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As a manuscript

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Study of the superconducting diode effect in superconductor/ topological insulator hybrid structures

Dissertation summary for the purpose of obtaining academic degree Doctor of Philosophy in Engineering

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Dissertation topic

Relevance

Superconducting electronics has become a steadily developing field of research from a relatively new direction. Due to its great application potential, as well as its ability to solve important problems in modern electronics, this area occupies a special place in modern science. In particular, one of these issues has recently become the search and development of a low-dissipative electronic component of the base. The key components of superconducting electronics are superconductors and superconducting structures. A superconductor is a macroscopic quantum object in which superconducting electrons (Cooper pairs) can be described by a single wave function. Thus, devices built on superconductors are systems that operate on quantum effects.

One of the objects of research in superconducting electronics is Josephson junctions. Two superconductors connected by a so-called weak link offer a fundamentally new functionality based on the tunneling of Cooper pairs through a non-superconducting intermediate material. In particular, Josephson junctions can be used as memory elements [1], qubits in a superconducting processor [2, 3], and also as key elements of a superconducting neural network [4]. In addition to Josephson junctions, hybrid structures operating on the proximity effect also have a wide range of potential applications in superconducting electronics and spintronics [5]. For example, superconducting hybrid structures in contact with ferromagnetic materials demonstrate a spin valve effect, making it possible to control superconductivity by tuning the parameters of the adjacent ferromagnet [6].

Semiconductor diodes are one of the fundamental electronic components that are widely used in modern electronics. However, semiconductor diodes are dissipative elements and silicon-based diodes can have high resistance at low temperatures, which in turn leads to energy losses and heating during their operation. Therefore, the quiet recently experimentally discovered diode effect in superconducting structures is capable of solving this problem. The superconducting diode effect operates at temperatures of the order of the superconducting transition, which is currently of the order of several Kelvin. In addition, superconducting diodes are quantum devices that are governed by certain symmetries and are described by the formalism of quantum mechanics. Such devices can be widely used in superconducting electronics, spintronics, quantum information, and communications technologies.

State of the art

The focus of this thesis is non-reciprocal electron transport in superconductors, i.e. the diode effect. The superconducting diode effect is becoming a rapidly developing area of research [7] and has enormous potential for applications in the fields of superconducting electronics [8] and spintronics [5]. This effect is analogous to the diode effect in classical electronics, except that instead of the usual electric current, a superconducting diode passes a superconducting current in a preferred direction, i.e., the current carried by the Cooper pairs. A superconducting diode is a non-dissipative element, that is, such a device does not dissipate heat. For the first time, the diode effect in a superconducting system was discovered experimentally in Nb/V/Ta superlattices [9]. Later, a series of theoretical papers were published, which proposed a theoretical description of the diode effect in distinct junction-free materials. It became clear that nonreciprocal superconducting transport can be obtained in systems with violation of time reversal and spatial inversion symmetries. The first condition can be achieved using an external magnetic field or the exchange field of a ferromagnet, and the second condition is satisfied in materials with spin-orbit interaction. In particular, superconducting devices based on materials with a topologically nontrivial band structure can typically exhibit significant spin-orbit coupling.

One of the promising platforms for realizing the superconducting diode effect is diodes based on topological insulators (TI) [10]. In TI based systems, such as Bi₂Te₃/FeTe and Bi₂Te₃/PdTe heterostructures in an external magnetic field, a significant nonreciprocity of the critical current was demonstrated [10, 11]. In such

structures, along with superconductivity, there is spin-orbit interaction due to the surface of the topological insulator Bi_2Te_3 . The TI surface provides a strong spin-orbit interaction, which makes it possible to demonstrate a significant magnetoelectric effect [12]. Particular attention was paid to the magnetoelectric effect in Josephson junctions based on TI materials, where it manifests itself in the form of the anomalous ground state phase shift [13].

The nature of the diode effect in systems with spin-orbit interaction can be explained by the so-called superconducting helical state [7]. A helical superconductor is characterized by a non-zero momentum of Cooper pairs, which leads to spatial modulation of the order parameter. In the case of a helical superconductor, the direction of the momentum of the Cooper pairs depends on the direction of the Zeeman field. The finite momentum of Cooper pairs, determined by the type of spin-orbit interaction and tied to the direction of the Zeeman field, leads to a non-reciprocal pairing current in various systems.

