NON-TRIVIALITY MATTERS

Examining the interplay between
s-wave superconductivity
and topological surface states

Marieke Snelder

Non-triviality matters

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and topological surface states

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NON-TRIVIALITY MATTERS
EXAMINING THE INTERPLAY BETWEEN S-WAVE
SUPERCONDUCTIVITY AND TOPOLOGICAL SURFACE STATES

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Contents

1	Introduction	1
1.1	Introduction	1
1.2	Braiding	2
1.3	Topological insulators	4
1.4	Majorana fermions and superconductors	6
1.5	Andreev bound states	7
1.6	Majorana mode in TI/S devices	8
1.7	Overview	9
2	Andreev bound states and current-phase relations in three-dimensional topological insulators	11
2.1	Introduction	11
2.2	The S/3DTI/S junction	12
2.3	Andreev bound states	14
2.4	Supercurrent	17
2.5	Signatures of 4π periodic ABS by means of Zener tunneling	19
2.6	Conclusions	21
2.7	Appendix: Eigenvectors and boundary conditions	22
3	Josephson supercurrent in a topological insulator without a bulk shunt	25
3.1	Introduction	25
3.2	Transport properties of exfoliated $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ flakes	26
3.3	Junction fabrication	29
3.4	Results	30
3.5	Discussion	33
4	Observability of surface Andreev bound states in a topological insulator in proximity to an s-wave superconductor	35
4.1	Introduction	35
4.2	Pairing wave function and Majorana-modes in nanowires	36
4.3	Pairing wave function in 3D topological insulators	42
4.4	Surface Andreev bound states and Majorana zero-energy modes . .	45
4.5	TI/STI tunneling conductance	48
4.6	TI/STI tunneling conductance with broken time-symmetry	49
4.7	Discussion and conclusion	51

5	Conductance spectroscopy of a proximity induced superconducting topological insulator	53
5.1	Introduction	53
5.2	Conductance measurements	56
5.3	Discussion	58
5.4	Noise measurements: initial results	62
5.5	Outlook beyond this thesis	66
6	Appendix: Tight binding model for a three dimensional topological insulator	69
6.1	Introduction	69
6.2	Tight binding model	70
6.3	Energy dispersion relations	72
6.4	The distribution of the wavefunction	75
6.5	Fitting STM data	76
6.6	Discussion and conclusions	77
	Bibliography	79
	Summary	93
	Samenvatting	95
	Dankwoord	99
	Publications	101

CHAPTER 1

Introduction

The search for a qubit immune to uncontrolled perturbations, has turned the relative new concept of topological insulators into one of the most active fields of research. It is theoretically predicted that the combination of a topological insulator and an s -wave superconductor can provide a stable building block for topological quantum computation. This chapter introduces the concept of topological quantum computation and how it is realized in topological insulator/superconductor heterostructures.

1.1 Introduction

The intensive study of condensed matter physics has increased our knowledge and allowed us to fabricate devices on the nanoscale. At this nanoscopic scale the behaviour of electrons and other particles start to deviate from classical Newtonian dynamics and are well-described by an alternative theory, quantum mechanics. Newton's third law in mechanics is then replaced by the Schrödinger equation to describe the quantum mechanical behaviour. The small dimensions of the devices nowadays provide novel opportunities to study quantum mechanics.

One particularly intriguing property of quantum mechanics is still challenging our understanding: a physical observable property of a quantum system is only determined when it is measured. Before the measurement, the system is described by a probability distribution of all the possible outcomes. Although we still do not know why the physical properties of particles are not known beforehand, a variety of (future) applications already relies on this property, for example quantum teleportation [1] and quantum computation [2, 3]. In the former example, the entanglement of two particles separated over a large distance is used to transport the property of a third particle. In quantum computation one uses the property that the quantum state is a superposition of the outcomes of a classical bit, a '0' and a '1'. This superposition makes the quantum bit (or qubit in short) more efficient than the regular bit for many purposes. The spin state is a promising candidate for realizing qubits [4], in which a spin up corresponds to the state $|1\rangle$ and spin down to the state $|0\rangle$. This qubit can, however, be easily disturbed by the environment such as a magnetic impurity. This disturbance can cause a switch from spin up to spin down and hence lead to computational errors. Topological quantum computation can prevent this type of problems. In topological quantum computation the total wavefunction of the qubit system is determined by the

Figure 1.1 (a) The propagation of a particle in two dimensions in the neighborhood of another particle. The particle is not returning necessarily to its original state after the round-trip. (b) Propagation of the same particle in three dimensions.

order in which particles are interchanged. This results in entanglement of the probability amplitudes of all the particles, making up the qubits [2, 3, 5–7]. Normally, the disturbance of a single wavefunction causes computational errors. In topological quantum computation the topology of the state of the system have to be changed, for example the order in interchanging the particles, to cause computational errors, making the entangled wavefunction more robust. The jargon for moving the particles around to perform a quantum computational operation is called braiding.

The combination of a topological insulator and a superconductor is one of the systems proposed to contain a state that can serve as a topological qubit [8]. The qubit is built out of two Majorana fermions. The field of topological insulators is new in condensed matter physics, as is their combination with superconductors. In order to create a useful Majorana state, one has to understand and control the physical properties at the interface between a topological insulator and a superconductor. This thesis is devoted to this topic. This chapter introduces the concept of braiding in topological quantum computation in section 1.2. We will briefly explain the concepts of topological insulators, Majorana fermions and Andreev bound states and how it relates to a topological qubit with statistics mentioned in section 1.2. Thereafter, we will discuss a theoretically proposed device to observe the Majorana fermion. It should, however, be noted that a more formal mathematical treatment is necessary to prove the statements made in this chapter. Finally, an overview of this thesis is given by the contribution of each chapter to this fast developing and exciting field.

1.2 Braiding

The formal definition of topology according to the encyclopedia [9] “*the study of the properties that are preserved through deformations, twisting, and stretching of objects. Tearing, however, is not allowed.*” From this definition an orange and a dish are topologically equivalent. But an orange is topologically different from a doughnut because an orange has to be torn open to create a hole in the middle to resemble the hole of the doughnut. In the same way, the traveled trajectories

Figure 1.2 (a) Four particles A, B, C and D are interchanged. First the particles at position A and B are interchanged followed by the particles now located at B and C. (b) Instead of interchanging the particles at location A and B first, we start with the particles at location B and C.

of particles can be topologically different from each other. This is the basis of the so-called anyonic statistics which are needed to create a qubit for topological quantum computation. In this section we will discuss the concept of anyons in more detail.

Consider two particles 1 and 2 in two spatial dimensions as drawn in Fig. 1.1(a). Particle 1 is moved to the position indicated by 1'. Thereafter it is moved back to its original position. If particle 1 encircles particle 2 it is not possible to deform the trajectory continuously without enclosing particle 2 in the area of the trajectory. This trajectory can be compared with the doughnut and is said to be non-trivial. The system does not have to return necessarily to its original state. The most general form to write this new state is $|\psi_{new}\rangle = |\psi_{original}\rangle e^{i2\theta}$. Particles that pick up a phase of θ when interchanged,* where $\theta \neq \{0, \pi\}$, are called anyons. Note, however, that interchanging anyons only results in multiplying the total wavefunction by a phase factor. To realize a qubit for topological quantum computation, the order of interchanging should also matter. To understand this, consider four particles at position A, B, C and D. First, we interchange particles A and B. Next, we interchange the anyons at location B and C. Particle D remains at the same position (Fig. 1.2(a)). Suppose, that instead of interchanging A and B first, we had started with B and C as depicted in Fig. 1.2(b). If the order of interchanging does not matter for the final total wavefunction then we end up with the same wavefunction multiplied by the same factor. However, if the order matters, then the phase factors picked up in the two situations differs. Assume now that we have eight particles where we interchange three of them as in the first case and the other three as in the second case. The interference of the wavefunctions will be different compared to the case where the order of interchanging does not matter due to the difference in phase picked up by the two sets of particles. Therefore, the total wavefunction can end up in another superposition of $|0\rangle$ and $|1\rangle$ states with different amplitudes

*The moving of particle 1 to 1' can be seen as an interchange of particle 1 and 2 by moving particle 2 towards position 1 and 1' to position 2. The full rotation can then be viewed as interchanging particle 1 and 2 two times.

(and not only a phase factor). In other words, we can define quantum operations by braiding the particles making up the qubits in a well-defined way.

In three dimensions the traveled path can also encircle particle 2 but it is always possible to deform the path such that the area of traveled trajectory does not enclose any other particle, just as the orange has no holes. One possible path where particle 2 is not enclosed by the area of the trajectory is shown by the dashed curve in Fig. 1.1(b). The traveled path in three dimensions is then said to be trivial and the particle returns to the same quantum state as before (assuming no magnetic field is present). Hence, to realize particles with anyonic statistics we need a two-dimensional system.

1.3 Topological insulators

The combination of an s -wave superconductor and a topological insulator is predicted to host a useful qubit to perform braiding operations. This particle is known as the Majorana fermion [8]. In this section we will explain the most important features of a topological insulator and its role in the formation of a qubit for topological quantum computation.

Three-dimensional topological insulators (3DTIs) are insulating in the bulk and have two-dimensional (2D) metallic surface states. The existence of metallic surface states is due to the strong spin-orbit coupling (SSOC) in the material which results in a band inversion. Fig. 1.3(a) shows the band structure of a normal insulator, which is topologically the same as the band structure of vacuum. This means that the two band structures can be continuously deformed into each other without closing the energy gap [10]. Fig. 1.3(b) shows the inverted band structure of a topological insulator compared to the normal insulator. The difference in band structure is indicated by the $\mathbb{Z}_2$ invariant which is 0 for the normal insulator and 1 for the topological insulator [6]. When a topologically trivial band structure (the normal insulator or vacuum) is connected to a non-trivial material (the topological insulator), the band structure cannot be continuously deformed into each other. Fig. 1.3(c) shows what happens at the surface of a TI when it is surrounded by a topologically trivial material. The form of the orange and the doughnut are drawn below the band structures. We have to close the band gap in order to change the order of the band structure. This closing of the gap is equivalent to cutting a hole in the orange and therefore the two band structures are said to be topologically different [10]. As a result, the topological insulator has metallic surface states. As long as the band order is reversed, the surface states are there. In the field of topological insulators it is therefore said that these surface states are topologically protected. The surface states have a linear dispersion relation where the spin is locked to the momentum due to the SSOC. Spin-orbit coupling can be viewed as an internal magnetic field in the topological insulator. It is well-known in quantum mechanics that a propagation of a particle in a magnetic field gives an additional phase which depends on the traveled path (think for example of the Aharonov-Bohm experiment). It can be shown that SSOC gives the two Majorana fermions (the qubit) in the

Figure 1.3 (a) Band order in a normal insulator. s indicates an s -wave atomic orbital and p a p -wave atomic orbital. (b) Due to SSOC the band order is inverted in a topological insulator. (c) When a topological insulator is connected to a trivial insulator or vacuum, the change from one band structure to the other causes a closing of the gap at the interface, leading to topologically protected surface states. (From our Dutch popular science article [11])

superconductor/topological insulator system an anyonic character where the order of interchanging determines the state of the wavefunction [2] (and references therein). The combination of a topological insulator and a so-called s -wave superconductor also provides the necessary p -wave superconducting correlations at the topological surface states to create a Majorana fermion. We will come back to this in section 1.4.

Other 2D or 1D systems with SSOC are, for this reason, also potential candidates for the realization of a topological qubit such as the semiconductors InAs and InSb [12–15]. In this thesis, we focus on the surface states of Bi-based 3DTIs. Strong evidence exists already for the existence of the topological surfaces in the Bi-based materials such as $\text{Bi}_{1-x}\text{Sb}_x$ [16], Bi_2Se_3 and Bi_2Te_3 [17]. The bottleneck with those materials is the presence of a large bulk contribution due to defects and impurities. The bulk contribution masks the topological properties of the surface states and should, therefore, be eliminated. To overcome this problem, the Se and Te atoms in these materials are replaced partly by other atoms to decrease the number of vacancies and defects. Materials such as $\text{Bi}_2\text{Te}_2\text{Se}$ [18–20] and $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_{3-y}\text{Se}_y$ [21] are examples of topological insulators where this atomic substitution is performed. The substitution of atoms resulted in relative high bulk resistivities.

1.4 Majorana fermions and superconductors

Majorana fermions were first proposed by Ettore Majorana in 1937 [22]. Theoretically, he predicted that there should exist a fermion that is its own anti-particle. This particle has not been found yet in particle physics but there are quasiparticle states in condensed matter systems that have the same characteristics as Majorana fermions. Superconductors are a logical starting point to search for Majorana fermions since the quasiparticles in superconductors are described as a superposition of electrons and holes. For a Majorana fermion we need a state that has equal electron and hole components. A state precisely in the middle of the superconducting gap will satisfy this condition [3].[†] However, not every Majorana fermion state is useful. If the wavefunctions of two Majorana's overlap, the particle and anti-particle can interact and, therefore, will annihilate. However, two isolated Majorana fermions can be used to create a qubit state which we will discuss in the following. Being in a state of half an electron and half a hole, two Majorana's can be described by a two level state where one corresponds to an empty (hole) $|0\rangle$ state and the other with the occupied (electron) $|1\rangle$ state. The Majorana mode is at zero-energy which means that there is no energy cost in occupying or emptying the state. In other quantum mechanical systems such as a particle-in-a-box we have to deliver a certain amount of energy to fill a level with an electron and get the same amount of energy back when we empty it. In the case of a ground state which contains the Majorana modes, we can just add and take away Majorana modes with no energy cost. The ground state is therefore degenerate and we can prepare the qubit system in any state as desired [2, 3, 5, 7].

There are different kinds of superconductors. In *s*-wave superconductors the superconducting gap is isotropic in space, just as an *s*-wave orbital band has a wavefunction that has the same phase and amplitude in every direction. Analogous to the *p*-wave atomic orbital, a *p*-wave superconductor has an anisotropic superconducting gap. He-3 and Sr_2RuO_4 are predicted to possess *p*-wave superconducting symmetry [26–33]. *p*-wave symmetry is of special interest for the creation of a Majorana zero-mode. It can be shown [34–36] that the additional phase shift between different directions in *p*-wave superconductivity, results in a zero-energy mode at the surface of a *p*-wave superconductor.[‡] A fruitful way to possibly observe a Majorana state is by studying the Andreev bound state spectrum in a superconductor/topological insulator Josephson junction.

[†]The term ‘Majorana fermion’ is often used in the field to denote this zero-energy state. It is a kind of misnomer. Ettore Majorana showed indeed that in principle there can be a fermion that is its own anti-particle, i.e. $\psi = \psi^*$. This relation is satisfied in the middle of the superconducting gap. However, this relation holds only for the Dirac equation in the Majorana representation. In all other representations, the condition for a Majorana fermion is $\psi = U\psi^*$ where U is a unitary matrix [23, 24]. In that sense, all Bogoliubov quasi-particles in superconductors are Majorana fermions [25]. Moreover, the zero-energy state scientists are looking for is not even a fermion but an anyon. However, we will keep to this nomenclature to be consistent with the literature.

[‡]In Chap. 4 we will show in more detail how *p*-wave superconductivity is realized in an *s*-wave superconductor/topological insulator system and how a zero-energy mode appears.

Figure 1.4 (a) The energy spectrum in the semiconductor picture. A hole branch and electron branch interact with each other so that a gap is opening which is 2 times the superconducting gap Δ . The Cooper pairs are at the chemical potential μ . (b) In the formation of Andreev bound states in a superconductor (S)/normal metal (N)/S Josephson junction, Andreev reflection has to be taken into account. (c) The Andreev bound states for an SNS junction with length smaller than the coherence length. For a transmission smaller than 1 a gap is opening at a phase difference of π .

