Wroclaw University of Science and Technology

Faculty of Fundamental Problems of Technology

Prof. Dr. Hab. Maciej Maśka *[professor, Ph.D., postdoctoral degree holder]*
Institute of Theoretical Physics
Faculty of Fundamental Problems of Physics
Wroclaw University of Science and Technology

Review of the doctoral dissertation of Nguyen Minh Nguyen, M.Sc., entitled:

Topological and non-topological boundary states in SnTe and HgTe materials

The reviewed dissertation was prepared at the Institute of Physics of the Polish Academy of Sciences. The Ph.D. candidate's supervisor was Dr. Hab. Wojciech Brzezicki *[Ph.D., postdoctoral degree holder]*, also received guidance from Dr. Tim Hyart.

I will start the review in an unconventional manner, specifically with the conclusion: I believe that the dissertation of Nguyen Minh Nguyen, M.Sc., **meets the minimum** standards for doctoral dissertations. Throughout the remainder of the review, I will endeavour to explain the reasons behind this "**minimal**" assessment and elaborate on how and why it "**meets**" these standards.

As the title suggests, the reviewed doctoral dissertation concerns boundary states in SnTe and HgTe, both topological states and topologically trivial states. Most of the dissertation consists of introductions to issues such as: symmetries important in the topological context, Qi-Wu-Zhang or Bernevig-Hughes-Zhang models, the Kitaev's model with the physics of Majorana modes (Chapter 1), classification of topological insulators and superconductors, SnTe material models (Chapter 2), classification of gapless topological phases, two-dimensional superconductors with nodes in the gap (nodal superconductors), Weyl semimetals (Chapter 3), classification of higher order topological phases, second-order topological phases with reflection symmetry (Chapter 4). A significant portion of these introductions is knowledge from books or available in review publications. If these chapters contain the Ph.D. candidate's **original** results, they are difficult to find there. Of course, there are calculations and their results, but either all of them, or at least the vast majority of them, are recreations of things already known.

Chapter 5 begins with a presentation of the Ph.D. candidate's results. Unfortunately, this presentation is limited to two one-and-a-half-page introductions to two of the Ph.D. candidate's publications and statements by the co-authors regarding their participation

in these papers. This is followed by publications and a one-page summary and list of references.

The main body of the dissertation contains 94 numbered pages, which does not differ significantly from the typical volume of doctoral dissertations in physics. What is not typical, however, is the fact that these pages include 3 completely blank pages, 9 pages with statements of co-authors, and 29 pages of attached publications. In addition, there are many pages that contain one illustration with a caption. Thus, the effective volume of the dissertation is reduced to 50, at most 60 pages, aligning more closely with standard master's dissertations than doctoral dissertations. The "Law on Higher Education and Science" Act in Art. 187, sec. 3, states that *"A doctoral dissertation may constitute (...) a collection of published and thematically related scientific articles",* suggesting that the Ph.D. candidate likely took advantage of this possibility. Consequently, the remaining modest section, after deducting the aforementioned fragments, should be regarded as an introduction to the main part, which encompasses the appended articles. Typically, such an introduction should provide a slightly more comprehensive overview of the publications than the two brief one-and-a-half-page summaries presented. Moreover, although it is not explicitly specified in the regulations, it is customary in Ph.D. dissertations in physics to adopt a "staple" format when the number of achievements is slightly higher. However, it is important to note that both papers are relatively extensive, justifying the approach adopted in the dissertation. Given this interpretation, the introductory sections do not constitute the core of the dissertation, and owing to their introductory nature, I will omit their substantive assessment. However, in the final section of the review, I will revisit their format. The critiques mentioned above contribute to the earlier assertion that the requirements are only met to a **minimal** extent.

After these general remarks, I would like to move on to discussing the main part of the dissertation, which includes two publications by the Ph.D. candidate. The above-mentioned act requires that in the field of exact and natural sciences, the subject of a doctoral dissertation must be an **original solution to a scientific problem**. I affirm that these papers meet this requirement, and the attached statements of the co-authors and the fact that the Ph.D. candidate is the first author in both papers indicate his indispensable role in their creation. Therefore, I argue that the requirements for doctoral dissertations **are met**.

The first paper, *"Corner states, hinge states, and Majorana modes in SnTe nanowires"* (Phys. Rev. B **105**, 075310 (2022)), concerns the properties of SnTe-based materials, whose non-trivial properties, including topological properties, can be controlled including through doping or gate potentials. The paper

