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

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

The doctoral dissertation of Nguyen Minh Nguyen, M.Sc., entitled "Topological and non-topological boundary states in SnTe and HgTe materials" contains comprehensive theoretical studies of the electronic properties of nanowires made of SnTe and two-dimensional heterostructures HgTe/CdTe, HgS/CdTe and InAs/GaSb/AlSb. All these materials belong to the group of so-called topological materials characterized by an unusual structure of electron systems, which are described using mathematical concepts taken from topology. The study of topological materials, initiated by the discovery of the total quantum Hall effect, has developed particularly in the last twenty years, mainly due to work on topological insulators, semimetals and superconductors. This thesis aligns with this extensive and presently very popular trend in the advancement of solid-state physics. The Ph.D. candidate presented two ambitious scientific issues. The first is the discovery of topological phases and associated boundary states in SnTe nanowires in the presence of a magnetic field and superconductivity. The second topic is finding the microscopic cause of the formation of non-topological edge states disturbing the quantum spin Hall effect in planar HgTe/CdTe, HgS/CdTe and InAs/GaSb/AlSb heterostructures. Both of these issues concern current and important problems for the further development of topological materials. There is also no doubt that these two research topics are difficult and their development required the Ph.D. candidate to have both the ability to use complex mathematical tools to describe the topological properties of materials and to conduct advanced numerical calculations of the band structure of one- and two-dimensional systems. The Ph.D. candidate's work on these issues under the supervision of both supervisors led to important results that made a significant contribution to the development of topological quantum structures, which were published in two scientific articles in the prestigious journal Physical Review B.

The doctoral dissertation consists of two parts preceded by an introductory chapter and concluded with a summary. The introductory chapter entitled "Motivation" contains a short introduction to topological materials and a justification for the undertaken scientific research on topological states in SnTe nanowires and HgTe/CdTe and InAs/GaSb/AlSb quantum wells. The author briefly presented various types of topological materials, focusing on crystalline topological insulators, which include SnTe and quantum spin Hall insulators discovered and studied in HgTe/CdTe and InAs/GaSb/AlSb heterostructures. The comprehensive examination of research advancements on these materials indicates that the subjects explored in the dissertation are thoroughly rooted and currently relevant. When presenting the history of the discoveries of topological insulators, on the first page, the author made two mistakes. The discovery of three-dimensional topological insulators was incorrectly attributed to the work of Hasan and Kane in 2010, while the discovery of two-dimensional topological insulators was credited to the work of Qi and Zhang in 2011. (Both of these papers have double numbers in the bibliography at the end of the dissertation. Unfortunately, the double numbering in the bibliography affects more articles.) In fact, two-dimensional topological insulators were discovered thanks to the theoretical work of Kane and Mele, as well as Bemevig, Hughes, and Zhang in 2005 and 2006, and were experimentally confirmed in HgTe/HgCdTe quantum wells by Kónig and colleagues in 2007. (The author mentioned these studies when discussing the quantum spin Hall effect.) Conversely, the theoretical prediction of three-dimensional topological insulators was made by Fu, Kane, and Mele, as well as by Moore and Balents in 2007. Subsequently, experimental confirmation in BiSb alloys was achieved by Hsieh and colleagues in 2008.

The first part of the dissertation, consisting of chapters one to four, is a thorough introduction to the topic of topological materials. It shows the foundation of knowledge on which the Ph.D. candidate based his own research. The first chapter entitled “Strong insulators and topological superconductors” begins with a discussion of non-spatial symmetries of Hamiltonians, i.e. time reversal symmetries, particle-hole symmetry and chiral symmetry, as well as canonical classes of Altland-Zimbauer symmetries, for which a classification of topological states in systems of different dimensions is presented. Then two models of two-dimensional topological insulators are presented: the Qi-Wu-Zhang model, describing the quantum anomalous Hall effect, and the Bemevig-Hughes-Zhang model, describing the quantum spin Hall effect. Topological indices are provided for both models, i.e. the Chem number for the Qi-Wu-Zhang model and the topological invariant Z_2 for the Bemevig-Hughes-Zhang model. Using these topological indices, topological phase diagrams were determined and examples of band structures for various topological phases were provided. The rest of the first chapter presents the Kitaev model describing a one-dimensional topological superconductor. Using the Bogoliubov-de Gennes approach, the topological invariant for this system was determined and the phase diagram was calculated. For the topologically non-trivial phase, unpaired zero-energy Majorana states were obtained in the open-edge system.

