries). At present, people usually take a very dense grid in the three dimensional Brillouin zone to search for Weyl fermions with zero band gap. Due to the large amount of computation required, this method is very inefficient. Therefore, it cannot be used to high-throughput search for Wey fermions. Considering the huge potential applications of Weyl semimetals, it is urgent to design a new algorithm or define a new topological invariant to search Weyl fermions accurately and quickly.

In a recent work published in *Science Bulletin*, Gao et al. proposed a new topological invariant χ in systems with S_4 symmetry, which can be used to diagnose the existence of Weyl fermions effectively. In addition, for magnetic systems, the nonzero χ can be revealed by the irreducible representations of occupied states on S_4 invariant k-points. Thus it greatly reduces the calculation cost for searching for Weyl fermions. It is worth noting that this new invariant χ works for both magnetic and nonmagnetic systems.

By applying this method to high-throughput screening in the firstprinciples calculations, the authors predicted a lot of new magnetic and nonmagnetic Weyl semimetals. The experimental observations have shown that these newly discovered Weyl semimetals possess many unique properties, such as magnetoresistance, superconductivity, and spin glassy states etc. These materials provide realistic platforms for future experimental study of the interplay between Weyl fermions and other exotic states.

More information: Jiacheng Gao et al, High-throughput screening for Weyl semimetals with S4 symmetry, *Science Bulletin* (2020). DOI: 10.1016/j.scib.2020.12.028

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