1.5 Andreev bound states

In BCS theory [37], developed by Bardeen, Cooper and Schrieffer, the s -wave superconducting state is described as an interaction between electrons with wavefunction f and holes with wavefunction g according to the equations [38]

$$\left[-\frac{\hbar^2}{2m} \nabla^2 - \mu + V \right] f + \Delta g = i\hbar \frac{\partial f}{\partial t}, \quad (1.1)$$

$$-\left[-\frac{\hbar^2}{2m} \nabla^2 - \mu + V \right] g + \Delta f = i\hbar \frac{\partial g}{\partial t}, \quad (1.2)$$

where V is a constant potential and Δ the superconducting gap. The corresponding energy spectrum is shown in Fig. 1.4(a).

A weak link between two superconductors is called a Josephson junction. This weak link can be a normal metal, insulator or a point contact [39]. Electrons close to the Fermi level are “trapped” in a potential well where the barrier height is given by the superconducting gap. Similar to a quantum mechanical model of a particle-in-a-box, only discrete energy levels are allowed. In a normal potential well we consider only single electrons that can be reflected at the potential wall. In the case of a superconductor we also have to take into account Andreev reflection which is the reflection of an electron into a hole or vice versa in the weak link and the transfer of a Cooper pair in the superconductor (S) as depicted in Fig. 1.4(b). The resulting discrete energy states are known as Andreev bound states (ABSs). The energy spectrum is shown in Fig. 1.4(c) and given by the formula [40]

$$E_{ABS}^{\pm} = \pm \Delta \sqrt{1 - \tau \sin^2 \left(\frac{\phi}{2} \right)}, \quad (1.3)$$

where τ is the transmission probability of the junction and ϕ is the phase difference between the leads. At low temperatures only the lowest branch is occupied. We see from this branch that after a phase change between the superconductors of 2π we return to the same state again. It is said therefore that a Josephson junction is 2π periodic.

When a p -wave superconductor is used instead of an s -wave superconductor, an additional phase shift is picked up due to the phase difference of the superconducting gap in specific directions similar to the p -wave orbital. In a p -wave superconductor the right moving Cooper pairs are shifted by a phase π compared to the left moving Cooper pairs. This phase shift is also picked up by the electrons in the normal metal when they are Andreev reflected. At first glance, the Andreev bound states of S/normal metal (N)/S and S/3DTI/S junctions may look similar, but the exact details are rather different.

1.6 Majorana mode in TI/S devices

In this section we will discuss shortly the properties of the ABS of a S/3DTI/S Josephson junction as discussed by Fu and Kane in Ref. [8] in order to observe the existence of a Majorana mode in superconductor/topological insulator devices [8]. The device is depicted in Fig. 1.5(a).

In Fig. 1.5(b) the Andreev bound spectrum for a S/3DTI/S Josephson junction is shown. On first sight, this looks the same as the Andreev bound state spectrum of a S/N/S junction as discussed in the previous section with a τ equal to 1. We will discuss the Andreev bound states of the two in more detail to clarify the differences between the two. As discussed in section 1.4, the qubit state consisting of two Majorana fermions could be either empty or occupied. The state is therefore degenerate with two eigenvalues where one eigenvalue corresponds with an occupied state (odd parity) and the other with an empty state (even parity). The dashed and solid branch in Fig. 1.5(b) correspond to the odd and even parity branch of this qubit state respectively in the S/3DTI/S Josephson

Figure 1.5 (a) Superconductor Josephson junction of an *s*-wave superconductor and topological insulator. The phase difference between the superconductors is ϕ . (b) Andreev bound state for superconductor/topological insulator Josephson junctions. (After [8])

junction. As the branches correspond to different eigenvalues, they are orthogonal and no interaction takes place. That means that instead of a phase change of 2π we have to change the phase by 4π in order to return to the original state [41]. We say, therefore, that the periodicity compared to a normal Josephson junction is doubled. In the normal Josephson junction both branches correspond to even parity eigen values [42]. The observation of this doubled periodicity is, therefore, a hallmark of the existence of Majorana modes in condensed matter systems.

1.7 Overview

As mentioned in the first part of this chapter, in order to realize the creation, detection and manipulation of the Majorana modes in the 3DTI/S systems, we have to understand first the influence of an *s*-wave superconductor on the topological surface states in more detail both theoretically and experimentally. This study should lead to a better picture of how to observe the Majorana mode and isolate them from other interactions that can mask their properties in experiments. Experiments should be performed in order to understand the S/3DTI interaction at the interface as the proposed models consider an ideal system with smooth interfaces.

In Chapter 2 we start with a detailed theoretical modelling study of ABSs and 4π periodicity in a 3D topological insulator/superconductor junction. We also model the effect of a ferromagnet on top of the TI in order to break time-reversal symmetry and its influence on the appearing of a 4π periodicity. From this study we make the important conclusion that the 4π periodicity is merely due to a single channel. In order to eliminate the other channels as much as possible, it is therefore necessary to fabricate small superconducting electrodes and to be able to gate tune the Fermi level. We will see that a ferromagnet can also be used to increase the 4π periodic signal.

Inspired by the conclusions of Chapter 2, Chapter 3 discusses the experimental realization of a Josephson junction on the 3DTI $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ (BSTS) with neglectable bulk conduction. The superconducting electrodes have a width of 40

nm in order to anticipate on future experiments to bring the device in a single channel regime to observe the doubled periodicity of the ABSs. The realization of the Josephson supercurrent shows that there is an interaction between the niobium *s*-wave superconductor and the topological surface states.

In Chapter 4, we study the superconducting correlations present at the *s*-wave superconductor/3DTI interface. We discuss different regimes and study the corresponding tunneling conductance spectra to determine the distinguished features of the *p*-wave superconducting correlations at the interface. Chapter 5 shows the results of the conductance spectra on Au/BSTS/Nb devices which are fabricated to investigate if the needed *p*-wave correlations can be observed. We end the chapter with an outlook on future experiments.

The thesis ends with an appendix that deals with a tight binding model to predict the necessary parameters needed for a 3D topological insulator thin film to turn it into a 2D topological insulator due to quantum confinement and interaction between the bottom and top surfaces. The presence of only edge state channels should make the observation of the 4π periodicity easier as there is no contribution from other topological channels with a 2π periodicity.

CHAPTER 2

Andreev bound states and current-phase relations in three-dimensional topological insulators

To guide the search for the Majorana fermion, we theoretically study superconductor/topological-insulator/superconductor (S/TI/S) junctions in an experimentally relevant regime. We find that the striking features present in these systems, including the doubled periodicity of the Andreev bound states (ABSs) due to tunneling via Majorana states, can still be present at high electron densities. We show that via the inclusion of magnetic layers, this 4π periodic ABS can still be observed in three-dimensional (3D) topological insulators, where finite angle incidence usually results in the opening of a gap at zero energy and hence results in a 2π periodic ABS. Furthermore, we study the Josephson-junction characteristics and find that the gap size can be controlled and decreased by tuning the magnetization direction and amplitude. These findings pave the way for designing experiments on S/3DTI/S junctions.

2.1 Introduction

The prediction of Fu and Kane [8] that Majorana fermions can be realized in superconductor–three-dimensional (3D) topological insulator structures, boosted theoretical predictions for the peculiar Majorana fermion properties [6, 7, 43–45]. Much progress has been made in the fabrication of two-dimensional [46–49] and three-dimensional topological insulators [16, 17, 49–55]. Recently, the three-dimensional topological insulators (TIs) based on the Bi compounds (e.g., Bi_2Te_3 , Bi_2Se_3) have already led to the realization of superconductor(S)/TI/S junctions [56–61] and superconducting quantum interference devices (SQUIDs) [62, 63]. From an experimental point of view it is difficult to realize topological-insulator materials with the chemical potential at or close to the Dirac point. It is therefore highly desirable to have a guiding theory in an experimentally relevant regime that can pave the way towards the verification of the Majorana fermion in S/TI hybrids.

Here we theoretically study superconductor/three-dimensional topological insulator Josephson junctions. In the calculations of Refs. [8, 44, 64–66], it is assumed that the Fermi level is close to the Dirac point. In addition, it is always assumed that the ferromagnet placed on top of a TI has a magnetization

Figure 2.1 (a) Schematic drawing of a topological insulator (TI) with a superconductor (S) and ferromagnet (F) on top. We consider the bound states at the surface of the TI with the proximity effect from both the superconductor and ferromagnet. (b) The energy dispersion at the TI surface (left) and at the S side (right). DP indicates the Dirac point. Here the case is shown without a F and with an incoming electron at the right interface.

$|M| > \mu$ in these calculations. In these systems, an Andreev bound state (ABS) with a doubled periodicity is predicted. We consider the experimentally relevant regime of high electron densities, and show that despite the chemical potential μ being situated far away from the Dirac point, this characteristic feature is still present. We furthermore consider the presence of a ferromagnetic layer with magnetization $|M| < \mu$ on top of the junction, and show that it can drastically alter the Josephson characteristics, even when $(|M|, \Delta) \ll \mu$. This is particularly interesting since the magnetization opens a gap not at the Fermi energy, as the superconducting correlations do, but at the Dirac point, far away from E_F . We show that a gap in the superconducting bound-states spectra always opens at a finite angle of incidence. However, the size of this gap can be tuned and decreased, and can, in principle, vanish by increasing the perpendicular magnetization amplitude.

The discussion of the bound states of a S/TI/S junction in this chapter is organized as follows: first we study the case without a ferromagnetic layer on top of the TI. Then we discuss the bound states with a ferromagnet. We will see that a 4π periodic Andreev bound state is still present in the 3D case, but only for one channel. This 4π periodic ABS is a feature of the presence of Majorana fermions. We show the supercurrent obtained by the bound states and discuss the observation of a 4π periodic ABS in a 3D topological insulator.

2.2 The S/3DTI/S junction

The configuration of the junction we consider is shown in Fig. 2.1(a). In the Nambu basis

$$\Psi = (\psi_1, \psi_l, \psi_1^\dagger, \psi_l^\dagger)^T \quad (2.1)$$

the Hamiltonian with a superconducting and magnetic proximity effect is [66]

$$H = \begin{pmatrix} H_0(\mathbf{k}) + M & \Delta(\mathbf{k}) \\ -\Delta^*(-\mathbf{k}) & -H_0^*(-\mathbf{k}) - M^* \end{pmatrix}, \quad (2.2)$$

where

$$H_0(\mathbf{k}) = v_F(\sigma_x k_x + \sigma_y k_y) - \mu_j, \quad M = \mathbf{m} \cdot \boldsymbol{\sigma}, \quad (2.3)$$

with M being the magnetization due to the ferromagnet and $\mathbf{m} = (m_x, m_y, m_z)$ being the exchange field. σ_i are the Pauli matrices and the index j of the chemical potential is S in the superconducting part and TI in the topological insulator. From this Hamiltonian, we calculated the eigenvectors of the TI in the presence of the proximity effects. We assume the superconductor to be an s -wave superconductor, $\Delta(\mathbf{k}) = \Delta e^{i\phi_S}$, where ϕ_S is the superconducting phase and $\Delta = 0$ outside the superconductor. This Heaviside function of the order parameter simplifies the calculations. However, it is not expected that there will be a qualitative difference with the results when a self-consistent order parameter is used, as, for example, is shown in Ref. [67] for a d -wave superconductor where the induced order parameter is taken into account in the normal metal, and the Andreev bound-state spectrum does not change near zero energy. It is this regime in the spectrum that is relevant for the appearance of a Majorana mode.

The nonsuperconducting part can be under the influence of a ferromagnetic proximity effect. In Majorana devices, the magnetization is taken perpendicular to the TI surface, $M = m_z \sigma_z$ (the resulting eigenvectors are listed in the Appendix). Magnetization parallel to the interface causes only a shift in the wave vector but does not open a gap. In the known topological insulators, the Dirac point is in the middle of the band gap or close to the valence band. The chemical potential is usually close to the conduction band as the topological insulators based on Bi compounds are not really good insulators yet. Therefore, the chemical potential $\mu_{TI,S}$ is much larger than the superconducting gap in experiments. In this case, we have only normal Andreev reflection at the interface and no specular Andreev reflection [68].

For most proposals, it is desired to have a ferromagnet on top of the TI (preferably an insulator so that practically no current flows through the ferromagnet) [44, 64–66]. We estimate here how much the gap at the Dirac point can be opened by such a ferromagnet. For a magnetic moment of $n\mu_B$ per unit cell of size a^3 , where n is an integer and μ_B is the Bohr magneton, we can estimate the value of the $m_z \sigma_z$ part of the Hamiltonian. By making the assumption that the atoms can be approximated by spheres with n elementary dipoles and perfect coupling to the TI, we estimate that the opened gap will be about $0.0002n/a^3$ eV, where a is in Ångström. This value is typically smaller than the value of the Fermi energy inside the gap (> 0.05 eV). We therefore study the relevant regime of $m_z < \mu_{TI,S}$.

With these assumptions, we solve the Andreev and normal reflection coefficients at both left and right interfaces for incoming electrons and holes by matching the wave functions at the interface. Following Kulik [69] (see example in Ref. [40]), the wave function in the topological insulator can be written as

$$\psi = a\psi_e^+ + b\psi_h^+ + c\psi_e^- + d\psi_h^-, \quad (2.4)$$

where the indices e and h indicate an electron and hole wave function, respec-

tively. The coefficients a, b, c, d are related by

$$\begin{aligned}
c\psi_e^- e^{-i|\mathbf{k}_e|\tilde{L}} &= r_{ee,r}a\psi_e^+ e^{i|\mathbf{k}_e|\tilde{L}} + r_{he,r}d\psi_h^- e^{-i|\mathbf{k}_h|\tilde{L}}, \\
b\psi_h^+ e^{i|\mathbf{k}_h|\tilde{L}} &= r_{eh,r}a\psi_e^+ e^{i|\mathbf{k}_e|\tilde{L}} + r_{hh,r}d\psi_h^- e^{-i|\mathbf{k}_h|\tilde{L}}, \\
a\psi_e^+ e^{-i|\mathbf{k}_e|\tilde{L}} &= r_{ee,l}c\psi_e^- e^{i|\mathbf{k}_e|\tilde{L}} + r_{he,l}b\psi_h^+ e^{-i|\mathbf{k}_h|\tilde{L}}, \\
d\psi_h^- e^{i|\mathbf{k}_h|\tilde{L}} &= r_{eh,l}c\psi_e^- e^{i|\mathbf{k}_e|\tilde{L}} + r_{hh,l}b\psi_h^+ e^{-i|\mathbf{k}_h|\tilde{L}},
\end{aligned} \tag{2.5}$$

where $\tilde{L} = \frac{L}{2} \cos \theta$. The second indices of the wave functions refer to the right (r) and left (l) interface. The right interface is placed at $L/2$ and the left interface is placed at $-L/2$. θ is the angle of incidence from the TI to the S where zero angle means orthogonal to the interface. The wave vectors k_h and k_e are the wave vectors of the hole and electron, respectively. They are given by

$$\begin{aligned}
|\mathbf{k}_h| &= \sqrt{(\mu_{TI} - E)^2 - m_z^2}/v_F, \\
|\mathbf{k}_e| &= \sqrt{(\mu_{TI} + E)^2 - m_z^2}/v_F,
\end{aligned} \tag{2.6}$$

where v_F is the Fermi velocity. The mismatch between these wave vectors and the wave vector in the superconductor causes an effective barrier at the interface. The superconducting gap can be neglected in this mismatch as $\Delta \ll \mu_{TI,S}$. Conservation of $k_{\parallel}$ (due to translational invariance) then gives, for the angle of transmission in the superconductor, $\theta_S = \arcsin \left(\sin \theta \sqrt{\mu_{TI}^2 - m_z^2}/\mu_S \right)$. Solving Eq. (2.5) gives the energy as a function of the phase difference, ϕ , between the superconductors.