The superconducting diode effect in hybrid structures in the absence of an external magnetic field is also interesting to study, since providing an external magnetic field, as well as its control inside an electronic circuit, can be challenging in practice. The diode effect without an external magnetic field was studied experimentally in Josephson diodes based on Van der Waals structures, as well as in ferromagnetic heterostructures [14, 15]. While in Ref. [14] the diode effect arises due to asymmetric tunneling of Cooper pairs at the interface, in Ref. [15] the effect is realized through a combination of superconductivity, spin-orbit interaction, and exchange field. In the latter case, by changing the parameters of the heterostructure, it is possible to control the diode effect. Thus, the diode effect in hybrid structures represents a promising area for research.

Experimentally studied heterostructures based on ferromagnets most often represent complex systems. In addition, creating a material that is a superconductor with spin-orbit interaction and has an effective exchange field can be quite problematic from a technological point of view. Therefore, there is a need to study hybrid systems that operate on the proximity effect with well-controlled parameters.

The idea of the diode effect occurring in superconductors is not novel. Back in 1996, Edelstein, following his work on the magnetoelectric effect in superconductors with broken spatial inversion symmetry (polar superconductors) [16], demonstrated within the framework of the Ginzburg-Landau formalism that non-reciprocal transport can be obtained in the same systems [17]. However, only after recent experimental work on the detection of the diode effect, interest in this topic has sharply increased. Theoretical predictions for detecting the diode effect have been made for many various systems [7]. Such systems can be roughly divided into individual superconducting materials [18] and Josephson junctions [19]. While the nonreciprocity of the depairing current is implied in the first case, in the second the nonreciprocity of the Josephson critical current is referred to as a diode effect.

At present, investigating the diode effect is relevant due to its widespread use in the field of superconducting electronics. This topic has not been widely studied in the context of superconducting hybrid structures based on a topological insulator. The devices where the conditions for the diode effect are combined with the proximity effect are of particular interest. The mechanism leading to the emergence of non-reciprocal superconducting transport in such structures has also not been thoroughly studied. Moreover, the parameters affecting the diode efficiency are also not well studied. An important point in the study of the superconducting diode effect in hybrid systems based on a topological insulator is the examination of hexagonal warping of the topological insulator lattice on superconducting transport. Warping can be crucial when considering diode effect in some topological insulators.

The **purpose** of this work is to study the mechanism of the diode effect in superconducting hybrid structures based on a topological insulator, as well as to identify parameters that affect its diode efficiency and find ways to increase its efficiency for applied superconducting electronics and spintronics.

To achieve this goal, it is necessary to solve the following tasks.

- Investigate the features of the superconducting state in the superconductor/ferromagnet/topological insulator structure, where superconductivity and ferromagnetism are separated in space. In particular, examine the ground state of the superconductor in such a system for the implementation of a spatially modulated order parameter.
- Study the conditions for the occurrence of the superconducting diode effect in a hybrid superconductor/ferromagnet/topological insulator structure and identify the parameters that control the efficiency of the diode effect.
- Obtain analytical expressions relating diode efficiency to control parameters.
- Investigating the effect of hexagonal warping of the topological insulator lattice on superconducting transport in the superconductor/topological insulator/superconductor Josephson junction. Particularly, one of the tasks is to study the influence of hexagonal warping on the diode effect.

Main results

Methods

The methods used in the dissertation research will be the microscopic quasiclassical Green's function method to describe superconductivity in hybrid structures. This method is microscopic and has proven its reliability in the study of numerous phenomena in superconducting systems. Along with the quasiclassical formalism, the framework of the Bogoliubov-de Gennes equations will be used. The object of research is superconducting hybrid structures. The subject of the research is non-reciprocal superconducting transport.