The second chapter is devoted to crystalline topological insulators. First, the classification of topological materials with reflection symmetries is discussed, with particular emphasis on crystalline insulators and topological superconductors.

The rest of the chapter deals with the bulk SnTe crystal, which is a crystalline topological insulator protected by reflection symmetries with respect to the (110) and (1-10) mirror planes. Using the tight-bonding Hamiltonian, the mirror Chern number was presented as a topological invariant for this material and the topological phase diagram was determined. For the crystalline topological insulator phase, the existence of surface Dirac cones on the (001) planes is shown, in accordance with the correspondence principle between volume and boundary for these materials.

Chapter three, entitled "Gapless topological phases," first discusses the classification of stable Fermi surfaces protected by nonspatial Altland-Zimbauer symmetries, and then presents two examples of gapless topological materials: a two-dimensional nodal superconductor and a three-dimensional Weyl semimetal. For both materials, appropriate topological invariants are given and the results of calculations of band structures containing topologically protected boundary states are shown.

The fourth chapter is devoted to the topological phases of higher orders. Using a generalized correspondence principle between the volume and the boundary of the system, nth-order topological phases are defined. Then, a two-dimensional superconductor was considered in a second-order topological phase, characterized by the presence of a pair of corner zero-energy Majorana states.

To sum up the first part of the dissertation, it can be stated that the Ph.D. candidate correctly discussed the electronic properties of basic types of topological materials, starting from strong insulators and topological superconductors, through crystalline topological insulators, gapless superconductors and semimetals, and ending with topological phases of higher orders. Topological invariants were presented for individual materials, phase diagrams and band structures for topological phases were calculated. The disadvantage of this section of the study includes several, albeit minor, errors and ambiguities that could have been easily eliminated through meticulous proofreading before submitting the dissertation. Moreover, the text exhibits stylistic deficiencies in various instances, accompanied by a considerable number of linguistic errors. In this review, I focus on substantial errors and present below a list of fragments in the first section of the dissertation that require correction or clarification.

1) On page 6, in formulas (1.1), the second Pauli matrix is multiplied by (-1).
2) On page 16, in Figures 1.4 (c)-(d), you can see small fluctuations in the energy gap near the topological phase transition. There is no explanation as to what causes these fluctuations.
3) There is a reference to Figure 1.2(d) on page 17 which is not included in the thesis.
4) On page 24, below formula (2.6), the AIII class is listed as a class without chiral symmetry, which does not agree with Table 1.1.

5) On page 25, line 5, the vague phrase “Cherna MZ_2 mirror numbers” is used.

6) On page 25, line 20, the abbreviation "TCIs" is erroneously used in the expression "which exist at any boundary between TCIs and TSCs". This expression should read "TIs" instead of "TCIs".

7) On page 28, Figure 2.2 (a) shows the energy gap divided by the parameter t_{12} as a function of the quotient of the parameters t_{11} and t_{12}. There is no explanation as to why the energy gap takes on non-zero values during a topological phase transition.

8) On page 32, the author first states that $d_{FS}=0$ for a Weyl semimetal, and in the next sentence he writes that d_{FS} is always positive. The statement that d_{FS} is always non-negative is correct.

9) On page 33, in formula (3.2), next to the symbol H’ there is an expression $k_y=0$, which requires explanation. Moreover, the right-hand sides of formulas (3.2) and (3.3) are the same, so the Hamiltonians H(**k**) and H’(**k**) are identical, which in turn makes formula (3.5) difficult to understand. Additionally, the phrase “Hamiltonian (3.4)” used by the author is unclear because formula (3.4) describes a topological index.

10) On page 39, the author incorrectly states that the conventional correspondence principle between a d-dimensional volume and a (d-1)-dimensional boundary applies only to crystalline topological insulators and not to strong topological insulators.