2.3 Andreev bound states

First we consider the case with no ferromagnet on top of the TI. For perpendicular incidence, we find a 4π periodic ABS with a gapless dispersion, even in the presence of a momentum mismatch (the solid curves in Fig. 2.2). However, in the presence of a momentum mismatch, a nonzero angle of incidence results in a nonzero scattering amplitude and a gap is always present (Fig. 2.2 (a)–2.2(c)). The larger the mismatch between the wave vectors, the larger is the gap that opens. For $\mu_{TI} = \mu_S$, the interface is effectively fully transparent and all trajectories give a 4π periodic ABS. This is a consequence of the model where the superconducting gap is neglected. The opening of the gap at finite angles is due to finite backscattering at nonzero angle of incidence. For a larger mismatch between the chemical potentials, the difference in angles of the particle in the TI and superconductor is larger. This causes also a larger mismatch in the spin direction, which increases the barrier and hence results in more reflected electrons. Only at zero angle of incidence is back scattering prohibited by the topological nature. So, in experiments, no 4π periodicity of the ABSs can be obtained for all angles; it is a single-channel effect, as is also concluded by Fu and Kane [8]

Figure 2.2 (a) Andreev bound states for different trajectories in a S/TI/S junction. A gap opens at finite angle. The arrows indicate which bound state branches are connected to form a 4π periodicity. In these branches a Majorana fermion is present at $\phi = \pi$. The legend applies to all the figures. $\mu_{TI}/\Delta = 100, \mu_S/\Delta = 1000$ and $L/L_0 = 0.01$ where $L_0 = v_f \hbar / \mu_{TI}$. (b) $\mu_{TI}/\Delta = 100, \mu_S/\Delta = 120$ and $L/L_0 = 0.01$. (c) $\mu_{TI}/\Delta = 100, \mu_S/\Delta = 120$ and $L/L_0 = 0.1$ and (d) $\mu_{TI}/\Delta = 100, \mu_S/\Delta = 120, m_z/\Delta = 60.0$ and $L/L_0 = 0.01$. (e) Bound state energy for different angles and phase difference $\phi = \pi$. Furthermore $\mu_S/\Delta = 120, \mu_{TI}/\Delta = 100, m_z/\Delta = 0$. The energy is oscillating with length. E_{gap} is defined as the distance from $E/\Delta = 0$ till the minimum of the ABS. (f) Bound state energy for fixed phase difference $\phi = \pi$ and angle using the formula from Ref. [70].

for a system with a small $\mu_{TI,S}$. Note that even when this 4π periodic ABS is present, it will only be noticeable in ac measurements since interactions with the environment already cause the system to reside in the lower (2π) ABS branches [65, 71–73].

For a different length (Fig. 2.2(c)), the curve corresponding to $\theta = 2\pi/5$ is now lower in energy than the bound states of $\theta = \pi/4$ and $\theta = \pi/3$ compared to the graphs of Figs. 2.2(a) and 2.2(b). In Fig. 2.2(e) the bound-state energy for specific angles at $\phi = \pi$ is plotted as a function of length. We see an oscillating behavior as a function of length due to a Fabry-Perot resonance. The oscillation period is determined by the Fabry-Perot resonant condition: $2Lk_{TI} \cos \theta = 2\pi n$ where k_{TI} is the wave vector in the topological insulator and n is an integer [70]. There is a strong similarity to a superconductor-normal-metal-superconductor (SNS) junction. In Fig. 2.2(f), a plot is made of the bound-state energy of a SNS junction for a fixed angle of $\pi/4$ and phase difference of π by determining the pole in the spectral supercurrent in Eq. (5) of Ref. [70], i.e.,

$$\begin{aligned} \Gamma_n = 0 = & (K^2 \Omega_n^2 + \omega_n^2) \cosh \left(\frac{2\omega_n L}{\hbar v_n} \right) + \\ & 2K\omega_n \Omega_n \sinh \left(\frac{2\omega_n L}{\hbar v_n} \right) - \\ & (K^2 - 1) \Omega_n^2 \cos(2k_N L) + \Delta^2 \cos \phi, \end{aligned} \quad (2.7)$$

where $\Omega_n = \sqrt{\omega_n^2 + \Delta^2}$, $\omega_n = \pi(2n+1)/\beta$, $\beta = 1/k_B T$, $k_S = \sqrt{\frac{2m}{\hbar} \mu - \mathbf{k}_{||}^2}$, $k_N = \sqrt{\frac{2m}{\hbar} (\mu - U) - \mathbf{k}_{||}^2}$, $K = \frac{k_N^2 + k_S^2}{2k_N k_S}$, and $v_{N(S)} = \frac{\hbar k_{N(S)}}{m}$. $\Gamma_n = 0$ corresponds to a pole in imaginary space which is equal to the energy of the Andreev bound state. The decrease of the amplitude is determined by the ratio of the length of the junction and the coherence length of the superconductor in the topological insulator. It should, however, be noted that varying the junction length will not result in a closing of the gap at a certain length. The calculation above is valid for every particular angle. When all angles are included, the oscillations will be averaged out.

When a ferromagnet is included, the magnetization is found to decrease the gap (see Fig. 2.2(d)). This can be understood by considering the extreme case where the magnetization m is close to the chemical potential so that the wave vectors of the electrons and holes are nearly zero (Eq. (2.6)). In that case, it also follows from the conservation of $k_{||}$ that θ_s is practically zero. Then, by using the eigenvectors (Eq. (2.10), (2.11), and (2.17)) in the Appendix and substituting these values of the wave vectors and angle into them, the resulting equations at the interfaces simplify. From these equations, it can be seen that there is perfect Andreev reflection. Quantitatively, it can be understood by noticing that the mismatch between the spins for the different particles in the system also causes a barrier. By the magnetization, this mismatch becomes smaller due to the alignment.

In Figs. 2.3(a) and 2.3(b), we show the bound states as a function of k_y , i.e.,

Figure 2.3 Bound state energy versus the wave vector parallel to the interface for different phase differences. For all the cases a nonhelical Majorana quantum wire is seen at $\phi = \pi$. The legend is shown in (a) and holds also for the other two. (a) $\mu_{TI}/\Delta = 100, \mu_S/\Delta = 1000$ and $L/L_0 = 0.01$. (b) $\mu_{TI}/\Delta = 100, \mu_S/\Delta = 110$ and $L/L_0 = 0.01$ and (c) $\mu_{TI}/\Delta = 100, \mu_S/\Delta = 1000, m_z/\Delta = 60$ and $L/L_0 = 0.01$.

the wave vector parallel to the interface. For a phase difference of π between the superconductors, we see that the zero-energy mode has a dispersion as a function of k_y . This is also called a nonchiral Majorana state [8]. For large mismatch between k_S and k_{TI} , the model of Fu and Kane applies [8] where the chemical potential is smaller than the superconducting gap. This situation resembles the case of a large mismatch at the interface, in our case, as the waves in the superconductor are then fully evanescent. For smaller mismatches, the gap is smaller, which results in smaller slopes in the $k_y - E$ graphs. A smaller slope indicates a smaller velocity of this propagating mode along the interface, as already noted in Ref. [74]. Based on the same reasoning as in the previous paragraph, the $k_y - E$ graphs have a smaller slope if magnetization is included. The result for $m_z/\Delta = 60.0$ is shown in Fig. 2.3(c).

2.4 Supercurrent

In this section, we numerically calculate the angle-averaged supercurrent of the Andreev bound states. We consider here only the supercurrents for small junction length, as longer lengths give no additional features regarding the 4π periodic

ABS and the influence of the chemical potential and magnetization on this. In the work of Ref. [75], discretized bound states were used but the continuum was missing in the calculation for larger length scales. Because we only consider here small length scales, only the discretized spectrum has to be considered,

$$I/I_0 = \int_{-\pi/2}^{\pi/2} d\theta \cos \theta \tanh \left(\frac{E}{2k_B T} \right) \frac{dE/\Delta}{d\phi}, \quad (2.8)$$

where $I_0 = eN\Delta/\hbar$. Three plots of this normalized Josephson supercurrent are shown in Fig. 2.4(a). The temperature is $T/T_c = 0.01$, where T_c is the critical temperature.

Although a 4π periodicity is present in the Andreev bound state for zero angle of incidence, the other channels are 2π periodic. Hence, the 2π periodic character is dominating the angle-averaged supercurrent and therefore this current will be 2π periodic in measurements. Moreover, the thermal equilibrium of the system even makes the ABS for zero angle of incidence 2π periodic since inelastic scattering can relax quasiparticles to an ABS that is lower in energy [41, 76, 77]. This thermal equilibrium is due to the exchange between the bulk superconducting electrodes and the Andreev bound-state levels in the junction [77].

We see that for larger mismatch, the supercurrent as a function of phase has a more sinusoidal shape. For small mismatches, there is a sharp transition at $\phi = \pi$ from positive to negative supercurrent, which is also the case in a normal superconducting junction [78]. Also, for a larger mismatch or for a magnetization, the slope of the energy-phase curves becomes less steep, causing a smaller supercurrent for both cases. In Fig. 2.4(b), we plot the dependence of the normalized $I_c R_N$ product as a function of mismatch in the Fermi level and as function of magnetization. R_N is here averaged over all angles. For larger mismatch in the Fermi level, the value of the $I_c R_N e/\Delta$ is saturating towards 0.8π which is between the value of 0.5π and π corresponding to the tunneling and ballistic limit respectively in normal SNS junctions. For small mismatch, the value is π . The critical current is also decreasing for a larger magnetization. However, we see that for values larger than $m_z/\Delta = 60$, the critical current is increasing again. When analyzing the Andreev bound states, we notice that there is a competition between the flattening of the bound states and the lowering of the barrier, both due to magnetization. The latter depends on the relative magnitude of the magnetization to the mismatch. In Fig. 2.4(b), the mismatch of the wave vectors due to a difference in the chemical potentials is relatively small: $\mu_{TI}/\Delta = 100$ and $\mu_S/\Delta = 120$. The aligning of the spins for larger magnetization can therefore make the interface almost transparent. The corresponding Andreev bound states also resemble therefore an almost transparent interface: small gap, and at $\phi = 0$ and 2π , the energy is $E/\Delta = \pm 1$. For a larger difference between μ_S and μ_{TI} , the effect is less and the critical current is monotonically decreasing for larger magnetization. However, if we analyze the normal resistance, the resistance increases for larger magnetization. This is because the spins in the topological insulator with the ferromagnet on top are now more *misaligned* compared to the topological insulator side without a ferromagnet on top. The combination of both an increasing I_c and R_N results in a normalized $I_c R_N e/\Delta$ product of 2π .

Figure 2.4 (a) Normalized Josephson supercurrent as a function of the phase difference between the superconductors. The numbers indicated in the inset correspond with the following parameters: (1) $\mu_S/\Delta = 1000, \mu_{TI}/\Delta = 100, m_z/\Delta = 0, L/L_0 = 0.01$, (2) $\mu_S/\Delta = 120, \mu_{TI}/\Delta = 100, m_z/\Delta = 0, L/L_0 = 0.01$ and (3) $\mu_S/\Delta = 120, \mu_{TI}/\Delta = 100, m_z/\Delta = 60.0, L/L_0 = 0.01$. (b) Dependence of the normalized $I_c R_N e / \Delta \pi$ product on both the magnetization (dashed line) and the chemical potential of the superconductor (solid line) separately. μ_{TI}/Δ is kept constant to 100. In the dependence of the magnetization, μ_S/Δ is kept constant to 120. The temperature is $T/T_c = 0.01$ in (a) and (b). (c) Sketch of an Andreev bound state at non-zero angle of incidence. Due to magnetization the gap of the ABS has become so small that through Zener tunneling the electron in the lower branch can be promoted to the upper branch around $\phi = \pi \pm n2\pi$ where n is an integer. (d) The influence of the magnetization and μ_S/Δ on the value of the gap. For both situations $\mu_{TI}/\Delta = 100, \theta = \pi/3$ and $L/L_0 = 0.01$.

2.5 Signatures of 4π periodic ABS by means of Zener tunneling

We have seen that the 4π periodic ABS is a single-channel effect for perpendicular trajectories only. Next to it, measuring in thermal equilibrium makes even the single 4π ABS 2π periodic because the electrons will follow the lowest ABS branches, i.e., below $E/\Delta = 0$. The latter can be solved by doing ac measurements such as Shapiro step and/or noise measurements. The 4π periodic ABS will only contribute to the Shapiro steps at a voltage equal to $n\hbar\omega/e$, where n is an integer and ω is the frequency of the applied microwave [65, 71]. A 2π periodic ABS will result in Shapiro steps at $V = n\hbar\omega/2e$, which is half the step

size of the 4π periodic bound state.

However, due to the presence of just one single 4π periodic ABS in 3D TIs/superconductor Josephson junctions out of many, one would expect that a 4π periodic signature in ac measurements is not visible due to angle averaging. Usually, one can enhance the zero-angle contribution by introducing a physical barrier of finite width due to the exponential dependence of the wave function on the width. It is, however, not possible to cancel the nonzero angles by introducing a physical barrier between the superconductor and TI because of Klein tunneling, which renders barriers effectively transparent (see, for example, the discussion of Klein tunneling in graphene in Refs. [68, 79]). So, in order to see a 4π periodic ABS, the ABSs of all angles should be 4π periodic. By means of Zener tunneling, this can be achieved.

In order to obtain Zener tunneling, a bias voltage across the junction is required (which is, for example, the case in Shapiro steps measurements). Due to this bias voltage, the quasiparticles in the junction can gain enough kinetic energy so that they can transfer from a lower Andreev bound state to an upper bound state despite the separation by a gap [80, 81]. It is noted in Ref. [82] that for large transparency of the interface, this can result in a 4π periodic ABS. So, when the gap is small, it can no longer be distinguished from an Andreev bound state without a gap. Hence, when electrons in the lower branch of these Andreev bound states with small gaps are promoted to the upper branch, it can result in 4π periodic signatures in ac measurements [72, 83]. In Fig. 2.4(c), a sketch is shown of an ABS with a finite but small gap. Due to magnetization, this can result in a 4π periodic signature in, for example, Shapiro step and/or noise measurements. Physically, the small gap is similar to having a finite length in the 1D Kitaev model, where also a gap is present due to the interaction of the Majorana fermions at the ends [5, 72, 84, 85]. A way to reduce the gaps of all nonzero angle of incidence channels in a 3D TI, in order to enhance the chance of Zener tunneling to get the 4π periodicity of all ABSs, is by exploiting magnetization, as is shown in Fig. 2.2(d).

The influence of the magnitude of the magnetization depends, first of all, on the relative magnitude of the chemical potentials to each other, as we can see from Fig. 2.4(d). The larger the mismatch, the less the influence is of the magnetization. Second, the influence of the magnetization depends on its magnitude compared to the absolute magnitude of the chemical potential. With a larger chemical potential, the influence of the magnetization is less. To get a clearer picture of the influence of the magnetization, we have plotted the gap in the Andreev bound state (at $\phi = \pi$) for several conditions in Fig. 2.4(d). For an increase of mismatch, we kept the magnetization constant to $m_z/\Delta = 0$, length $L/L_0 = 0.01$, and angle $\theta = \pi/3$. A similar result is obtained for other angles. Furthermore, $\mu_{TI}/\Delta = 100$ for both graphs. We see that the gap is a strong function of magnetization in the beginning, but saturates at larger mismatches in the chemical potentials. The graph that shows the influence of the magnetization has a constant (small) mismatch, $\mu_S/\Delta = 140$ and $\mu_{TI}/\Delta = 100$. When the magnetization energy is half the value of the Fermi level in the TI, the energy gap is already decreased by 50% of its original value at zero magnetization.

However, we have estimated before that the magnetization energy is typically on the order of 1% of the Fermi energy, i.e., $\mu \gg m_z$, in experiments. So only for small mismatches in the chemical potentials is it possible to reduce the gap so that by means of Zener tunneling, the 4π periodicity of the ABSs remains for all angles. This reduction of the gap can be made visible in SQUID experiments, as proposed in Refs. [86, 87], where it is shown that the reduction of the gap size results in a different critical current modulation of the SQUID as a function of the applied flux through the ring. These results hold even in equilibrium experiments, so that these SQUID devices can be used for ABS spectroscopy.

