

TopologicalNumbers.jl: A Julia package for calculating topological numbers

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DOI: [10.xxxxxx/draft](https://doi.org/10.xxxxxx/draft)

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Submitted: 01 January 1970

Published: unpublished

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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 ([Du et al., 2017](#); [Hirayama et al., 2015, 2017](#); [Yang et al., 2011](#)) in three-dimensional.

There is no Julia package yet that comprehensively implements these methods. The basic topological numbers in this package can be calculated if only the Hamiltonian is given. The calculations can be performed with a minimum number of arguments, making them easy to use even for Julia beginners and beginning students of condensed matter physics. 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.

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