Main results submitted for defense

The main statements of the research:

- 1. The ground state of the superconductor is helical in the superconductor/ferromagnet/topological insulator structure with some features. The order parameter is modulated in space by a finite momentum q, while the system has a nonuniform distribution of superconducting current density with zero total current. The sign of the momentum q depends on the direction of the exchange field in the ferromagnet.
- 2. In the superconductor/ferromagnet/topological insulator structure, nonreciprocal superconducting transport occurs, i.e. the diode effect. The nature of the diode effect is explained by the magnetoelectric effect, as well as the helical state realized in the hybrid structure. The efficiency of the diode effect is controlled by the parameters of the system (exchange field of the ferromagnet, width of the ferromagnetic and superconducting regions) and the proximity effect. The efficiency in such a system reaches several percent.
- 3. The Josephson diode effect that takes place in the superconductor/ferromagnet/topological insulator hybrid structure when considering hexagonal warping of the crystal lattice in a topological insulator has significant anisotropy under certain parameters. The possibility of controlling the diode effect by rotating the surface of a topological insulator is shown.

Scientific novelty:

- It has been demonstrated that the ground state of the superconductor is helical in the hybrid superconductor/ferromagnet/topological insulator system. The possibility of implementing a superconducting diode in such a structure has been demonstrated.
- The parameters that control the superconducting diode effect have been identified, and analytical relationships have been obtained for the efficiency of the diode in the superconductor/ferromagnet/topological insulator system.

• The anisotropy of the diode effect in superconducting hybrid structures with a topological insulator in the presence of hexagonal warping of the topological insulator Fermi surface has been demonstrated. Due to the anisotropy of the diode effect, significant control over the effect can be achieved under certain parameters.

Theoretical significance of the work

The theoretical significance of the dissertation work lies in expanding knowledge about the diode effect in topological hybrid structures. In this research we have determined the parameters that have impact on the diode effect. In particular, the parameters of the proximity effect were found to influence the effect. The constructed models can be used to describe the diode effect for thin layer hybrid structures. Moreover, the analytical expressions obtained to describe the efficiency of the diode complement the knowledge about the parameters affecting the efficiency. As a result of the work, a comparison of linear and nonlinear methods for calculating the nonreciprocity of the critical current was obtained.

Practical significance

The results obtained during the theoretical study can be used for further development of the theory of the diode effect in hybrid structures operating on the proximity effect. The obtained dependences of diode efficiency on various parameters of the hybrid structure can be useful in describing experimental data. Additionally, they can be used in the design of superconducting diodes to achieve better efficiency. Some conclusions obtained in the work, for example, the anisotropy of the Josephson diode effect, may serve as a basis for experimental research.

Reliability of the obtained results

The reliability of the results obtained is confirmed by the reliability of the methods used in the study. In addition, the results obtained are in agreement with the conclusions of the works of other authors who considered similar systems.

Author's personal contribution

The author of the thesis participated in the formulation of problems, construction of models for calculations, implementation of numerical algorithms for solving equations, as well as obtaining analytical results. The author also took part in the analysis and discussion of the results of this work.

Approbation of the results

The results of the dissertation research were presented by the author of the work at international conferences:

- XXVII International Symposium "Nanophysics and Nanoelectronics", report "Hybrid helicoidal state and superconducting diode effect in S/F/TI heterostructures", Nizhny Novgorod, March 11-15, 2023.
- 8th International Conference on Superconductivity and Magnetism-ICSM2023, report "Effects of a helical state on the dynamic properties of the topological superconducting systems", Turkey, Fethiye, May 4-11, 2023.
- 9th International Conference on Superconductivity and Magnetism-ICSM2024, report "Controllable topological superconducting diode", Turkey, Fethiye, April 27- May 4, 2024.

In addition to delivering talks at conferences, the author of the dissertation research reported the results at laboratory seminars, as well as at seminars at MIPT and Lebedev Physical Institute.

List of publications

1. Karabassov T., Bobkova I. V., Golubov A., Vasenko A. Hybrid helical state and superconducting diode effect in superconductor/ ferromagnet/ topological insulator heterostructures // Physical Review B: Condensed Matter and Materials Physics. 2022. Vol. 106. No. 22. Article 224509. Karabassov T., Emir Amirov, Bobkova I. V., Golubov A., Kazakova
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3. Karabassov T., Bobkova I. V., Silkin V. M., Lvov B. G., Golubov A., Vasenko A. Phase diagrams of the diode effect in superconducting heterostructures // Physica Scripta. 2024. Vol. 99. No. 1. Article 015010.