2.6 Conclusions

We studied the Andreev bound states and the resulting supercurrent for S/TI/S junctions with and without a ferromagnet on top of the TI. In experiments, it is often the case that $\mu \gg \Delta$ and $m_z < \mu$, and therefore we extended the model (by Fu and Kane [8] and Linder *et al.* [66]) towards this regime. The bound states are solved by means of the total wave function in the topological insulator and its relation to the reflection coefficients, providing insight in the process. The important conclusion is that the results from Fu and Kane [8] (e.g., the 4π periodic ABS existing only for $\theta = 0$) are confirmed, even for large chemical potentials. Therefore, these features are also valid in actual experiments on TIs. The 4π periodicity of the bound states only remains in a 3D topological insulator for zero angle of incidence. This 4π feature cannot be observed, as all of the other angles, which give 2π periodic bound states, cause the 2π periodicity to dominate. However, Zener tunneling can cause a transition from the lower branches to the upper branches of the Andreev bound states, even when a gap is present. We can enhance this Zener tunneling, and hence enhance the 4π periodicity of the nonzero angle ABSs, by depositing a ferromagnet on top. The magnetization effectively lowers the barrier, which causes the gap in the Andreev bound states to become smaller.

2.7 Appendix: Eigenvectors and boundary conditions

The eigenvectors in the topological insulator are calculated to be

$$\psi_1 = n_1 \begin{pmatrix} -m + \sqrt{m^2 + v^2|\mathbf{k}_1|^2} \\ -v|\mathbf{k}_1|e^{i\theta} \\ 0 \\ 0 \end{pmatrix}, \quad (2.9)$$

$$\psi_2 = p_2 \begin{pmatrix} 0 \\ 0 \\ m + \sqrt{m^2 + v^2|\mathbf{k}_2|^2} \\ -v|\mathbf{k}_2|e^{-i\theta} \end{pmatrix}, \quad (2.10)$$

$$\psi_3 = p_3 \begin{pmatrix} m + \sqrt{m^2 + v^2|\mathbf{k}_3|^2} \\ v|\mathbf{k}_3|e^{i\theta} \\ 0 \\ 0 \end{pmatrix}, \quad (2.11)$$

$$\psi_4 = n_4 \begin{pmatrix} 0 \\ 0 \\ -m + \sqrt{m^2 + v^2|\mathbf{k}_4|^2} \\ v|\mathbf{k}_4|e^{-i\theta} \end{pmatrix}, \quad (2.12)$$

where $n_j = 1/\sqrt{2(m^2 + v^2|\mathbf{k}_j|^2 - m\sqrt{m^2 + v^2|\mathbf{k}_j|^2})}$ with $j = 1, 4$ for ψ_1 and ψ_4 , respectively. Furthermore, $p_j = 1/\sqrt{2(m^2 + v^2|\mathbf{k}_j|^2 + m\sqrt{m^2 + v^2|\mathbf{k}_j|^2})}$ with $j = 2, 3$ for ψ_2 and ψ_3 respectively. The eigenvalues are

$$E_1 = -\mu - \sqrt{m^2 + v^2|\mathbf{k}_1|^2}, \quad (2.13)$$

$$E_2 = \mu - \sqrt{m^2 + v^2|\mathbf{k}_2|^2}, \quad (2.14)$$

$$E_3 = -\mu + \sqrt{m^2 + v^2|\mathbf{k}_3|^2}, \quad (2.15)$$

$$E_4 = \mu + \sqrt{m^2 + v^2|\mathbf{k}_4|^2}. \quad (2.16)$$

ψ_1 and ψ_3 are the electrons belonging to the lower and upper half of the Dirac cone, respectively. ψ_2 and ψ_4 are the holes corresponding, respectively, to the lower and upper half of the cone. The wave function in the superconductor is given by

$$\psi_s = \frac{1}{2\sqrt{E}} \begin{pmatrix} e^{i\phi}\sqrt{E - \mu + v|\mathbf{k}_s|} \\ e^{i\phi}e^{i\theta}\sqrt{E - \mu + v|\mathbf{k}_s|} \\ -\Delta e^{i\theta} \\ \sqrt{E - \mu + v|\mathbf{k}_s|} \\ \Delta \\ \sqrt{E - \mu + v|\mathbf{k}_s|} \end{pmatrix} \quad (2.17)$$

with an energy given by $E = \sqrt{\Delta^2 + (v|\mathbf{k}_s| - \mu)^2}$.

The reflection and transmission coefficients can differ at both interfaces due to magnetization. If we consider the electrons at the upper cone, as depicted in Fig. 2.1(a), we need the wave functions ψ_2 and ψ_3 . By taking the direction of the particles into account in the angle θ in the TI and θ_s in the superconductor, we arrive at the following set of equations.

Right interface, incoming electron

$$\begin{aligned}
 p_{m,3}(1 + r_{ee}) &= \frac{e^{i\phi}}{2\sqrt{E}} (c_1 t_{ee} + d_1 t_{eh}), \\
 p_{k,3}(e^{i\theta} - r_{ee}e^{-i\theta}) &= \frac{e^{i\phi}}{2\sqrt{E}} (c_1 t_{ee}e^{i\theta_s} - d_1 t_{eh}e^{-i\theta_s}), \\
 p_{m,2}r_{eh} &= \frac{\Delta}{2\sqrt{E}} \left(-t_{ee} \frac{e^{i\theta_s}}{c_2} + t_{eh} \frac{e^{-i\theta_s}}{d_2} \right), \\
 -p_{k,2}e^{-i\theta}r_{eh} &= \frac{\Delta}{2\sqrt{E}} \left(t_{ee} \frac{1}{c_2} + t_{eh} \frac{1}{d_2} \right), \tag{2.18}
 \end{aligned}$$

where

$$\begin{aligned}
 |\mathbf{k}_{se}| &= \mu/v + \sqrt{E^2 - \Delta^2}/v, \\
 |\mathbf{k}_{sh}| &= \mu/v - \sqrt{E^2 - \Delta^2}/v, \\
 c_1 &= \sqrt{E - \mu + v|\mathbf{k}_{se}|}, \\
 d_1 &= \sqrt{E - \mu + v|\mathbf{k}_{sh}|}, \\
 c_2 &= \sqrt{E - \mu + v|\mathbf{k}_{se}|}, \\
 d_2 &= \sqrt{E - \mu + v|\mathbf{k}_{sh}|}, \\
 p_{m,j} &= \frac{m + \sqrt{m^2 + v^2|\mathbf{k}_j|^2}}{\sqrt{2(m^2 + v^2|\mathbf{k}_j|^2 + m\sqrt{m^2 + v^2|\mathbf{k}_j|^2})}}, \\
 p_{k,j} &= \frac{v|\mathbf{k}_j|}{\sqrt{2(m^2 + v^2|\mathbf{k}_j|^2 + m\sqrt{m^2 + v^2|\mathbf{k}_j|^2})}}. \tag{2.19}
 \end{aligned}$$

Right interface and incoming hole

$$\begin{aligned}
 p_{m,3}r_{he} &= \frac{e^{i\phi}}{2\sqrt{E}} (c_1 t_{ee} + d_1 t_{eh}), \\
 -p_{k,3}r_{he}e^{-i\theta} &= \frac{e^{i\phi}}{2\sqrt{E}} (c_1 t_{ee}e^{i\theta_s} - d_1 t_{eh}e^{-i\theta_s}), \\
 p_{m,2}(1 + r_{hh}) &= \frac{\Delta}{2\sqrt{E}} \left(-t_{ee} \frac{e^{i\theta_s}}{c_2} + t_{eh} \frac{e^{-i\theta_s}}{d_2} \right), \\
 p_{k,2}(e^{i\theta} - r_{hh}e^{-i\theta}) &= \frac{\Delta}{2\sqrt{E}} \left(t_{ee} \frac{1}{c_2} + t_{eh} \frac{1}{d_2} \right). \tag{2.20}
 \end{aligned}$$

Left interface, incoming electron

$$\begin{aligned}
p_{m,3}(1 + r_{ee}) &= \frac{e^{i\phi}}{2\sqrt{E}} (d_1 t_{eh} + c_1 t_{ee}), \\
p_{k,3}(-e^{-i\theta} + r_{ee}e^{i\theta}) &= \frac{e^{i\phi}}{2\sqrt{E}} (d_1 t_{eh}e^{i\theta_s} - c_1 t_{ee}e^{-i\theta_s}), \\
p_{m,2}r_{eh} &= \frac{\Delta}{2\sqrt{E}} \left(-t_{eh} \frac{e^{i\theta_s}}{d_2} + t_{ee} \frac{e^{-i\theta_s}}{c_2} \right), \\
p_{k,2}r_{eh}e^{i\theta} &= \frac{\Delta}{2\sqrt{E}} \left(t_{eh} \frac{1}{d_2} + t_{ee} \frac{1}{c_2} \right). \tag{2.21}
\end{aligned}$$

Left interface, incoming hole

$$\begin{aligned}
p_{m,3}r_{he} &= \frac{e^{i\phi}}{2\sqrt{E}} (d_1 t_{eh} + c_1 t_{ee}), \\
p_{k,3}r_{he}e^{i\theta} &= \frac{e^{i\phi}}{2\sqrt{E}} (d_1 t_{eh}e^{i\theta_s} - c_1 t_{ee}e^{-i\theta_s}), \\
p_{m,2}(1 + r_{hh}) &= \frac{\Delta}{2\sqrt{E}} \left(-t_{eh} \frac{e^{i\theta_s}}{d_2} + t_{ee} \frac{e^{-i\theta_s}}{c_2} \right), \\
p_{k,2}(-e^{-i\theta} + r_{hh}e^{i\theta}) &= \frac{\Delta}{2\sqrt{E}} \left(t_{eh} \frac{1}{d_2} + t_{ee} \frac{1}{c_1} \right). \tag{2.22}
\end{aligned}$$

These equations can be used to calculate the coefficients that are used in Eq. (2.5) in the main part of the chapter.

CHAPTER 3

Josephson supercurrent in a topological insulator without a bulk shunt

A Josephson supercurrent has been induced into the three-dimensional topological insulator $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$. We show that the transport in $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ exfoliated flakes is dominated by surface states and that the bulk conductivity can be neglected at the temperatures where we study the proximity induced superconductivity. We prepared Josephson junctions with widths in the order of 40 nm and lengths in the order of 50 to 80 nm on several $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ flakes and measured down to 30 mK. The Fraunhofer patterns unequivocally reveal that the supercurrent is a Josephson supercurrent. The measured critical currents are reproducibly observed on different devices and upon multiple cooldowns, and the critical current dependence on temperature as well as magnetic field can be well explained by diffusive transport models and geometric effects.

3.1 Introduction

Topological insulators (TIs) have conducting surface states with a locking between the electron momentum and its spin [6, 16, 17, 50, 53, 54, 88–90]. Besides bearing promise for high temperature spintronic applications [91–93], TIs are also candidate materials to host exotic superconductivity. For example, $p + ip$ order parameter components [94, 95] and Majorana zero energy states [7, 43–45] have been theoretically predicted. The topological superconductivity can either be intrinsic [96] or proximized by a nearby superconductor [8, 56, 97].

The first generation of topological insulators, Bi-based materials as $\text{Bi}_{1-x}\text{Sb}_x$ alloys, and later Bi_2Te_3 and Bi_2Se_3 compounds, exhibit topological surface states but also have an additional shunt from the conducting bulk, mainly due to anti-site defects and vacancies [19, 21, 54]. Josephson junctions [56–61, 63, 98–102] and SQUIDs [62, 63, 101–103] have been realised in these topological surface states, but the practical use of these topological devices is limited by the bulk shunt [62, 87]. Secondary and ternary compounds have been engineered to increase the bulk resistance and increase the stability of the surface states. The most promising examples of the latest generation three-dimensional TIs are $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_{3-y}\text{Se}_y$ [104] and strained HgTe [46, 48, 105].

In this work we report the realization of a Josephson supercurrent across 50 nm of topological insulator $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$. We first show that in our

$\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ no bulk conduction is present at low temperatures and that the observed surface states are of a topologically non-trivial nature. We then demonstrate Josephson junction behaviour reproducibly on different flakes and during multiple cooldowns. The width of the superconducting Nb electrodes is very narrow, of the order of 40 nm, anticipating future work on topological devices with only a few modes [106–108].

3.2 Transport properties of exfoliated $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ flakes

$\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ single crystals were obtained by melting stoichiometric amounts of the high purity elements Bi (99.999 %), Sb (99.9999 %), Te (99.9999 %) and Se (99.9995 %). The raw materials were sealed in an evacuated quartz tube which was vertically placed in the uniform temperature zone of a box furnace to ensure the homogeneity of the batch. The molten material was kept at 850 °C for 3 days and then cooled down to 520 °C with a speed of 3 °C/h. Next the batch was annealed at 520 °C for 3 days, followed by cooling to room temperature at a speed of 10 °C/min [109].*

Smooth flakes are prepared using mechanical exfoliation on a silicon-on-insulator substrate. To determine the transport characteristics of $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$, Hall bars are prepared using e-beam lithography and argon ion etching on exfoliated flakes with a thickness ranging from 80 till 200 nm. Au electrodes are defined by photolithography and lift-off. During all the fabrication steps the Hall bar is covered with either e-beam resist or photoresist protecting the surface from damage or contamination. The Hall bars are 7 μm long and 700 nm wide. Figure 3.1(a) shows a SEM image of such a Hall bar.

A typical temperature dependence of the resistance of the Hall bars is shown in Fig. 3.1(b). At high temperature, the crystal exhibits semiconductor-like thermally activated behaviour. Below 150 K the resistance stabilises, indicating metallic surface channels. At high temperatures the transport properties are determined by the bulk of the crystal, while at low temperatures the surfaces provide the dominant charge carriers. To verify this, the RT curve is modelled by a semiconductor bulk part and metallic surface part, i.e. the total resistance is given by $R = (G_b + G_s)^{-1}$. Where $G_b = (R_{b0}e^{\Delta/k_B T})^{-1}$ and $G_s = (R_{s0})^{-1}$ with R_{b0} a constant depending on the flake dimensions and resistivity of the bulk at high temperature and R_{s0} the resistance of the surface states. The best fit is obtained for $\Delta = 50$ meV. This means that the Fermi energy is positioned 50 meV below the bottom of the conduction band. The entire bulk band gap would be larger than 50 meV. At 300 K, the bulk contribution is dominant and allows for a one-band interpretation of the Hall effect measurement (Fig. 3.1(c)) at this temperature, giving a bulk carrier density of 10^{17} cm^{-3} . Extrapolating

*Crystal growth is done by Y. (Yingkai) Huang and D. (Dong) Wu at the Van der Waals-Zeeman Institute in Amsterdam. Yu Pan was involved in the transport characterisation, as were others including Anne de Visser also from the Van der Waals-Zeeman Institute in Amsterdam.

Figure 3.1 (a) Scanning electron microscopy image of a Hall bar of $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$. The dimension of this Hall bar is different from the Hall bar of the measurements shown in Fig. 3 (c–e). The Hall bar of the measurements has a width of 560 nm and a length of 6.8 μm . The dark grey part is etched away. The light gray part between the electrodes is the topological insulator. The white scale bar is 5 μm . The longitudinal resistance is measured between V1+ and V- and the Hall resistance between V- and V2+. (b) Typical temperature dependence of the resistance of an exfoliated flake of $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$, measured in a Hall bar configuration. The fitting function is $(G_s + G_b)^{-1}$. (c) A typical Hall effect measurement at 2K (black) and 300 K (red). The negative slope implies that the charge carriers are electrons. (d) Measured magnetoconductance, together with a fit of the HLN theory to the data. The best fit is obtained for $B_\phi = 0.003\text{T}$ and $B_e = 0.25\text{T}$. (e) The temperature dependence of the coherence length fitted by the relation in Eq. (3.3) for $p' = 1$ and $p = 2$ which implies contribution of both electron-electron and electron-phonon interactions. (f) Measurements of the magnetoresistance at different angles of the applied magnetic field on a different Hall bar at 12 K. The scaling with $\cos \theta$ indicates that the sample is in the 2D regime.

the carrier freeze out to low temperatures we find a negligible bulk conduction at low temperatures. At low temperatures all transport is due to the surface states. Hall and longitudinal resistance measurements at 2 K are used to determine the electron density and mobility of the surface states. We reproducibly obtain surface electron densities in the range of 10^{12} - 10^{13} cm^{-2} with mobilities between 120 and 450 cm^2/Vs . The resulting mean free path of the order of 10 to 40 nm is comparable to the mean free path of the electron-like surface states found by Taskin *et al.* [104].

