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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"

Topological insulators hold the potential for a revolutionary advancement in electron device technology owing to their unique properties related to the presence of surface or edge ballistic conduction channels while blocking electron transport in the bulk. The existence of low-dimensional surface states is forced, or as currently referred to, "protected", by the global topological properties of the band structure of a given material. Topology, in turn, is intricately linked to the global symmetry of the system. This situation motivates research on the relationships between the so-called topological invariants and ballistic quantum transport via non-trivial surface states. The basic issue is to determine whether non-trivial topological properties are a necessary and sufficient condition for the occurrence of "protected" surface states and what topological invariants should be considered as critical in this respect. Issues of this type are the axis of the reviewed doctoral dissertation. In particular, the subject of the dissertation is theoretical research on the electron properties of boundary states on the example of SnTe quantum wires and HgTe/CdTe quantum wells.

The dissertation was prepared at the Institute of Physics of the Polish Academy of Sciences under the supervision of Dr. Hab. Wojciech Brzezicki *[Ph.D., postdoctoral degree holder]* and Dr. Timo Hyart *[Ph.D.]* and is written in English. The introductory material, consisting of 17 pages numbered with Roman numerals, includes acknowledgments, an abstract in Polish and English, a list of abbreviations, a table of contents, and a list of figures and tables. The main part, covering a total of 94 pages, consists of six chapters and a summary and list of literature (101 items). The last two chapters contain, preceded by short introductions, reprints of two multi-authored articles published together with the supervisors in Physical Review B in 2022 and 2023. In both publications, Nguyen Minh Nguyen, M.Sc., is the first author, and the attached statement precisely defines his contribution to their creation. The structure of the work indicates that the main achievements are contained primarily in these two articles. From the reviewer's point of view, however, the dissertation constitutes an inseparable whole and is assessed as such.

The first four chapters introduce the elements necessary to understand the main theses contained in the articles and in the summary. They are quite short and do not fully fulfill their role, which I will refer to in the summary.

Chapter 1 is devoted to the discussion of the classification of topological insulators based on the occurrence of discrete symmetries not related to the crystal structure, such as time reversal symmetry, particle-hole symmetry and chiral symmetry, which are the basis for the standard division into ten basic classes. The author discusses the representative Qi-Wu-Zhang and Bernevig-Hughes-Zhang models. The presentation is illustrated with carefully prepared phase diagrams for these models in an appropriately selected range of parameters. Basically, the thesis focuses on systems of non-interacting electrons or, more generally, on systems described by one-electron Hamiltonians. As part of the extension to systems interacting in the mean-field approximation, there is a discussion of the so-called Kitaev model of so called Majorana modes in the presence of superconductivity, according to the Bogoliubov-De Gennes scheme. The topological characterization of superconductors based on the properties of the Bogoliubov-De Gennes Hamiltonian is convincingly illustrated with appropriate phase diagrams and band diagrams.

The next chapter discusses the properties of crystalline topological insulators on the example of systems based on SnTe, which constitute the basis of the first article included in the dissertation. Crystal symmetry, and in particular specular reflection, can modify the topological classification depending on the previously introduced symmetry elements by introducing additional topological invariants, such as mirror Chern numbers, etc. In this way, the correspondence between the topology of the bands in the interior and the states on the walls of the system is modified. For example, it turns out that a non-zero energy gap in a band of boundary states inconsistent with spatial symmetry does not necessarily indicate a trivial topology of the bulk band structure. Within the framework of the tight bond model, an example of a topological transition in a thick SnTe layer perpendicular to the direction (001) is presented. This example confirms the correlation between the value of the topological invariant and the appearance of an even number of Dirac cones on the boundary plane symmetrical with respect to the reflection plane.

The rest of the thesis (Chapter 3 titled “Gapless topological phases”) discusses the topological properties of the Fermi surface in materials with zero gap and given global symmetries. The topological classification of Fermi surfaces is related to their stability due to perturbations and is based on the well-known “ten-fold” classification of topological insulators due to different classes of extra-spatial symmetries. This classification can be carried out using topological invariants or by the construction of minimal Hamiltonians, which, depending on the imposed symmetry, allow or do not allow perturbations leading to the opening of a gap, thus allowing to distinguish topologically trivial from non-trivial cases. This approach is illustrated by the analysis of two standard model Hamiltonians relating to Weyl semimetals and nodal superconductors. In both cases, appropriate topological invariants were indicated, showing their connection with the closure of the energy gap in the bulk crystal. A correlation was also demonstrated between the internal Fermi points and the band structure of surface states. In particular, it was demonstrated how the presented four-band model with broken time reversal symmetry relates Weyl cones in the interior of the crystal to the formation of flat bands of surface states. The existence of a topologically stable Fermi surface in a bulk crystal can lead to the appearance of zero-energy bands on the crystal surface.

The short fourth chapter discusses higher-order topological phases, characterized by the occurrence of states in the energy gap located at the junction of the boundary planes. Their presence is forced by the topological properties of the band structure inside the material, which is characterized by a non-zero energy gap. For example, three-dimensional topological insulators can be considered which do not have zero-gap states on the surface, but have states propagating along the edges (“hinge” states) or located at the vertices. They can be protected by time reversal symmetry and crystal rotation symmetry, or by specular reflection. As an example, the model Hamiltonian proposed in ref [48] is discussed. In this model, the topological invariant belonging to the Z_2 class, responsible for the topological transition, was identified as the Pfaffian of a specific block within the Hamiltonian in the basis of the eigenstates of the reflection operator. Numerical calculations confirm the correlation of this invariant with the occurrence of the “hinge” states.