4. Karabassov T. Anisotropic Josephson Diode Effect in the Topological Hybrid Junctions with the Hexagonal Warping // JETP Letters. 2024. Vol. 119. No. 4. Article 308.

Dissertation structure

In the first part of the work (Appendix 1), the superconducting state in the hybrid superconductor/ferromagnet/topological insulator (S/F/TI) structure was studied. Such a hybrid structure is shown in Fig. 1(a). The superconducting region S is characterized by order parameter Δ , and the ferromagnetic region F is described by exchange field h. The paper considers a two-dimensional system in which the dispersion of quasiparticles is described by the dispersion of surface states of the topological insulator TI.

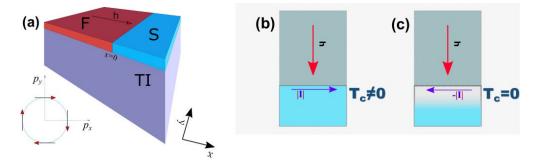


Fig. 1 - (a) Schematic geometry of an S/F bilayer on the surface of a topological insulator TI. (b)-(c) Illustration of the superconducting diode effect. The application of an external supercurrent along the interface in one direction occurs at a non-zero critical temperature (b); when the direction of the current is reversed, the superconducting state can be completely suppressed, since the critical temperature drops to zero (c).

In the S/F/TI hybrid structure, it was shown that the ground state of the superconducting part S corresponds to a helical state, in which the order parameter is characterized by a spatially modulated behavior $\Delta(r) = \Delta(x)e^{iq_s y}$, where q_s - momentum of the Cooper pair. This order parameter is realized even though superconductivity and the exchange field of a ferromagnet are spatially separated.

In the ground state, the momentum q_s depends on the direction of the exchange field *h* and is an odd function of *h*, which is a characteristic feature of the helical state. Next, we calculated the superconducting current density distribution and the total supercurrent through the hybrid structure. In the ground state, it was demonstrated that the supercurrent has a non-uniform distribution over the structure. However, the total supercurrent is zero. This situation is caused by a combination of the inverse magnetoelectric effect and superconductivity.

Then in the work we discuss the results for the diode efficiency, which is determined as follows:

$$\eta = \frac{I_c^+ - |I_c^-|}{I_c^+ + |I_c^-|},\tag{1}$$

where I_c^+ and I_c^- are critical supercurrents in opposite directions. It was shown how the efficiency depends on the S/F interface parameters γ and γ , i.e. parameters that describe the proximity effect. The γ parameter is proportional to the ratio of conductivities in the S and F parts and describes the strength of the inverse proximity effect. The γ parameter is proportional to the resistance at the S/F boundary and describes the mutual influence of the S and F regions. We also present some analytical results. In the limit of a thin S layer, it was found that the efficiency is inversely proportional to temperature and proportional to the exchange field.

To calculate the supercurrent in the hybrid structure, the nonlinear Usadel equation was used. The work also provides a comparison of efficiency calculations using the linearized Usadel equation (Appendix 2). It is shown that the two calculation methods, under certain parameters, provide only a small quantitative difference when calculating the diode efficiency. In order to get an idea of how the diode efficiency depends on the system parameters, phase diagrams of the diode effect in the S/F/TI system were constructed (Appendix 3).

In the last part of the dissertation research (Appendix 4), the effect of hexagonal warping of the Fermi surface of topological states on the surface of a topological insulator on superconducting transport, including non-reciprocal transport, was studied. For this purpose, a Josephson junction superconductor/topological insulator/superconductor (S/TI/S) in a Zeeman field was considered (See Fig. 2).

To construct a Josephson junction model, the formalism of the Bogoliubov– de Gennes equations in the tight-binding approximation was used. This method makes it possible to quite simply describe superconducting transport in such a system. To take into account the warping of the Fermi surface, it is necessary to add the corresponding term to the Hamiltonian of the system

$$H_w = \lambda k_x \left(k_x^2 - 3k_y^2 \right) \hat{s}_z \otimes \hat{\sigma}_z, \tag{2}$$

where λ is responsible for the degree of hexagonal warping, k is the momentum of the quasiparticle, \hat{s}_z and $\hat{\sigma}_z$ are the corresponding Pauli matrices in the spin and electron-hole spaces, respectively.