Figures 3.1(c) shows the change in longitudinal conductance as function of applied perpendicular magnetic field. When spin scattering from magnetic impurities is neglected, the full expression for the quantum correction to conductivity in an out of plane magnetic field is described by the Higami-Larkin-Nagaoka (HLN) equation [110]

$$\begin{aligned}
& -\frac{\pi\hbar}{e^2} (\Delta\sigma(B) - \Delta\sigma(0)) \\
& = \psi\left(\frac{1}{2} + \frac{B_e + B_\phi}{B}\right) - \psi\left(\frac{1}{2} + \frac{2B_{so}^z + 2B_{so}^x + B_\phi}{B}\right) \\
& + \frac{1}{2}\psi\left(\frac{1}{2} + \frac{B_\phi}{B}\right) - \frac{1}{2}\psi\left(\frac{1}{2} + \frac{4B_{so}^x + B_\phi}{B}\right) \\
& - \ln\left(\frac{B_e + B_\phi}{B}\right) + \ln\left(\frac{2B_{so}^z + 2B_{so}^x + B_\phi}{B}\right) - \frac{1}{2}\ln\left(\frac{B_\phi}{B}\right) \\
& + \frac{1}{2}\ln\left(\frac{4B_{so}^x + B_\phi}{B}\right), \tag{3.1}
\end{aligned}$$

where ψ is the digamma function, B_e , B_ϕ and B_{so} ($B_i = \frac{\hbar}{4eL_i^2}$) characterize the effective dephasing length scale for electron-electron interaction, inelastic scattering and spin-orbit scattering respectively. This formula is fitted to the magnetoresistance data. In Fig. 3.1(c) a typical fitting is shown for a measurement at 10K. From this fitting we obtain that $B_{so} \gg B$ and $B_\phi = 0.003\text{T}$ and $B_e = 0.25\text{T}$.

When $B_e \gg B$ the HLN equation can be simplified to

$$\Delta\sigma(B) - \Delta\sigma(0) = \alpha \frac{e^2}{2\pi^2\hbar} \left[\psi\left(\frac{1}{2} + \frac{B_\phi}{B}\right) - \ln\left(\frac{B_\phi}{B}\right) \right]. \tag{3.2}$$

α is a parameter indicating the strength of the spin-orbit interaction. For weak spin-orbit interaction $\alpha = 1$ as opposed to strong spin-orbit interaction where a negative value of -0.5 is expected. Due to the chiral-spin texture of a topological insulator and the contribution of both top and bottom surfaces in the transport measurements, an α parameter of -1 is expected. To verify the topological character of the surface states this simplified HLN equation is used to fit the data in the magnetic field range below B_e . Up to 40 K the parameter of $\alpha = -1.01$ with an error of 0.2 at 40 K and 0.05 at 10 K. The corresponding phase coherence lengths L_ϕ is plotted in Fig. 3.2(e). The dependence of L_ϕ as a function of

temperature is fitted with the formula [111, 112]

$$\frac{1}{L_\phi^2} = A'_{ee}T^{p'} + A'_{ep}T^p \quad (3.3)$$

where the first term represents the contribution from the electron-electron interaction and the second term from the electron-phonon interaction. The best fit is obtained for $p' = 1$ and $p = 2$ which implies electron-transverse phonon interactions are dominant above the electron-longitudinal phonon interactions [113, 114]. However, the data below 10 K results in phase coherence length that deviates from the best fit. We think this is due to the fact that the phase coherence length at 4 K according to the fit is about the same size as the width of the measured Hall bar. The HLN formula is only applicable at 2D and therefore if the phase coherence length becomes of the order of the width of the Hall bar, the HLN formula can't be used to fit this data.

At last, we measured the magnetoresistance under different angles of applied field (Fig. 3.2(f)). The scaling of the magnetoresistance with $\cos\theta$ implies that the sample is in the 2D regime. Note however that this does not verify that we have surface states as the phase coherence length is larger than the thickness of the flake at low temperatures which would also force the bulk to behave two dimensionally in those measurements. Despite of that, it is a verification that the HLN equation could be used to fit all the data without making corrections for 3D channels.

However, we cannot rule out the presence of additional trivial two-dimensional metallic surface states that could originate from surface band bending. The possibility of the conduction band bending down below the Fermi energy has been observed in $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ [104]. Angle resolved photo-electron spectroscopy has revealed that the presence of these non-topological surface states is depending on surface absorbents and could vary over time [115].

3.3 Junction fabrication

Now that we have verified the topological nature of our crystals we turn to fabricating Josephson junctions with $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ as the weak link. Transferred similarly to the devices for determining the transport properties, smooth flakes on Si/SiO_2 substrates are used for devices. E-beam lithography is used to define the junctions and the contact pads. Thereafter we perform a 30 second low voltage etching step to avoid large damage to the surface followed by sputtering in-situ 25 nm Nb and 2.5 nm Pd to protect the Nb layer, and lift-off of the excess material. The resulting $\text{Nb}/\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}/\text{Nb}$ junction has been covered by photoresist during the entire process and no damage from etching or growth has occurred to the crystal surface between the electrodes. In figure 3.2(a) a junction is visible in a SEM image, and similar junctions have been prepared on different flakes. The width is about 40 nm and the electrode separation is about 50 nm. The motivation for the junction length is based on our earlier work on Bi_2Te_3 with junctions ranging from 50-250 nm [59]. The mean free path in

Figure 3.2 (a) Scanning electron microscopy image of a Nb/Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}/Nb junction. The Nb layer has been coloured yellow for clarity. The junction is 57 nm long and 38 nm wide. (b) The dependence of the critical current of the Nb nanowire as function of temperature. From the linear fit to the data point in the range of 300–850 mK, the critical temperature is extrapolated to be 1.4 K. Close to the transition temperature, the gap and therefore the critical current can be approached by a linear dependence [116].

Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3} is ten times smaller compared to Bi₂Te₃ which implies that the junction length should also be reduced by a factor of ten to realise sufficient coupling between the electrodes. Simultaneously, this design takes a step forward towards experiments for the observation of a quantized supercurrent where only a few modes should be present [106–108]. In order to achieve the presence of a few modes, the junction width should be of the order of the Fermi wave length. For a 40 nm wide junction and a Dirac velocity of 4.5×10^5 m/s this means that the Fermi level would have to be tuned within 50 meV from the Dirac point by means of gating, which is quite reasonable. To realise these dimensions a thin layer of PMMA (80 nm) is used which limits the thickness of Nb that could be grown. The reduction of the dimensions of the Nb leads reduces the gap of Nb. A 40 nm wide and 250 nm long Nb nanowire is prepared in the same run to determine the properties of the niobium with these dimensions. In figure 3.2b the critical current of this nanowire as a function of temperature is presented, and a reduction of the critical temperature from 9 K of the Nb of our thin film process to about 1.4 K is visible.

3.4 Results

Measurements are performed in a cryogen free dilution refrigerator with low pass filtering of current and voltage signals using pi filters, printed circuit board copper powder filters [117], and RC filters. We measured the critical current as function of temperature and the modulation of the critical current by an applied magnetic field at 30 mK. We will start this section with a discussion of the temperature dependence followed by an analysis of the Fraunhofer pattern.

3.4.1 Temperature dependence of the critical current

At 30 mK we observe a critical current of 14 nA for a junction with 57 nm electrode separation, visible in figure 3.2(a), and 4.8 nA for a 80 nm long junction. Using the extracted critical temperature of the Nb nanowire as the transition temperature for the leads, the normalised temperature dependence of the critical current is plotted in figure 3.3(a) for the 57 nm junction. The boundary between Josephson coupling and thermal noise $(\hbar I_0/e)/(k_B T) = 1$ is illustrated with the dashed line. In figure 3.3(b) the dV/dI characteristics around the thermal limit reveal indeed that a zero resistance state and coherence peaks are only visible below the thermal limit. The coherence peaks are used for determining the critical current below the thermal limit. Above the thermal limit the width of the resistance valley is used as an estimate.

The nature of weak link is determined by fitting the temperature dependence of the supercurrent. For diffusive SNS junctions, i.e. junctions where the junction length L is larger than the electron mean free path, the Usadel equation is used to describe the temperature dependence [118–120],

$$J = \frac{2\pi k_B T}{e\rho_N} \text{Im} \sum_{\omega_n > 0} \frac{G_N^2}{\omega_n^2} \Phi_N \frac{d}{dx} \Phi_N, \quad (3.4)$$

where ρ_N is the resistivity of the N layer, Φ_N is the self-consistently determined induced order parameter function in the N layer with G_N the corresponding normal Green function and $\omega_n = \pi k_B T(2n + 1)$ the Matsubara frequencies, where $n \geq 0$ is integer. As there is no analytical expression for arbitrary length and barrier transparency, the expression was solved numerically with three fitting parameters [121], $\gamma = \frac{\rho_S \xi_S}{\rho_N \xi_N}$, $\gamma_B = \frac{R_B}{\rho_N \xi_N}$ and ξ_N . Here, γ is the ratio between the resistivities and coherence lengths in the superconducting leads and the topological insulator surface state. The resistivity of Nb is much smaller than that of $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ which gives $\gamma \ll 1$. γ_B is proportional to the interface resistance per unit area R_B between the S and N layers. Finally, ξ_N is the coherence length in the normal region at T_C . For the junction illustrated in figures 3.2(a) and 3.3, the best fit is obtained for $\gamma_B = 5$ and $\xi_N = 11.4$ nm. The other junctions give values of the same order of magnitude. The large γ_B is in good agreement with the low excess current in the IV curves which implies a large barrier or low transparency at the interface. Taking the T_c of the Nb wire, we get for $\xi_N(T_c) = \sqrt{\frac{\hbar D}{2\pi k_B T_c}}$ a value of 28 nm which is also in good agreement with the fitting parameters. We note, that the junctions have a small $I_C R_N$ product, $\sim 7 \mu\text{V}$. We argued that $\gamma \ll 1$. Together with the fitted values of γ_B and ξ_N the $I_C R_N$ product is either of the form $\propto V_0/\gamma_B$ or $I_C R_N \propto V_0 e^{-L/\xi_N}$ [78]. Substitution of γ_B , ξ_N and the junction length L we estimate from this relation that the $I_C R_N$ should be in the order of 1-10 μV which is in good agreement with the measured product value.

Figure 3.3 Josephson characteristics of the Nb/Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}/Nb junction illustrated in Figure 3.2. (a) Temperature dependence of the critical current. Above the thermal limit, indicated by the black dashed line, the critical current is determined by the resistance peaks. Below the thermal limit the width of the resistance dip is used as estimate. The red dashed line is a fit for diffusive junctions with the Usadel equation, see main text. (b) Derivative of the current-voltage characteristic above, at, and below the thermal limit. Below the thermal limit the resistance is zero and coherence peaks are visible. These peaks disappear above the thermal limit of 200 mK and only a resistance valley remains. (c) Modulation of the critical current by an applied perpendicular magnetic field. The upper and lower frames are measurements during different cooldown cycles. The upper frame was the first cooldown using Al bond wires which have reduced cooling power below 10 mT, resulting in a sharp step in the critical current at this point. The bottom frame uses Au bond wires. This second cooldown exhibited a slightly reduced critical current and ergo reduced visibility of the first lobe of the diffraction pattern. The dotted line is a model of the critical current by Barzykin *et al.* [122] using the junction parameters found in (a). (d) Current-voltage characteristic and derivative at base temperature. The critical current of 14 nA and normal state resistance of 460 Ω result in an $I_c R_N$ product of 6.4 μ V, consistent with a junction with high γ_B and $L \geq \xi_N$.

3.4.2 Critical current as a function of magnetic field

In Fig. 3.3(c) measurements during two separate cooldowns of the $I_c(B)$ pattern at 30 mK are shown for the same junction. The changes in the supercurrent in the second cooldown indicate a slight evolution in time. The upper frame shows the Fraunhofer pattern of the first measurement. Due to the use of Al bond wires, the cooling of the sample is reduced below the critical field of Al. These measurements are greyed out because the temperature increased in that region, we estimate by 100 mK. A second cooldown using Au bonds results in the lower

panel Fraunhofer pattern. Here, the critical current has reduced slightly resulting in a decreased visibility of the lobes of the Fraunhofer pattern. The Fraunhofer patterns are fitted by the critical current derived from the Usadel equations for arbitrary W and L with open boundaries, as described by Barzykin *et al.* [122],

$$I_c \sim \sum_{l=-\infty}^{\infty} (-1)^l S_l(L/2) S'_l(L/2) \left(\frac{\sin \pi(\nu + l)/2}{\pi(\nu + l)/2} - (-1)^l \frac{\sin \pi(\nu - l)/2}{\pi(\nu - l)/2} \right)^2,$$

$$S_l(u) = \sqrt{|u|/2\pi} (q_T^2 + \pi^2 l^2 / W^2)^{1/4} K_{1/2} \left(\sqrt{u^2 (q_T^2 + \pi^2 l^2 / W^2)} \right),$$

$$S'_l(u) = \frac{d}{du} S_l(u), \quad (3.5)$$

where $\nu = \phi/\phi_0$ with $\phi_0 = \hbar/2e$ is the normalised flux, $q_T = 1/\xi_N^2$ and $K_{1/2}$ is a modified Bessel function of the second kind. For our junction dimensions it follows from this model that the first period is tripled, i.e. the first minimum is at $\Phi = 3\Phi_0$ and the following minima are separated by $2\Phi_0$ intervals. The doubling of the period is not restricted to diffusive junctions and was, in fact, also predicted [122] and observed [123] in ballistic junctions for width and length ratios in the order of one. The first minimum in the measurements occurs at a field value of 0.07 T. The width of the junction is 37 nm. For a flux of $3\phi_0 = 6.2 \cdot 10^{-15} \text{ Wb}$ this implies that the junction effective length (including the penetration depths) is about 2 μm . The obtained London penetration depth is then about 1 μm . This large London penetration depth compared to bulk Nb (47 nm)[124] can be explained by the reduced dimensions of the junctions. The increase of the London penetration depth with decreasing film thickness is studied in Ref. [125]. A film thickness of 25 nm gives a London penetration depth above 100 nm and a decrease of the critical current to 8 K. Due to the reduction of width of the junction in our devices, we end up with a T_C of 1.4 K which consistently implies an even larger increase of the London penetration depth. The coherence length found from the fitting of the critical current together with the width and the length of the junction and London penetration depth serve as inputs for the model described in Eq. (3.5). The theoretical expectation is shown in figure 3.3(c). The relative small critical current of the higher order peaks in the data is found to be well explained by the model.

3.5 Discussion

We showed that the transport in the $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ flakes is dominated by surface states at low temperatures where we study proximity induced superconductivity. We prepared Josephson junctions with widths in the order of 40 nm and lengths in the order of 50 to 80 nm on several $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ flakes and measured them during several cooldowns to 30 mK. The Fraunhofer patterns unequivocally reveal that the supercurrent is a Josephson supercurrent. The measured critical currents are reproducibly observed on different devices and

upon multiple cooldowns, and the measurement can be well explained by diffusive transport models and geometric effects. The predicted 4π periodic Josephson effect can only be observed in the future for similar devices with just a single perpendicular mode (see Chap. 2) and when measured faster than the relaxation rate of a quasiparticle inside an Andreev bound state.