The second part of the dissertation, consisting of chapters five and six, contains a description of two of the Ph.D. candidate’s own research works. Each of these chapters consists of a short summary, an article published in the journal Physical Review B, and the authors’ statements, which clearly show that the contribution of M.Sc. Nguyen Minh Nguyen was instrumental in the creation of the article. The fifth chapter entitled “Corner states, hinge states, and Majorana modes in SnTe nanowires” contains an article by the Ph.D. candidate and both supervisors under the same title, which presents a comprehensive study of the topological quantum phases formed in SnTe nanowires in the presence of a magnetic field and superconductivity. Calculations of quantum states in nanowires were carried out using the tight binding method described in section II and appendix A. Section III discusses four topological phases formed in nanowires of different thickness in the presence of a Zeeman magnetic field, i.e.: (a) trivial insulator, (b) a one-dimensional Weyl semimetal characterized by localized hinge states, (c) an inverted band structure insulator having a non-trivial spin texture and corner boundary states, (d) a skewed semimetal having no corner boundary states. Section IV is devoted to hinge and corner states in one- and two-dimensional systems, which exist due to non-trivial higher-order topology. For the two-dimensional Hamiltonian, a topological invariant Z_2 was discovered, which precisely determines the formation of corner states. Section V concerns the Majorana states formed in SnTe nanowires in the presence of s-type superconductivity. Using the Bogoliubov-de Gennes approach, the authors of the article performed numerical calculations and conducted a theoretical analysis of the topological properties of the system, which clearly show that bulk Majorana modes can exist in nanowires constructed from SnTe when inversion symmetry is preserved, and when this symmetry is broken, topologically protected zero-energy Majorana states can be obtained at the ends of the nanowires.

Chapter six contains an article entitled “Unprotected edge modes in quantum spin Hall insulator candidate materials”, whose authors, apart from the Ph.D. candidate and supervisors, are three people, i.e. Giuseppe Cuano, Rajibul Islam and Carmine Autieri, dealing with *ab-initio* calculations of the band structure of topological materials. The main topic of this article is to investigate the microscopic cause of the formation of non-topological edge states in HgTe/CdTe, HgS/CdTe and InAs/GaSb/AlSb heterostructures. These unprotected boundary states can disturb the quantum spin Hall effect and therefore their thorough study is of great importance for the development of two-dimensional topological insulators, which was clearly presented in section I of the above-mentioned article. Section II describes the tight-binding model used to calculate two-dimensional volume states and one-dimensional boundary states in the studied heterostructures. The parameterization of three-dimensional tight-binding Hamiltonians was based on calculations of the band structure of electron systems for bulk semiconductors, carried out within the framework of density functional theory. Figures 3 to 5 clearly show the existence of non-topological edge states in HgTe/CdTe, HgS/CdTe and InAs/GaSb/AlSb heterostructures. Section III presents the so-called minimal model for the analyzed heterostructures. This model, characterized by a limited number of parameters, facilitates the exploration of the overarching properties inherent in these systems. The band structure of this model contains flat bands with non-trivial geometric Zak phases, leading to the accumulation of electric charge at the edges of the system. Sections IV and V illustrate, using the example of HgS/CdTe heterostructures, that the non-topological edge states in these systems stem from the flat bands within the minimal model. These states can be removed by adding an external electrostatic potential at the structure’s edge.

To summarize the second part of the dissertation, it can be certainly stated that the results presented therein constitute a significant contribution to the global advancement of research on topological materials. The author of the dissertation has demonstrated proficiency in utilizing advanced numerical and analytical methods for exploring the topological properties of quantum structures. It is noteworthy that there is a clear description of the theoretical models and a thorough analysis of the obtained results. However, a minor critique of this part of the dissertation pertains to an article presented in chapter six, where on page 6, in the first column, there is an incorrect reference to Figure 1(b), as a figure with this number is not included in the article.

In my assessment, the presented dissertation contains novel and important theoretical findings, making a significant contribution to the advancement of topological quantum structures. These findings were published in two articles in the prestigious journal Physical Review B and there is no doubt that the Ph.D. candidate played a dominant role in contributing to these publications. Therefore, despite the relatively numerous yet minor errors in its initial segment, this dissertation merits recognition. A particular strength of this dissertation lies in the adept integration of advanced numerical calculations based on the tight binding method and a comprehensive theoretical analysis of the topological properties of the tested materials. The use of this approach has yielded highly valuable and reliable theoretical results that have captured the attention of specialists worldwide.

Finally, I affirm that the dissertation by Nguyen Minh Nguyen, M.Sc., meets all the criteria outlined for doctoral dissertations in Art. 187 of the Act of 20 July 2018 - "Law on higher education and science" (Journal of Laws of 2020, item 85, as amended) and I hereby petition the Scientific Council of the Institute of Physics of the Polish Academy of Sciences for the admission of Nguyen Minh Nguyen, M.Sc., to the subsequent stages of the doctoral process.

[legible signature] ***Sławomir Paweł Łepkowski***

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