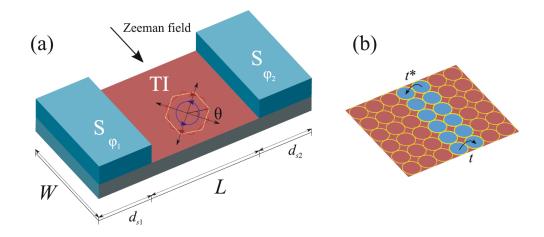


Fig. 2 – (a) Schematic representation of the Josephson hybrid structure. (b) Central region of the topological insulator surface in the tight-binding representation.

In order to understand how the warping will affect transport, the Fermi surface rotation angle θ is introduced, while making the angle finite, the Fermi surface is rotated in *k* space. In this case, by rotating the Fermi surface in *k* space we can calculate the supercurrent through the Josephson junction and study the effect of the finite angle on the transport.

The work showed that hexagonal warping affects the superconducting current and the current-phase relationships of the S/TI/S hybrid structure. In addition, anisotropy of the Josephson critical current with respect to the angle θ was demonstrated. Figure 3 shows a diagram for a possible experiment to observe the anisotropy effect of superconducting transport in a hybrid S/TI/S structure. In such a structure, the Josephson critical current between two opposite superconducting regions S can be measured, and the theory predicts an anisotropic critical current in the absence of the magnetic field and an anisotropic diode effect in the presence of the magnetic field.

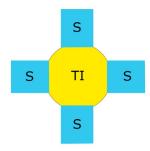


Fig. 3 – Scheme of a possible experiment to observe the anisotropy of the Josephson critical current, as well as the anisotropy of the diode effect.

Conclusion

In conclusion, we can highlight the main results obtained in this dissertation research.

• A review of the current state of the issue regarding the mechanisms of the superconducting diode effect, as well as experimental work in which the operation of the diode was performed.

- The features, advantages and disadvantages of existing materials and structures that have the property of nonreciprocal superconducting transport are determined. One of the most promising areas is the research and development of a diode based on topological insulators and ferromagnetism.
- The geometry of the hybrid structure of a superconducting diode superconductor/ferromagnet/topological insulator without an external magnetic field is proposed. A quasiclassical model of such a system in the diffusive regime has been constructed.
- It has been shown that in such a structure a helical state with some features is realized.
- Parameters that influence the efficiency of the diode effect have been identified. Thus, the diode effect is influenced by both geometric parameters and parameters of the proximity effect.
- Analytical relations were obtained in the limiting case of a smallwidth superconductor. The key factors controlling the efficiency of the diode have been identified: the size of the ferromagnetic region, as well as its exchange field.
- Phase diagrams have been constructed showing at what parameters the diode effect reaches its maximum values.
- In the Josephson diode superconductor/topological insulator/superconductor, significant anisotropy of the diode effect is demonstrated when taking into account the hexagonal warping of the crystal lattice of the topological insulator.
- Based on the anisotropic Josephson diode effect, a controlled superconducting diode is proposed.

The superconducting diode effect in hybrid structures is a promising direction for research due to its wide application potential. The diode effect in

hybrid superconductor/ferromagnetic/topological insulator structures allows for a controlled diode effect with controlled efficiency. In addition, the considered system does not require the application of an external magnetic field, which is a significant simplification for practical use. The dissertation research showed that by using various parameters of the hybrid system, better diode efficiency can be achieved.

Based on the results of the work done, directions for further research can be identified. In particular, it is important from the point of view of experimental implementation to study the influence of the gap between the superconducting and ferromagnetic parts in a planar superconductor/ferromagnet/topological insulator structure, since current technological capabilities do not always allow the implementation of an ideal superconductor/ferromagnet interface. In addition, based on this research, it is possible to theoretically study the possibility of controlling a superconducting diode by applying a potential difference, similar to the gate in a field-effect transistor. Such a system will make it possible to control the diode effect without the need to change the magnetizations of ferromagnetic regions.

Another promising direction for research is the study of dynamic phenomena in ferromagnet/topological superconductor systems.

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