The realization of a Josephson supercurrent in junctions with dimensions in the order of tens of nanometers on a topological insulator dominated by surface states at low temperatures, is an important technological step towards advanced devices necessary for the observation of a quantized supercurrent and confirming the presence of a Majorana bound states in such devices [8]. Future work will focus on top and bottom gating of the surface states to eliminate potential additional trivial surface states from band bending.

CHAPTER 4

Observability of surface Andreev bound states in a topological insulator in proximity to an s -wave superconductor

To guide experimental work on the search for Majorana zero-energy modes, we calculate the superconducting pairing symmetry of a three-dimensional topological insulator in combination with an s -wave superconductor. In analogy to the case of nanowires with strong spin-orbit coupling we show how the pairing symmetry changes across different topological regimes. We demonstrate that a dominant p -wave pairing relation is not sufficient to realize a Majorana zero-energy mode useful for quantum computation. Our main result of this paper is the relation between odd-frequency pairing and Majorana zero energy modes by using Green functions techniques in three-dimensional topological insulators in the so-called Majorana regime. We discuss thereafter how the pairing relations in the different regimes can be observed in the shape of the tunneling conductance of an s -wave proximized three-dimensional topological insulator. We will discuss the necessity to incorporate a ferromagnetic insulator to localize the zero-energy bound state to the interface as a Majorana mode.

4.1 Introduction

The search for a qubit that is robust against local decoherence has led to extensive studies of the so-called Majorana zero-energy mode in materials with strong spin-orbit coupling (SOC) combined with s -wave superconductors. Nanowires and topological insulators are promising candidate materials with strong spin-orbit coupling [8, 12–15, 41, 44, 64, 65, 126–131]. Experimentalists have already reported to have observed signatures of the Majorana zero-energy mode [132–134], where zero-bias conductance peaks are the main features observed in this context.

Besides the possibility to host Majorana modes, topological materials are also interesting for the study of unconventional p -wave superconductivity by itself. p -wave superconductivity gained renewed interest after the prediction that the p -wave pairing symmetry in He^3 would lead to half-quantum vortices with potential application to the field of quantum computing. Sr_2RuO_4 is believed to have p -wave symmetry and together with the prediction of the existence of a nodal gap it has led to an extensive study of this material [26–33]. Also supercon-

ductor/ferromagnet/superconductor junctions are studied for their prospective to switch from a dominant s -wave state to a p -wave state [135–138]. Also these devices have potential application to quantum computation, through which the understanding of the behaviour of p -wave superconductivity has become a field on its own.

In this paper we study the s and p -wave correlations that exist both in semiconductor nanowires as well as in three-dimensional topological insulators (3DTIs). The superconducting symmetry in nanowires with strong spin-orbit coupling is well understood to arise from the presence of two Fermi surface sheets with opposite spin helicity when no magnetic field is applied. We use the nanowire case as an introduction to topological insulators where only one spin branch is present. A single spin branch is only achieved in nanowires after applying a Zeeman magnetic field. We review in which regime a dominant p -wave correlation is present and under which conditions a dominant p -wave correlation can lead to a zero-energy Majorana bound state. Our main theoretical results are expressions for the bound state formed at a 3DTI in the “Majorana” regime. We show the relation between odd-frequency pairing and Majorana zero-energy modes by using a Green function approach. We use those new insights to calculate the conductance spectra of proximity induced superconducting 3DTIs with and without broken time-reversal symmetry. The main focus in this part of the paper is to understand how the modelled tunneling conductance spectra arise from the s and p -wave correlations. We will see that the combination of a zero-bias conductance peak together with conductance dips at the gap energy are distinguished features for p -wave correlations. We shall demonstrate that it is not necessary to be in the “Majorana” regime in order to observe signatures of the required p -wave correlations.

4.2 Pairing wave function and Majorana-modes in nanowires

In order to determine the pairing relations for a nanowire with strong SOC we start with the relation $[E - H]\mathbf{G} = \mathbb{1}$ where $\mathbf{G}$ is the Green function of the system, $\mathbb{1}$ the identity matrix and H is in the basis $[\psi_1, \psi_1, \psi_1^\dagger, \psi_1^\dagger]$ [130]. For a system with spin orbit coupling $[E - H]$ is given by

$$\begin{bmatrix} E + \epsilon_p + M & -\lambda_x k_x - i\lambda_y k_y & 0 & -\Delta \\ -\lambda_x k_x + i\lambda_y k_y & E + \epsilon_p - M & \Delta & 0 \\ 0 & \Delta & E - \epsilon_p - M & -\lambda_x k_x + i\lambda_y k_y \\ -\Delta & 0 & -\lambda_x k_x - i\lambda_y k_y & E - \epsilon_p + M \end{bmatrix}, \quad (4.1)$$

where $\epsilon_p = \mu - \frac{\hbar k^2}{2m}$. Here, $\lambda_{x,y}$ is the SOC strength in x and y -direction. At the end we will set $k_x = 0$ and $\lambda_y = \lambda$ to discuss a nanowire extending in the y -direction. μ is the chemical potential, Δ is the induced superconducting gap and M is the energy of a perpendicular magnetic field, either externally

applied (Zeeman term) or due to an exchange interaction. Note, that the Zeeman contribution of a magnetic field can be considerable, due to the large g -factor of most relevant materials. We neglect the orbital contribution of the applied field.

By taking the inverse of this matrix equation we can obtain the Green's function $\mathbf{G}$, expressed as

$$\begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix}. \quad (4.2)$$

The elements G_{ij} are blocks of 2×2 matrices. The diagonal blocks describe the propagation of the electrons and holes separately. The off-diagonal blocks describe the combined electron and hole propagation, i.e. they describe the propagation of the Cooper pairs in the s -wave proximized nanowire which is the quantity of interest in this paper. When we represent

$$E - H(\mathbf{k}) = \begin{bmatrix} \hat{a} & \hat{b} \\ \hat{c} & \hat{d} \end{bmatrix}, \quad (4.3)$$

the Green function is given by

$$\mathbf{G}(\mathbf{k}, E) = \begin{bmatrix} (\hat{a} - \hat{b} \hat{d}^{-1} \hat{c})^{-1} & (\hat{c} - \hat{d} \hat{b}^{-1} \hat{a})^{-1} \\ (\hat{b} - \hat{a} \hat{c}^{-1} \hat{d})^{-1} & (\hat{d} - \hat{c} \hat{a}^{-1} \hat{b})^{-1} \end{bmatrix}. \quad (4.4)$$

We find

$$G_{12} = i \frac{\Delta}{Z} [(E^2 - B_{k,M}) \hat{\sigma}_0 + 2(-\lambda_x k_x \epsilon_p + i \lambda_y k_y M) \hat{\sigma}_1 - 2(-\lambda_y k_y \epsilon_p - i \lambda_x k_x M) \hat{\sigma}_2 - 2ME \hat{\sigma}_3] \hat{\sigma}_2, \quad (4.5)$$

with

$$Z = -(E^2 - B_{k,M})^2 - 4(-\lambda_x k_x \epsilon_p + i \lambda_y k_y M)^2 - 4(-\lambda_y k_y \epsilon_p - i \lambda_x k_x M)^2 - 4E^2 M^2, \quad (4.6)$$

and

$$B_{k,M} = \epsilon_p^2 + \Delta^2 + (\lambda_x k_x)^2 + (\lambda_y k_y)^2 - M^2 \quad (4.7)$$

To discuss the symmetry of the anomalous Green functions, we use the Matsubara representation which can be obtained by analytical continuation, $E + i\delta \rightarrow i\omega_n$,

$$\begin{aligned} G_{12} = & i \frac{\Delta}{Z} [(-\omega_n^2 - B_{k,M}) \hat{\sigma}_0 + 2(-\lambda_x k_x \epsilon_p + i \lambda_y k_y M) \hat{\sigma}_1 \\ & - 2(-\lambda_y k_y \epsilon_p - i \lambda_x k_x M) \hat{\sigma}_2 - i 2M \omega_n \hat{\sigma}_3] \hat{\sigma}_2 \\ \equiv & i(f_0 + \mathbf{f} \cdot \boldsymbol{\sigma}) \hat{\sigma}_2, \end{aligned} \quad (4.8)$$

$$Z = -(\omega_n^2 - B_{k,M})^2 - 4(-\lambda_x k_x \epsilon_p + i\lambda_y k_y M)^2 - 4(-\lambda_y k_y \epsilon_p - i\lambda_x k_x M)^2 + 4\omega_n^2 M^2, \quad (4.9)$$

$$f_0(\mathbf{k}, i\omega) = \frac{\Delta}{Z}(-\omega_n^2 - B_{k,M}), \quad (4.10)$$

$$f_1(\mathbf{k}, i\omega) = 2\frac{\Delta}{Z}(-\lambda_x k_x \epsilon_p + i\lambda_y k_y M), \quad (4.11)$$

$$f_2(\mathbf{k}, i\omega) = -2\frac{\Delta}{Z}(-\lambda_y k_y \epsilon_p - i\lambda_x k_x M), \quad (4.12)$$

$$f_3(\mathbf{k}, i\omega) = -2i\frac{\Delta}{Z}M\omega_n. \quad (4.13)$$

The total wave function of a pair of fermions should be asymmetric and the total wave functions can be described by the product of an orbital (or parity), spin and frequency term. Even-frequency pairing means that a function is even in ω_n . If we consider singlet (which is an odd function under spin permutation) s -wave (orbitally symmetric) pairing, the pairing wave function $F(= G_{12})$ should satisfy the relation $F_s(k) = F_s(-k)$ in order for the wave function to be antisymmetric when the pairing is even in frequency. For p -wave triplet pairing the relation $F_p(k) = -F_p(-k)$ applies [139].

We note that Z is an even function of ω_n and is an even-parity function. The singlet component f_0 belongs to the even-frequency even-parity class (ESE). The two equal-spin components (f_1 and f_2) are even-frequency spin-triplet odd-parity class (ETO). Finally, f_3 belongs to odd-frequency spin-triplet even-parity class (OTE).

The chemical potential is usually close to the conduction band so that $\mu \gg \Delta$. If we also consider low energy excitations we obtain for the nanowire ($k_x = 0, \lambda_y = \lambda$)

$$G_{12} = \begin{bmatrix} F_{1\uparrow} & F_{1\downarrow} \\ F_{1\downarrow} & F_{1\uparrow} \end{bmatrix}, \quad (4.14)$$

where

$$\begin{aligned} F_{1\uparrow} &\sim -2\Delta i k \lambda \left(M + \frac{\hbar^2 k^2}{2m} - \mu \right) / Z_{nw}, \\ F_{1\downarrow} &\sim \Delta \left(M^2 - k^2 \lambda^2 - \left(\frac{\hbar^2 k^2}{2m} \right)^2 + \frac{\hbar^2 k^2}{m} \mu - \mu^2 \right) / Z_{nw}, \\ F_{1\downarrow} &\sim -\Delta \left(M^2 - k^2 \lambda^2 - \left(\frac{\hbar^2 k^2}{2m} \right)^2 + \frac{\hbar^2 k^2}{m} \mu - \mu^2 \right) / Z_{nw}, \\ F_{1\uparrow} &\sim 2\Delta i k \lambda \left(M - \frac{\hbar^2 k^2}{2m} + \mu \right) / Z_{nw}, \end{aligned} \quad (4.15)$$

$$\begin{aligned} Z_{nw} &= -B_{nw}^2 - 4(i\lambda k M)^2 - 4(\lambda k \epsilon_p)^2 \\ B_{nw}^2 &= (\epsilon_p^2 + \lambda^2 k^2 - M^2)^2 + 2\Delta^2 (\epsilon_p^2 + \lambda^2 k^2 - M^2). \end{aligned} \quad (4.16)$$

G_{21} is related to G_{12} by complex conjugation.

For the moment we assume that we have even-frequency symmetry. (f_3 in Eq. (4.13) can be neglected in the regime of low energy excitations. The appearance of non-negligible odd-frequency symmetry terms will be discussed in section III.) The second and third relation in Eq. (4.15), therefore, correspond to s -wave pairing and the other two with p -wave pairing relations.

The energy dispersion relation of the s -wave proximized nanowire can be obtained by diagonalizing the corresponding Hamiltonian as described above, and is found to be

$$E = \pm \sqrt{E_t \pm 2\sqrt{E_s}}, \quad (4.17)$$

where $E_t = \Delta^2 + \epsilon_p^2 + \lambda^2 k^2 + M^2$ and $E_s = \epsilon_p^2 \lambda^2 k^2 + \Delta^2 M^2 + \epsilon_p^2 M^2$. In the limit of $\mu \gg \Delta$ this can in a good approximation be written as

$$E = \pm \epsilon_p \pm \sqrt{\lambda^2 k^2 + M^2}.$$

Now we have all the formal work done to consider the pairing symmetry in three different regimes: $M \ll \sqrt{\Delta^2 + \mu^2}$, $M = \sqrt{\Delta^2 + \mu^2}$ and $M \gg \sqrt{\Delta^2 + \mu^2}$.

4.2.1 Regime $M \ll \sqrt{\Delta^2 + \mu^2}$

In this case we have four superconducting gaps as indicated in Fig. 4.1(a). Δ_1 and Δ_2 indicate the position for positive wave vector momentum. At Δ_1 (and for the corresponding gap at negative k) it follows from the dispersion relation that $\mu = \frac{\hbar^2 k_F^2}{2m} - \lambda |k_F|$ and for Δ_2 $\mu = \frac{\hbar^2 k_F^2}{2m} + \lambda |k_F|$. Using the relations for the anomalous Green function, Eq. (4.15), we get for Δ_1

$$\begin{aligned} F_{11} &\sim -2\Delta i k k_f \lambda^2 / Z_{nw}, \\ F_{1\downarrow} &\sim -2\Delta \lambda^2 k^2 / Z_{nw}, \\ F_{\downarrow 1} &\sim 2\Delta \lambda^2 k^2 / Z_{nw}, \\ F_{\downarrow\downarrow} &\sim 2\Delta i k k_f \lambda^2 / Z_{nw}. \end{aligned}$$

Expressions such as $\frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 k_F^2}{2m}$ are set to zero in the above equations as we consider low energy excitations. For Δ_2 we obtain

$$\begin{aligned} F_{11} &\sim 2\Delta i k k_f \lambda^2 / Z_{nw}, \\ F_{1\downarrow} &\sim -2\Delta \lambda^2 k^2 / Z_{nw}, \\ F_{\downarrow 1} &\sim 2\Delta \lambda^2 k^2 / Z_{nw}, \\ F_{\downarrow\downarrow} &\sim -2\Delta i k k_f \lambda^2 / Z_{nw}. \end{aligned}$$

We see from the above that the matrix elements corresponding to the s -wave pairing are in magnitude as large as the matrix elements corresponding to the p -wave relations. So in the case of negligible M we have an equal admixture of s -wave and p -wave for both gaps.

As soon as time-reversal symmetry is broken the increase in M causes the p -wave component to become larger in magnitude than the s -wave component.

Figure 4.1 (a) Energy dispersion relation for a nanowire with $M \ll \sqrt{\Delta^2 + \mu^2}$. The solid line corresponds to the relation $\sqrt{E_t - 2\sqrt{E_s}}$ and the dashed line to $\sqrt{E_t + 2\sqrt{E_s}}$. (b) In the regime $M = \sqrt{\Delta^2 + \mu^2}$ the gap at $k = 0$ is closing. Because of the finite magnetic field there is another gap indicated by Δ_3 . (c) In the regime $M \gg \sqrt{\Delta^2 + \mu^2}$ a dominant topological non-trivial p -wave gap exist at Δ_1 . (d) Energy dispersion relation for a 3D topological insulator in the regime $|M| \ll \mu$. The solid line corresponds to $\sqrt{E_{t'}} - 2\sqrt{E_{s'}}$ and the dashed line to $\sqrt{E_{t'}} + 2\sqrt{E_{s'}}$. The graphs are plotted for Δ in the order of μ for clarity.

