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TopologicalNumbers.jl: A Julia package for topological number computation

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.

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Summary

Topological insulators have been of considerable interest in the last decades (Hasan & Kane, 2010; Qi & Zhang, 2011). These materials show new states of matter that are insulating in the bulk but have conducting states on their surfaces. The conducting states on the surface are protected by the topology of the bulk band structure, and topological numbers, such as first Chern number, second Chern number, $\mathbb{Z}_2$ number, etc., are used to characterize them. As a typical example, the quantum Hall effect has the quantized Hall conductivity, which can be calculated by the first Chern number. Other topological numbers similarly become important physical quantities that characterize the system, depending on the system dimension and symmetry classes (Ryu et al., 2010).

To obtain the topological numbers, we often need numerical calculations, and it may require an enormous amount of computation before convergence is achieved. Therefore, creating tools to easily compute these numbers will lead to advances in research for the topological phase of matters. So far, several methods have been reported that suggest that some topological numbers can be computed efficiently (Fukui et al., 2005; Fukui & Hatsugai, 2007; Mochol-Grzelak et al., 2018; Shiozaki, 2023). However, since each method is specialized for a specific dimension or symmetry class, it is necessary to implement the algorithm for each problem, respectively. Our project, `TopologicalNumbers.jl`, aims to provide a package that can easily and efficiently compute topological numbers comprehensively in various dimensions and symmetry classes.

Statement of need

`TopologicalNumbers.jl` is an open-source Julia package for computing various topological numbers. This package currently includes various methods for calculating topological numbers. The first is the Fukui-Hatsugai-Suzuki (FHS) method for computing first Chern numbers in two-dimensional solid-state systems (Fukui et al., 2005). First Chern numbers are obtained by integrating the Berry curvature, derived from the eigenstates of the Hamiltonian, in the Brillouin zone. The FHS method enables us to compute the numbers efficiently by discretizing Berry curvature in the Brillouin zone. Based on the FHS method, several calculation methods have been proposed to compute various topological numbers. One is the method of second Chern number calculation in four-dimensional systems (Mochol-Grzelak et al., 2018). $\mathbb{Z}_2$ numbers can also be calculated in two-dimensional systems with time-reversal symmetry (Fukui & Hatsugai, 2007; Shiozaki, 2023). The FHS method is also applied to find Weyl points and Weyl nodes in three-dimensional systems (Du et al., 2017; Hirayama et al., 2015, 2018; Yang et al., 2011).

Currently, there is no comprehensive Julia package that implements all these calculation methods. Users can easily calculate topological numbers using these methods included in our package. In the simplest case, users only need to provide a function of the Hamiltonian matrix with wave numbers as arguments. Computations can be performed by creating a corresponding `Problem` and calling the `solve` function (`solve(Problem)`). The package also offers a `calcPhaseDiagram` function, enabling the computation of topological numbers in one-dimensional or two-dimensional parameter spaces by providing a `Problem` and parameter ranges (`calcPhaseDiagram(Problem, range...)`).

For the calculation of $\mathbb{Z}_2$ invariants, which require the computation of pfaffian, we have ported `PFAPACK` to Julia. `PFAPACK` is a Fortran/C++/Python library for computing the pfaffian of skew-symmetric matrices (Wimmer, 2012), and our package includes a pure-Julia implementation of all the functions originally provided. While `SkewLinearAlgebra.jl` exists as an official Julia package for computing pfaffians of real skew-symmetric matrices, `TopologicalNumbers.jl` is the first official package to offer a pure-Julia implementation for handling complex skew-symmetric matrices. Additionally, several utility functions are available, such as `showBand`/`plot1D`/`plot2D` for visualizing energy band structures and phase diagrams. We also provide various model Hamiltonians (e.g., `SSH`, `Haldane`) to enable users to quickly check the functionality and learn how to use these features. Moreover, the package supports parallel computing using `MPI.jl`. Consequently, `TopologicalNumbers.jl` is the first comprehensive Julia package for computing topological numbers in solid-state systems, and we believe that it will be useful for researchers in the field of solid-state physics.

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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 InNbX2 (x = s,se). *Phys. Rev. B*, *96*(23), 235152. https://doi.org/10.1103/PhysRevB.96.235152

Fukui, T., & Hatsugai, Y. (2007). Quantum Spin Hall Effect in Three Dimensional Materials: Lattice Computation of Z2 Topological Invariants and Its Application to Bi and Sb. *J. Phys. Soc. Jpn.*, *76*(5), 053702. https://doi.org/10.1143/JPSJ.76.053702

Fukui, T., Hatsugai, Y., & Suzuki, H. (2005). Chern Numbers in Discretized Brillouin Zone: Efficient Method of Computing (Spin) Hall Conductances. *J. Phys. Soc. Jpn.*, *74*(6), 1674–1677. https://doi.org/10.1143/JPSJ.74.1674

Hasan, M. Z., & Kane, C. L. (2010). Colloquium: Topological insulators. *Rev. Mod. Phys.*, *82*(4), 3045–3067. https://doi.org/10.1103/RevModPhys.82.3045

Hirayama, M., Okugawa, R., Ishibashi, S., Murakami, S., & Miyake, T. (2015). Weyl Node and Spin Texture in Trigonal Tellurium and Selenium. *Phys. Rev. Lett.*, *114*(20), 206401. https://doi.org/10.1103/PhysRevLett.114.206401

Hirayama, M., Okugawa, R., & Murakami, S. (2018). Topological Semimetals Studied by Ab Initio Calculations. *J. Phys. Soc. Jpn.*, *87*(4), 041002. https://doi.org/10.7566/JPSJ.87.041002

Mochol-Grzelak, M., Dauphin, A., Celi, A., & Lewenstein, M. (2018). Efficient algorithm to compute the second Chern number in four dimensional systems. *Quantum Sci. Technol.*, *4*(1), 014009. https://doi.org/10.1088/2058-9565/aae93b

Qi, X.-L., & Zhang, S.-C. (2011). Topological insulators and superconductors. *Rev. Mod. Phys.*, *83*(4), 1057–1110. https://doi.org/10.1103/RevModPhys.83.1057

The Journal of Open Source Software

Ryu, S., Schnyder, A. P., Furusaki, A., & Ludwig, A. W. W. (2010). Topological insulators and superconductors: Tenfold way and dimensional hierarchy. *New J. Phys.*, *12*(6), 065010. https://doi.org/10.1088/1367-2630/12/6/065010

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

Wimmer, M. (2012). Algorithm 923: Efficient Numerical Computation of the Pfaffian for Dense and Banded Skew-Symmetric Matrices. *ACM Trans. Math. Softw.*, *38*(4), 30:1–30:17. https://doi.org/10.1145/2331130.2331138

Yang, K.-Y., Lu, Y.-M., & Ran, Y. (2011). Quantum Hall effects in a Weyl semimetal: Possible application in pyrochlore iridates. *Phys. Rev. B*, *84*(7), 075129. https://doi.org/10.1103/PhysRevB.84.075129