The first of two articles containing the main results of the dissertation is included in Chapter five and is entitled “Corner states, hinge states and Majorana modes in SnTe nono-wires”. Tin telluride, exemplifying a crystalline topological insulator, has been extensively studied in the literature. However, the exploration of the topological properties of quantum wires made of this material is notably lacking in comparison to the broader research on tin telluride. Taking up this topic in the article is therefore very timely. An attempt is presented to find mutual connections between the symmetry of the system and its topological properties represented by topological invariants. Within the framework of the tight binding model, possible mechanisms for generating various topological states by means of symmetry breaking were investigated. Breaking the time reversal symmetry by adding an axial magnetic field leads, among others, to the appearance of a one-dimensional Weyl semi-metal type phase protected by rotational symmetry around the wire axis and an insulator phase with an inverted band structure. Numerical calculations indicate the appearance of "hinge" states at the edges. Such states also appear without a magnetic field, which may indicate the existence of higher-order topological phases in SnTe. A topological invariant responsible for the occurrence of topologically protected vertex states was identified. The conclusion was that localized surface topological states and higher-order topological states can coexist in SnTe quantum wires. A striking statement was made that the $k \bullet p$ method, unlike the tight binding method, is unable to describe this system. The question arises: why should it be any different? In the segment devoted to the study of the Majorana mode in the superconducting state, it was shown that the inversion symmetry maintains the zero-gap Majorana mode throughout the entire volume of the wire, while its breaking may result in the zero-gap mode being located at the ends of the wire. This is an important tip for experimenters.

The last chapter contains an article entitled "Unprotected edge modes in quantum spin Hall insulator candidate materials". An attempt was made to analyze the heterostructures of HgTe/CdTe and HgS/CdTe. While these structures were incorporated into the realm of topological materials some time ago, the application of the tight binding method has yielded novel and unexpected results. It turns out that in the topologically trivial state of the system, edge states appear, which, for example in the case of HgS/CdTe, may enter the energy gap and affect the ballistic transport studied experimentally. These states can be removed by turning on a perturbation potential at the ends of the sample, so they are not topologically protected. An important result of this work is to relate the occurrence of these states to the presence of a flat zero-energy band in the ribbon geometry. This mechanism is elegantly illustrated using a minimal tight-binding model that considers only sigma bonds and neglects spin-orbit coupling and is associated with Zak phases for flat bands.

Moving on to the assessment of the dissertation, it should be emphasized, first of all, that the subject matter covered is extremely complex, but also very topical. Nevertheless, drawing from my past reviewing experiences, I expected that the introductory section (Chapters 1-4) would serve as a favorable preamble to the main body, namely the two aforementioned articles. To my dismay, this expectation was not met. The language and style employed in this section of the dissertation are subpar. Frequently, sentences lack a clear subject or predicate, and some sentences without verbs result in incomprehensible word clusters. As an example, we can mention the last sentence of subsection 1.2, or the text around equation (2.5), or the sentence „Thus, we open the Hamiltonian respect to n_z-direction to show the surface Dirac cones” (page 29). Numerous editorial errors are also noteworthy, such as the challenge in comprehending the reference and relation between equation (3.3) and (3.2). A similar problem arises in equation (4.1): the connection between k_1 and k_2 with k_x and k_y is unclear. However, it is essential to commend the exceptional quality of the charts produced.

My assessment of the main content encompassed in the articles incorporated into the dissertation is exceedingly positive, both in terms of presentation and their scientific significance. As previously highlighted, a noteworthy accomplishment of the Ph.D. candidate, presented in the initial article, is the identification of the potential emergence of higher-order topological states in SnTe quantum wires. Another important outcome is the investigation of the mechanism leading to the localization of topologically protected zero Majorana modes at the wire’s ends and the connection of this effect with inversion symmetry breaking. It is worth mentioning that this article, published last year, has already garnered 7 citations.

The most important achievement contained in the second article is the indication of the existence of non-topological edge states in HgTe/CdTe or HgS/CdTe heterostructures and the demonstration that this effect cannot be described based on model $k \cdot p$ type Hamiltonians. Since its publication in January this year, this article was cited three times.

In conclusion, I affirm that notwithstanding certain linguistic and editorial shortcomings in the first section, the submitted doctoral dissertation maintains a commendable scientific standard. The Ph.D. candidate has demonstrated substantial research maturity within the intricate domain of the physics of topological insulators.

In my opinion, the presented dissertation fulfills the standard criteria for a doctoral dissertation and aligns with the stipulations outlined in the Act of 20 July 2018 “Law on Higher Education and Science” (consolidated text: Journal of Laws of 2023, item 742). Consequently, I recommend the admission of Nguyen Minh Nguyen, M.Sc., to the subsequent stages of the doctoral process.

[illegible signature]

Warsaw, 4 December 2023 prof. dr hab. Witold Bardyszewski

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