This can be intuitively understood by notifying that a magnetic field aligns the spins parallel to the field. Therefore spin triplet pairing is favoured above spin singlet pairing.

A Majorana zero-energy mode is defined as a *single, localized* zero-energy mode satisfying the relation $\gamma = \gamma^\dagger$ where γ is the creation/annihilation operator of the Majorana mode. Despite the dominant p -wave order parameter a single Majorana zero-energy mode is not yet appearing since there are two branches.

4.2.2 Regime $M = \sqrt{\Delta^2 + \mu^2}$

This case is shown in Fig. 4.1(b), where the superconducting gap at $k = 0$ is closed. At Δ_2 the anomalous Green function parts are zero because $k = 0$. Because we have turned on a magnetic field, the bands corresponding to different helicity are not orthogonal anymore. Therefore, there exist an interaction between the two in this regime and another superconducting gap is opening above

μ (Δ_3 in the Fig. 4.1(b)) [140]. For Δ_3 the relation $\mu = \frac{\hbar^2 k^2}{2m}$ holds so that

$$\begin{aligned} F_{\uparrow\uparrow} &\sim -2\Delta ik\lambda\mu/Z_{nw}, \\ F_{\uparrow\downarrow} &\sim -\Delta(k^2\lambda^2 - \mu^2)/Z_{nw}, \\ F_{\downarrow\uparrow} &\sim \Delta(k^2\lambda^2 - \mu^2)/Z_{nw}, \\ F_{\downarrow\downarrow} &\sim 2\Delta ik\lambda\mu/Z_{nw}. \end{aligned}$$

For a typical [132] spin orbit strength of $\lambda = 0.2 \text{ eV}\cdot\text{\AA}$ and $m = 0.015m_e$ where m_e is the free electron mass, it follows that the magnitude of the spin-singlet order parameters in this regime are larger than the p -wave components. However, since the energy level of Δ_3 increases with M , i.e. $E_{\Delta_3} \approx \sqrt{\lambda^2 k^2 + M^2}$, for low energy excitations this superconducting contribution can be neglected.

At Δ_1 , $\frac{\hbar^2 k_F^2}{2m} - \mu - \sqrt{\lambda^2 k_F^2 + \mu^2} = 0$ so that we get the following relations for the anomalous Green function part:

$$\begin{aligned} F_{\uparrow\uparrow} &\sim -2\Delta ik\lambda \left(\mu + \sqrt{\lambda^2 k_f^2 + \mu^2} \right) / Z_{nw}, \\ F_{\uparrow\downarrow} &\sim -2\Delta \lambda^2 k^2 / Z_{nw}, \\ F_{\downarrow\uparrow} &\sim 2\Delta \lambda^2 k^2 / Z_{nw}, \\ F_{\downarrow\downarrow} &\sim 2\Delta ik\lambda \left(\mu - \sqrt{\lambda^2 k_f^2 + \mu^2} \right) / Z_{nw}. \end{aligned}$$

Here, we see that $F_{\downarrow\downarrow}$ becomes gradually smaller and $F_{\uparrow\uparrow}$ becomes larger than the s -wave pairing parts, assuming M to be positive. As already noted in the previous section, we obtain a dominant p -wave component for the spin triplet component where the spins are parallel to the magnetic field.

Because Δ_2 is zero we enter the regime of a single non-degenerate branch. Therefore, a single zero-energy Majorana mode appears. However, due to the gap closing at $k = 0$ the Majorana mode is not localized yet. For localization, the gap has to open again and that is the regime we are going to discuss in the next subsection.

4.2.3 Regime $M \gg \sqrt{\Delta^2 + \mu^2}$, “Majorana” regime

The situation is sketched in Fig. 4.1(c). The gap at $k = 0$ reopens. The pairing wave function at Δ_1 satisfies

$$\begin{aligned} F_{\uparrow\uparrow} &\sim -2\Delta ik\lambda \left(M + \sqrt{\lambda^2 k_f^2 + M^2} \right) / Z_{nw}, \\ F_{\uparrow\downarrow} &\sim -2\Delta \lambda^2 k^2 / Z_{nw}, \\ F_{\downarrow\uparrow} &\sim 2\Delta \lambda^2 k^2 / Z_{nw}, \\ F_{\downarrow\downarrow} &\sim 2\Delta ik\lambda \left(M - \sqrt{\lambda^2 k_f^2 + M^2} \right) / Z_{nw}. \end{aligned}$$

We see that for increasing M the p -wave part becomes more pronounced and that $F_{\uparrow\uparrow}$ becomes larger than $F_{\downarrow\downarrow}$. $F_{\downarrow\downarrow}$ actually goes to zero for increasing positive field. For negative field $F_{\downarrow\downarrow}$ will be dominant as one would expect for the

opposite field direction. Around $k = 0$ there is no interaction anymore between the hole and electron branches and, as noted before, the degeneracy in the p -wave order parameters disappears in this regime. Since the gap at $k = 0$ has reopened again we also have a proper localized single Majorana mode at the ends of the nanowire. Just as the surface states of a topological insulator are localized to a surface, the Majorana mode in a nanowire is localized at the ends of the nanowire due to the vacuum gap at one side and the superconducting gap with a reversed band order on the other side. The reversed band order ensures that the bands are crossing at the ends of the nanowire resulting in a localized end mode similar to the topological surface and edge states in topological insulators.

At Δ_3 we have

$$\begin{aligned} F_{\uparrow\uparrow} &\sim -2\Delta ik\lambda M/Z_{nw}, \\ F_{\uparrow\downarrow} &\sim 2\Delta (M^2 - k^2\lambda^2)/Z_{nw}, \\ F_{\downarrow\uparrow} &\sim -2\Delta (M^2 - k^2\lambda^2)/Z_{nw}, \\ F_{\downarrow\downarrow} &\sim 2\Delta ik\lambda M/Z_{nw}. \end{aligned}$$

Hence, the s -wave pairing becomes dominant for increasing magnetic field at Δ_3 , but as discussed before it is safe to ignore it in the low excitation regime.

Note, that all of the expressions in this section can be generalized to two dimensions. This could be relevant for InAs thin films for example. The scalar k has to be replaced by a $\mathbf{k}$ -vector with an amplitude $|\mathbf{k}|$ and phase $e^{i\theta}$ analogous to the 3D topological insulator discussed below. The $e^{i\theta}$ factor denotes the chirality of one branch and $e^{-i\theta}$ the chirality of the other branch present at the Fermi level. Apart from an additional $e^{i\theta}$ and $e^{-i\theta}$ factor in the expressions of the order parameter, the given conclusions would still be valid.

4.3 Pairing wave function in 3D topological insulators

For a 3D topological insulator ϵ_p and the SOC strength in x and y -direction in Eq. (4.1) are equal to μ and the Fermi velocity v respectively. The matrix $[E - H]$ in the relation $[E - H]\mathbf{G} = \mathbb{1}$ is then given by

$$\begin{bmatrix} E + \mu - M & -v|k|e^{i\theta} & 0 & -\Delta \\ -v|k|e^{-i\theta} & E + \mu + M & \Delta & 0 \\ 0 & \Delta & E - \mu + M & -v|k|e^{-i\theta} \\ -\Delta & 0 & -v|k|e^{i\theta} & E - \mu - M \end{bmatrix}, \quad (4.18)$$

where M is a magnetization term and θ is the angle between k_x and k_y . We assume in this section that $\mu > E_{DP}$ where DP stands for the Dirac point, but the opposite “hole” regime of $\mu < E_{DP}$ can also easily be obtained. The energy dispersion relations are

$$E = \pm \sqrt{E_{t'}^2 \pm 2\sqrt{E_{s'}}} \quad (4.19)$$

where $E_{t'} = M^2 + \Delta^2 + \mu^2 + |k|^2 v^2$ and $E_{s'} = M^2 \Delta^2 + M^2 \mu^2 + |k|^2 v^2 \mu^2$. Also here we assume that $\mu \gg \Delta$. The anomalous part of the Green function matrix then becomes

$$\begin{aligned} F_{\uparrow\uparrow} &\sim 2\Delta|k|ve^{i\theta}(M + \mu)/Z_{TI}, \\ F_{\uparrow\downarrow} &\sim \Delta(M^2 - |k|^2 v^2 - \mu^2)/Z_{TI}, \\ F_{\downarrow\uparrow} &\sim -\Delta(M^2 - |k|^2 v^2 - \mu^2)/Z_{TI}, \\ F_{\downarrow\downarrow} &\sim 2\Delta|k|ve^{-i\theta}(M - \mu)/Z_{TI}, \end{aligned} \quad (4.20)$$

$$\begin{aligned} Z_{TI} &= -B_{TI}^2 - 4(-vk_x\mu - ivk_yM)^2 - 4(-vk_y\mu + ivk_xM)^2, \\ B_{TI}^2 &= (\mu^2 + v^2|k|^2 - M^2)^2 + 2\Delta^2(\mu^2 + v^2|k|^2 - M^2). \end{aligned} \quad (4.21)$$

Following the same argumentation as in the nanowire case, opposite spin elements correspond to s -wave pairing and the other with p -wave pairing. We see that in contrast to the 1D nanowire case, an additional $e^{\pm i\theta}$ factor appears in the triplet pairing amplitudes. This factor shows the chiral p -wave character of an s -wave proximized 3D topological insulator. We will also consider here three regimes: $|M| = 0$, $M < \mu$ and the “Majorana” regime.

4.3.1 Regime $|M| = 0$

Assume a homogenous magnetization term (for example an external magnetic field as in the nanowire case). In the regime $|M| \ll \mu$ we have the situation as depicted in Fig. 4.1(d). There is only one gap opening because the branch with opposite helicity is not present in the TI case. The branch that is present corresponds to the branch in the nanowire where Δ_1 is opening. The magnitude of the anomalous Green function relations reduces in this limit at Δ_1 to

$$\begin{aligned} F_{\uparrow\uparrow} &\sim 2\Delta|k||k_f|e^{i\theta}/Z_{TI}, \\ F_{\uparrow\downarrow} &\sim -2\Delta|k|^2/Z_{TI}, \\ F_{\downarrow\uparrow} &\sim 2\Delta|k|^2/Z_{TI}, \\ F_{\downarrow\downarrow} &\sim -2\Delta|k||k_f|e^{-i\theta}/Z_{TI}. \end{aligned}$$

So also in the 3DTI an equal admixture of p and s -wave pairing exists in the regime $M = 0$. This result is similar to the result found by Tkachov in Ref. [141, 142] for a topological insulator. In Ref. [8] Fu and Kane transform to another basis, $c_k = (\psi_{1k} + e^{i\theta}\psi_{1k})$, in which the Hamiltonian becomes equivalent to a spinless $p_x + ip_y$ (dominant p -wave). Although this transformation is an elegant way to show that p -wave relations are present, when doing predictions for the experimental outcome in this basis, a transformation also has to be made to the s -wave superconductor deposited on top. This would also cause an additional phase shift in the normal superconductor through which one can then conclude that p -wave is not longer dominant. Nonetheless, the existing proposals of Fu and Kane for Majorana devices [8] still hold as it was already noted that breaking time-reversal symmetry can make $p_x + ip_y$ dominant, as we will see next.

4.3.2 Regime $M < \mu$

As soon as we turn on the perpendicular magnetization term, so that we have a finite M , the relations become

$$\begin{aligned} F_{\uparrow\uparrow} &\sim 2\Delta e^{i\theta} \sqrt{(\mu - M)(\mu + M)^3} / Z_{TI}, \\ F_{\uparrow\downarrow} &\sim -2\Delta (\mu^2 - M^2) / Z_{TI}, \\ F_{\downarrow\uparrow} &\sim 2\Delta (\mu^2 - M^2) / Z_{TI}, \\ F_{\downarrow\downarrow} &\sim -2\Delta e^{-i\theta} \sqrt{(\mu - M)^3(\mu + M)} / Z_{TI}. \end{aligned}$$

In analogy to the nanowire case, one of the p -wave correlations becomes larger than the s -wave correlations as soon as time-reversal symmetry is broken. Opposite to the nanowire case, there is no degeneracy and only a single dominant p -wave pairing gap is present. Unfortunately, this still does not mean that a Majorana zero-energy mode exists as soon as we apply magnetization, because the zero-energy mode is not yet fully localized as one would have in the nanowire Majorana regime. As already noted by Fu and Kane [8], the 2DTI surface has no edge, which prevents a localized Majorana bound state to form. The same is true in a 2D topological insulator where 1D edge states can go around the 2D topological insulator. We therefore need a different device in order to localize the zero-energy mode.

Note, that in this regime a single dominant p -wave component is already present. It is therefore possible to already observe dominant p -wave features. This is also true for the nanowire albeit with a degenerate p -wave order parameter.

4.3.3 The “Majorana” regime

One way to create an edge *and* break time-reversal symmetry is shown in Fig. 4.2(a). The M denotes the magnetization induced by the ferromagnet. We assume here that we have an insulating ferromagnet so that the current is only going through the surface states. A different way is to have a Josephson junction with a phase difference between the two superconductors [8]. For now, we focus on the device in Fig. 4.2(a). In order to have a localized zero-energy mode, the Majorana mode needs to be localized both at the superconducting side and at the ferromagnet side. At the superconducting side the superconducting gap is doing the job. At the ferromagnet side, the magnetization has to be large enough such that the Fermi level is inside the gap (see Fig. 4.2(b)). Then, the zero-energy mode is fully localized. To be more specific, in order to have a proper localized Majorana mode one has to satisfy the relation $M(x) > \sqrt{\Delta(x)^2 + \mu^2}$ at the ferromagnet side. We also included the superconducting gap as a function of position to take the proximity effect into account.

Figure 4.2 (a) A ferromagnet insulator(FI) can both break time-reversal symmetry and localize the Majorana zero-energy mode in a TI. The location of the Majorana mode is indicated by the white arrow. (b) The dispersion relation of the topological insulator at the ferromagnet side for a magnetization smaller and larger than the chemical potential. In the former, the chemical potential still lays in the Dirac cone. In the latter, the states around the chemical potential are gapped out and the zero-energy mode is localized at the interface between the superconductor and ferromagnet. (c) Calculation of the surface Andreev bound state. To model the suppression of the superconducting gap of the superconducting topological insulator (STI) we assume a normal part in the order of the coherence length ξ_0 at the interface between the superconductor and the ferromagnet.

4.4 Surface Andreev bound states and Majorana zero-energy modes

So far we have looked at properties of the bulk, i.e. the inner part of the nanowire or the s-wave proximized 2D surface states of the topological insulator. We are now going to discuss the properties at the interface between the superconductor and ferromagnet where the Majorana zero mode is formed in the Majorana regime. It is expected that different symmetries are present at the surface or edge of a superconducting system as noticed in Ref. [55, 143]. Due to a finite size, translational symmetry is broken in that direction. The orbital symmetry (even or odd) is then not a well-defined parameter anymore, giving rise to mixed odd and even symmetry at the interface. The spin pairing symmetry, however, is not affected by the finite size. The only option, then, to have an asymmetric wave function is to allow for odd-frequency states at the interface.

Figure 4.2(a) shows the superconductor/ferromagnet device needed to localize a Majorana state. In experiments it is useful to use a ferromagnetic *insulator* (FI) to ensure that the magnet itself does not shunt the device [66]. We will, therefore, indicate the ferromagnet by FI in the remaining part of the paper.

Assume, that we are in the regime with a fully localized Majorana state, i.e. $M > \mu$. The resulting SABSs can be calculated by considering a small non-superconducting region in the order of the coherence length to model the suppression of the gap near the edge (Fig. 4.2(c)). We use the wave functions described in Chap. 2 to calculate the SABSs. The direction of the transmitted waves in the superconductor is chosen such that k is conserved parallel to the interface. We assume that the electrons in the non-superconducting part are confined and therefore, that they completely reflect back at $x = -L$.

