TopologicalNumbers.jl: A Julia package for calculating topological numbers

Keisuke Adachi[1,2*¶] **and Minoru Kanega**[2*¶]

1 Department of Physics, Ibaraki University, Mito, Ibaraki, Japan **2** Department of Physics, Chiba University, Chiba, Japan ¶ Corresponding author * These authors contributed equally.

DOI: 10.xxxxxx/draft

Software

- Review
- Repository
- Archive

Editor: Open Journals

Reviewers:

- @openjournals

Submitted: 01 January 1970
Published: unpublished

Summary

Recently, topological phase transitions have been of considerable interest in recent condensed matter physics. The topological number is a physical quantity that plays an important role in characterizing topological phase transitions in condensed matter physics. A typical example is the integer quantum Hall transition, where the quantized Hall conductivity can be calculated by the first Chern number, one of the topological numbers. Other topological numbers can be also calculated in various ways depending on each dimension and symmetry class. The quantization of such physical quantities is closely related to the concept of topology. However, the calculation of this topological number often requires numerical calculations. In addition, it may require an enormous amount of computation before convergence is achieved. Creating tools to easily calculate the topological numbers will lead to advances in condensed matter physics. In fact, several papers (Fukui et al., 2005),(Shiozaki, 2023) have been reported that suggest that some topological numbers can be computed efficiently. We have taken these papers as references and produced a package that easily and efficiently computes topological numbers.

Statement of need

`TopologicalNumbers.jl` is an open-source Julia package for computing various topological numbers. These numbers are very important physical quantities in the study of condensed matter physics. However, their calculation can be very computationally intensive. In addition, the computation of topological numbers is often not the essence of the study. Most researchers in the field of condensed matter physics calculate topological numbers as an assistance to their research. Therefore, this package is very useful and practical for them. The package is also useful for beginning students of condensed matter physics.

There are currently various methods for computing topological numbers, the first of efficient calculation methods was the Fukui-Hatsugai-Suzuki (Fukui et al., 2005) in 2005 for method of computing two-dimensional Chern numbers. In general, topological numbers are obtained by integrating the eigenstates of the Hamiltonian in the Brillouin zone, and this method can efficiently calculate them by discretizing the Brillouin zone, which is the integral range. This method can be useful in a practical computation for more complicated systems with a topological order for which a number of data points of the wave functions cannot easily be increased. Also, methods have been proposed to compute various topological invariants using this method. One is the method of (Shiozaki, 2023), which computes the Z2 numbers in two-dimensional with time-reversal symmetry in 2023. This method does not require any gauge fixing conditions and is quantized for any discrete approximation of the Brillouin zone. It is also used for methods to find Weil points and Weyl node (Hirayama et al., 2017),(Yang et al., 2011),(Hirayama et al., 2015),(Du et al., 2017) in three-dimensional.

There is no Julia package yet that comprehensively implements these methods. This package is easy for beginners to use because calculations can be done with a minimum of arguments. It is also easy for researchers to use because it is designed with many optional arguments so that it can be used for general-purpose calculations. It is designed to be more accessible and with clear documentation.

Mathematics

Citations

Figures

Acknowledgements

The authors are grateful to Takahiro Fukui for fruitful discussions. M.K. was supported by JST, the establishment of university fellowships towards the creation of science technology innovation, Grant No. JPMJFS2107.

References

Du, Y., Bo, X., Wang, D., Kan, E., Duan, C.-G., Savrasov, S. Y., & Wan, X. (2017). Emergence of topological nodal lines and type-II weyl nodes in the strong spin-orbit coupling system InNb x 2 (x = s ,se). *Physical Review B*, *96*, 235152. https://doi.org/10.1103/PhysRevB.96.235152

Fukui, T., Hatsugai, Y., & Suzuki, H. (2005). Chern numbers in discretized brillouin zone: Efficient method of computing (spin) hall conductances. *Journal of the Physical Society of Japan*, *74*, 1674–1677. https://doi.org/10.1143/JPSJ.74.1674

Hirayama, M., Okugawa, R., Ishibashi, S., Murakami, S., & Miyake, T. (2015). Weyl node and spin texture in trigonal tellurium and selenium. *Physical Review Letters*, *114*, 206401. https://doi.org/10.1103/PhysRevLett.114.206401

Hirayama, M., Okugawa, R., & Murakami, S. (2017). Topological semimetals studied by ab initio calculations. *Journal of the Physical Society of Japan*, *87*, 041002. https://doi.org/10.7566/JPSJ.87.041002

Shiozaki, K. (2023). *A discrete formulation of the kane-mele $\mathbb{Z}_2$ invariant* (No. arXiv:2305.05615). arXiv. https://doi.org/10.48550/arXiv.2305.05615

Yang, K.-Y., Lu, Y.-M., & Ran, Y. (2011). Quantum hall effects in a weyl semimetal: Possible application in pyrochlore iridates. *Physical Review B*, *84*, 075129. https://doi.org/10.1103/PhysRevB.84.075129