is devoted to examining how the Zeeman field, evaporation and inversion symmetry breaking lead to the formation of topological states in these systems. It begins by introducing the Hamiltonian in the tight-bond approximation. The system under consideration is an infinite nanowire with a square cross-section. The first case examined is the Zeeman field, which breaks the time reversal symmetry and several mirror symmetries. The paper shows that, depending on the field intensity and the nanowire thickness, a wide range of phases can be observed: the system can be in the state of a trivial insulator, a one-dimensional Weyl semimetal or an inverted band insulator, among others. The next chapter is devoted to hinge states. These are among the states whose presence is expected in higher-order topological insulators, i.e. those in which not only the interior is insulating, but also the walls. These states, topologically protected, are located along the edges. The paper shows that even in the absence of the Zeeman field, these states should exist in SnTe, which may make these materials interesting, e.g. for spintronics. The chapter also shows the presence of corner states. Using a detailed analysis of the system's symmetry, topological invariants characterizing these non-trivial states were defined. The next chapter analyzed the influence of superconductivity, which in the tested system can be induced, for example, by the proximity effect, i.e. after placing a nanowire on a superconducting substrate. Combining non-trivial topological properties with superconductivity is attractive due to the hopes related to topological quantum computers in which logical operations would be implemented by "weaving" non-Abelian objects. In this paper, the authors argue that SnTe may also be a promising material in this aspect. By introducing the Bogoliubov-de Gennes formalism, they show the existence of Majorana modes and determine phase diagrams defining the conditions under which topological superconductivity is possible. In particular, it was shown there that it is necessary to introduce a field that breaks the inversion symmetry so that the Majorana modes are localized and topologically protected, which is necessary for their possible practical application in quantum computers. The paper is written clearly, and five extensive appendices help to understand the calculations carried out in it. The discussion in the final part of the paper also includes proposals for experimental confirmation of the presence of the suggested non-trivial states. However, I would have two questions regarding the paper. An elongated geometry of the system is assumed there, but it has a finite width. In the cases studied, is this width so small that the orbital effects of the magnetic field, which were not taken into account in the calculations, can actually be neglected? Or does the very large gyromagnetic factor make the importance of orbital effects negligible compared to the Zeeman effect? The second question concerns correlation effects, also omitted from the calculations. How good is this approximation? It is known that in one-dimensional systems, weak shielding enhances the importance of the Coulomb interaction. Even a very weak interaction can change the nature of the system from a Landau liquid to a Luttinger liquid. There are suggestions (e.g. Phys. Rev. Lett. **116**, 026803 (2016)) that it may also play a role in SnTe.

The second paper included in the dissertation, *“Unprotected edge modes in quantum spin Hall insulator candidate materials”* (Phys. Rev. B **107**, 045138 (2023)), focuses on the derivation from first principles of effective Hamiltonians in the tight bond approximation for heterostructures that are candidates for materials exhibiting the quantum spin Hall effect. In particular, Hamiltonians for HgTe/CdTe, HgS/CdTe and InAs/GaSb are formulated and analyzed. The parameters of the “bulk” Hamiltonians, such as the hop integrals, energies at the nodes and the spin-orbit coupling amplitude, were determined by fitting tight-binding models to the band structures obtained using density functional theory methods. Then, “sandwiches” were constructed from layers of different materials, which are models of heterostructures with quantum wells. Studies of the band structures of these models have revealed the presence of additional edge states, albeit not topological states. The authors of the paper believe that the microscopic source of these states is the “buckled” lattice of anions and cations forming a honeycomb structure, which they consider an elementary block, serving as the basis for the construction of the studied heterostructures. For this purpose, they introduce approximations leading to a minimal model. This model is characterized by flat bands and it is their presence that causes the emergence of boundary states. Additionally, they show that these states are sensitive to the type of termination of the system, which may allow the use of potential at the edge of the system, for example by gating or doping, to remove these states from the energy gap. This work additionally ends with some appendices that allow to understand some of the technical details. In relation to this study, I would like to ask whether the Ph.D. candidate could, as he did in the case of the previous paper, propose an experimental verification of the existence of these states. I would also have a general question about both publications, namely what was done by the Ph.D. candidate in each of the papers? The dissertation contains statements from the co-authors specifying their participation, so it can be assumed that everything that is not included there was the work of the Ph.D. candidate. However, I would like to ask that this contribution is calculated as precisely as possible.

The dissertation concludes with a concise, one-page summary of the principal findings. Similar to the introductions of papers, it is regrettable that these summaries predominantly consist of references to content already presented in the papers. Providing a more expansive context for these results would be more advantageous.

Finally, I would like to return to the introductory section, i.e. the first four chapters of the dissertation. Unfortunately, I regret to say that it is written extremely carelessly. There are many more errors, both substantive and editorial, than in typical doctoral dissertations, which makes it much more difficult to follow the progress of the dissertation.

To conclude, as I wrote at the beginning of the review, despite significant shortcomings, I affirm that the dissertation meets the requirements set by the *“Law on Higher Education and Science”* Act. Therefore, I am requesting that the Ph.D. candidate be admitted to the subsequent stages of the doctoral process.

[illegible signature]
Maciej Maśka

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Wroclaw University of Science and Technology

Wybrzeże Wyspiańskiego 27
50-370 Wrocław

building A-1, room 234

Tel.: +48 71 320 25 79,
+48 71 320-23-95

dziekan.wppt@pwr.edu.pl
http://wppt.pwr.edu.pl

REGON *[National Business Registry No.]*: 000001614
NIP *[taxpayer ID No.]*: 896-000-5851
Bank account No.:
37 1090 2402 0000 0006 1000 0434