The phase difference that is picked up in one round trip (Fig. 4.2(c)) is

$$\begin{aligned} 2L(|k_e| - |k_h|) - 2\theta + 3\pi + 2 \arccos E/\Delta &= 2\pi n \\ &= \frac{4LE}{\hbar v_f \cos \theta} - 2\theta + 3\pi + 2 \arccos E/\Delta \end{aligned} \quad (4.22)$$

so

$$\frac{E}{\Delta} = \cos \left(-3\pi/2 + \theta + \frac{2LE}{\hbar v_f \cos \theta} \right) \quad (4.23)$$

$$= -\sin \left(\theta + \frac{2LE}{\hbar v_f \cos \theta} \right). \quad (4.24)$$

Taking the limit $L \rightarrow 0$ we have

$$\frac{E}{\Delta} = -\sin(\theta) \quad (4.25)$$

$$= -k_y/|k|. \quad (4.26)$$

When the magnetization of the FI is in the exact opposite direction, the resulting ABS is $\frac{E}{\Delta} = \sin(\theta)$. This is exactly the SABS of a chiral p -wave superconductor [34].

In order to determine the features of the SABS and its relation to Majorana zero energy modes, we consider the regimes around $E = 0$ and $E \neq 0$ in more detail in the following.

4.4.1 Around $E = 0$

In Fig. 4.2(c) we can calculate the reflection and transmission coefficients of the electron and holes at the interface by using continuation of the wave function. From these coefficients it follows that the total wave function in the superconducting part in the electron-hole basis $[\psi_{k\uparrow}, \psi_{k\downarrow}, \psi_{-k\uparrow}^\dagger, \psi_{-k\downarrow}^\dagger]$ is given by

$$\Psi = \frac{e^{i\theta}}{\Delta} \begin{pmatrix} (E - i\tilde{\Omega}) \\ -e^{-i\theta}(E - i\tilde{\Omega}) \\ \Delta e^{-i\theta} \\ \Delta \end{pmatrix} e^{-ikr} e^{-r/\xi_0}$$

$$+ \frac{1}{E + i\tilde{\Omega}} \begin{pmatrix} (E + i\tilde{\Omega}) \\ (E + i\tilde{\Omega})e^{i\theta} \\ -\Delta e^{i\theta} \\ \Delta \end{pmatrix} e^{ikr} e^{-r/\xi_0}, \quad (4.27)$$

where $\tilde{\Omega} = \sqrt{\Delta^2 - E^2}$ and $\xi_0 = \sqrt{\Delta^2 - E^2}/v_F$. Around $E = 0$ (and so around $\theta = 0$) the expression for the Majorana zero mode becomes

$$\Psi = e^{-x/\xi_0} \begin{pmatrix} 2e^{-i\pi/4} \cos(kx + \pi/4) \\ 2e^{i\pi/4} \cos(kx - \pi/4) \\ 2e^{i\pi/4} \cos(kx + \pi/4) \\ 2e^{-i\pi/4} \cos(kx - \pi/4) \end{pmatrix}. \quad (4.28)$$

Note, that this expression is consistent with the result found by Tanaka and Asano in a semiconductor/superconductor device [130]. In their case, an additional magnetic field is applied through which only the spin up part survives of Eq. (4.28).

To give a complete picture of the properties of these Majorana zero-energy mode, we calculated the frequency symmetry of this zero-energy state. The anomalous Green's function can be obtained by the relation

$$F(E, r, r'; \theta)_{\uparrow\downarrow} = \Sigma_n \left[\frac{u_{n\uparrow}(r)v_{n\downarrow}^*(r')}{E + i\delta - E_n} + \frac{v_{n\uparrow}^*(r)u_{n\downarrow}(r')}{E + i\delta + E_n} \right]. \quad (4.29)$$

where u and v are the electron and hole parts respectively.

The relationship at $x = x' = 0$ satisfies

$$\bar{F}_{\beta,\alpha}(\mathbf{r}, E, \mathbf{p}) = -[F_{\alpha,\beta}(\mathbf{r}, -E, \mathbf{p})]^* \quad (4.30)$$

where $\bar{F}$ denotes the conjugated of F and α and β are the spin-indices [139], which means the Cooper pairs are odd-frequency pairs. The spatial symmetry of Eq. (4.28) satisfies the s -wave symmetry. Therefore the boundary of a pure p -wave even-frequency superconductor is a pure s -wave, odd-frequency state. The appearance of odd-frequency states near zero-energy is also noted in calculations on spinless p_x and $p_x + ip_y$ superconductors [144].

4.4.2 $E \neq 0$

In a similar way as discussed for zero energy we can calculate the anomalous Green function for energies larger than zero. We find that there is an admixture between even and odd-frequency. The odd and even-frequency parts are, respectively, given by

$$F_{\text{odd}} \sim \sqrt{1 - E^2/\Delta^2}, \quad (4.31)$$

$$F_{\text{even}} \sim E/\Delta. \quad (4.32)$$

Near zero-energy, the odd-frequency part is dominant and the even-frequency contribution grows with E . The emergence of a (partly) odd-frequency amplitude at the surface/interface due to spatial non-uniformity is well-known for

Figure 4.3 (a) In the calculation of the conductance we consider two electrodes: the proximized TI by the FI and the proximized TI by the s -wave superconductor. (b) In order for the Andreev formalism to hold, the distance between the FI and the superconductor should be smaller than the mean free path and the coherence length.

superconducting systems [55, 145–147]. However, in this case, we have a full odd-frequency state at zero energy. Therefore the conclusion of Asano and Tanaka [130] holds that in these devices pure odd-frequency Cooper pairs and the Majorana zero-energy mode are one and the same thing.

4.5 TI/STI tunneling conductance

In the study of the conductance we consider the system where one electrode consists of the topological insulator proximized by the FI and the other electrode of the topological insulator proximized by the s -wave superconductor as depicted in Fig. 4.3(a). We assume here that the magnetization is smaller than the chemical potential in the magnetic topological insulator electrode. We modelled this magnetic TI/STI interface by using the wave functions in the magnetic TI and STI as described in Chap. 2 and match them at the interface such that

$$\psi_{in} + a\psi_h + b\psi_e = t_e\psi_{Se} + t_h\psi_{Sh} \quad (4.33)$$

where ψ_h is the reflected hole, ψ_e the reflected electron, ψ_{Se} the transmitted quasi-particle in the electron branch of the superconductor, ψ_{Sh} the transmitted quasi-particle in the hole branch of the superconductor and a , b , t_e and t_h are the Andreev, normal, electron transmission and hole transmission coefficients respectively. We calculated then the conductance by using the relation

$$\frac{G}{G_0} = \frac{\int_{-\pi/2}^{\pi/2} d\theta \cos(\theta) T(\theta, eV)}{\int_{-\pi/2}^{\pi/2} d\theta \cos(\theta) T(\theta, eV) |_{\Delta=0}}, \quad (4.34)$$

where $T(\theta, E) = 1 + |a|^2 - |b|^2$ and θ is the angle between k_x and k_y . The Andreev formalism holds when the distance between the superconducting and the ferromagnet side is smaller than the coherence length and the mean free path

(l_{mean}) as drawn in Fig. 4.3(b). We choose here to divide the conductance by the energy dependent normal conductance to ensure that the normalized conductance goes to one at large voltage.

We first consider the case with time-reversal symmetry, i.e. without the FI on top of the TI. By means of a gate electric field, the chemical potential at the superconductor side can be tuned independently from the non-superconductor side. Therefore, we make from now on a distinction between the chemical potential at the superconductor and non-superconductor side. In Fig. 4.4(a) we plotted the normalized conductance for different ratios of the STI chemical potential, μ_S , and TI chemical potential, μ_{TI} . A conductance peak at $eV = \Delta$ is appearing for larger barriers due to Andreev resonance at this energy, similar to the s-wave case. Opposite to the s-wave case, the value of the conductance never drops to zero, even for a large mismatch where the barrier height goes practically to infinity ($\mu_S/\mu_T = 1/100$). The conductance inside the gap is close to one instead which can be understood by considering different angles of incidence. The large barrier causes the propagation direction in the superconductor to be almost equal to $\theta = 0$ as follows from the conservation of parallel momentum: $\theta_S = \arcsin(\sin \theta \mu_{TI}/\mu_S)$. The spin in the topological insulator with $\theta = 0$ sees no barrier because of Klein tunneling (which gives perfect Andreev reflection for all energies) and for $\theta = \pi/2$ the spin mismatch is the largest which results in the lowest transparency (perfect normal reflection). For angles inbetween, the transparency of the barrier increases continuously from one to zero for increasing angle of incidence. The angle averaged conductance is therefore close to one.

The presence of a non-zero conductance for energies below the gap, even for large barriers, distinguishes the proximized TI surface from conventional s-wave symmetry superconductors. Although the *p*-wave pairing is not dominant in the time symmetric situation, the *p*-wave correlations are encoded in the non-zero conductance for energies below the gap in the presence of a barrier. The fact that the gap does not go to zero is due to the spin-momentum locking which is also responsible for the *p*-wave correlations.

4.6 TI/STI tunneling conductance with broken time-symmetry

To modulate the TI/STI tunneling conductance with broken time-reversal symmetry we take the set-up as displayed in Fig. 4.3(a). We will use a relatively large chemical potential compared to the superconducting gap to model the experimentally realistic regime. The topological insulators so far have the Dirac point close or at the same energy as the bulk bands so as long as the chemical potential is in the gap, the chemical potential is likely much larger than the superconducting gap. We argued in Chap. 2, that a magnetization in the case of a ferromagnet insulator will only be a few percent of the chemical potential. However, to see the effect of the broken time-symmetry we also modulated the conductance spectrum for a magnetization value of $0.95\mu_{TI}$. This result is shown in Fig. 4.4(b). There are two distinguished features compared to an N/S interface, namely a

Figure 4.4 (a) Conductance spectra for a TI/STI configuration for different mismatches in chemical potential. (b) Conductance spectra for a magnetization $M/\Delta=95$, $\mu_{TI}/\Delta=100$ and different mismatches in chemical potential. (c) Conductance spectra for a magnetization $M/\Delta=10$, $\mu_{TI}/\Delta=100$ and different mismatches in chemical potential. (d) The conductance spectra for different values of magnetization and $\mu_{TI}/\Delta = \mu_S/\Delta=100$. Even if the magnetization is smaller than the chemical potential, clear signatures of the SABSs are still visible.

zero-bias peak (ZBP) and a conductance dip at $eV = \Delta$. The appearance of these two features for large magnetization is also reported by Linder *et al.*[66]. Both features are due to the formation of SABSs at the interface. In fact, the SABSs have a constant density of states at energies between $-\Delta$ and $+\Delta$ as follows from Eq. (4.26), but from conservation of parallel momentum it follows that the angles near zero have a larger transparency. The coherence peaks at the gap energy in the low barrier limit, are replaced by resistance peaks at the same energy. The coherence dips at Δ arise from the spectral weight transfer from high to low energy due to the formation of SABSs. This results in a decrease of the density of states at Δ . Therefore, next to a zero bias conductance peak, also coherence dips are a distinguished feature of a p -wave order parameter compared to s -wave.

Note, that the surface states are not fully gapped yet with a magnetization of 95% of the chemical potential, i.e. the chemical potential is not inside the gap at the FI side. We are therefore not in the topologically non-trivial regime. However, the increased reflection at the interface or enhanced p -wave pairing symmetry due to magnetization, causes the SABS to form at the interface. If we use a

magnetization value of 10% of the chemical potential in the TI, Fig. 4.4(c) is obtained. We see there is only a small effect on the conductance spectra around zero energy at Δ compared to the time-reversal symmetry case in Fig. 4.4(a). Figure 4.4(d) shows the effect of increasing the magnetization for $\mu_{TI} = \mu_S = 100\Delta$. Gradually, the conductance at zero energy increases while at Δ the conductance decreases due to the formation of SABSs for larger magnetization. It shows that the ZBP and conductance dip at the gap energy come together. That is, if one has a dominant p -wave pairing wave function and if one observes a ZBP, then also the conductance dips are present. As soon as the ZBP becomes less pronounced, as is the case for lower magnetizations, the conductance dip at $eV = \Delta$ is less pronounced. The observation of *both* a ZBP and a conductance dip is a strong signature for a p -wave state. For practical ferromagnets that have a magnetization in the order of a few percent of the chemical potential of the TI, it is not expected to see this particular p -wave signatures back in the conductance spectra. A pronounced deviation from s -wave behaviour starts to occur when $M/\Delta = 60$ (see Fig. 4.4(d)). With a typical exchange energy of 40 meV [148, 149] it means that one has to gate tune the chemical potential to about 70 meV from the Dirac point, which seems doable experimentally [150, 151].

4.7 Discussion and conclusion

An equal admixture of s and p -wave correlations exists in a 3D topological insulator proximized by an s -wave superconductor. By inducing a perpendicular magnetization, the p -wave pairing becomes dominant. For a magnetization energy as large as the chemical potential, the topological regime is entered with Majorana modes.

We studied the symmetry of the bound state of a 3D topological insulator in the Majorana regime. Green function techniques show us that the pure odd-frequency pairing state at interfaces is equivalent to a zero-energy Majorana mode.

In the conductance spectra the increasing p -wave pairing can be observed by the presence of a ZBP together with a conductance dip at the gap energy. In the time-reversal symmetric case, the non-zero sub-gap conductance in the presence of large interface barriers, indicates that p -wave correlations are present.

CHAPTER 5

Conductance spectroscopy of a proximity induced superconducting topological insulator

We study the proximity effect between a superconducting topological insulator (STI) and the normal part of a topological insulator (TI) in $\text{Au}/\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}/\text{Nb}$ devices. The conductance spectra of the devices show the presence of an induced gap in the STI as well as induced superconducting correlations in the normal part of the TI on the order of the Thouless energy. The shape of the conductance modulation around zero-energy varies between devices and can be explained by existing theory of *s*-wave induced superconductivity in SNN' devices. All the conductance spectra show a conductance dip at the induced gap of the STI.

5.1 Introduction

The proximity effect between an *s*-wave superconductor and a three-dimensional topological insulator (3DTI) or nanowire with strong spin-orbit coupling has been predicted to create a Majorana zero-energy mode that may serve as the building block of a topological quantum computer [2, 5, 8, 12, 13, 41, 44, 64, 65, 126, 128, 152, 153]. The presence of peaks in the conductance at zero-energy has been interpreted as experimental evidence for the existence of Majorana modes in such systems [132–134, 154]. It is also known from theoretical studies that a zero-bias conductance peak and conductance dips at the characteristic gap energy are typical features of Majorana zero-energy modes [8, 34, 66, 130, 155–157] (see also Chap. 4).

We study the proximity effect between an *s*-wave superconductor (Nb) and a 3DTI with dominant surface transport ($\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$, BSTS) in more detail. Although no Majorana zero-energy modes are expected in these devices, it has been predicted that unconventional superconducting correlations are already present [141, 142] (see also Chap. 4) at the interface between a topological insulator and an *s*-wave superconductor. We performed differential conductance measurements on Nb/BSTS/Au devices (see Fig. 5.1). Here, the normal metal reservoir (Au) was placed close to the superconductor-3DTI interface with a

Figure 5.1 (a) A schematic view of the device and SEM picture of the small area indicated in the schematic view for a typical Au/Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}/Nb trilayer. For clarity, the BSTS flake is not shown in the schematic view. Two contacts are used for applying a current. The other two contacts are used to measure the voltage across the trilayer. The spacing between the Au and Nb leads is 50 nm and the width of the contacts is around 300 nm. (b) Side view of the device.

lateral spacing comparable to the mean free path in BSTS to obtain information about the induced pairing in the 3DTI material.

Fabrication

All devices were prepared by exfoliation from a single crystal of BSTS. BSTS crystals were grown using the Bridgman method briefly described in Chap. 3.* Flakes were transferred from a BSTS crystal to a Si/SiO₂ substrate by the use of mechanical exfoliation. Device 2 and 3 were fabricated simultaneously on a single substrate with flakes that originated from the same cleavage. Device 1 was prepared separately with a flake from a different exfoliation cycle. By means of e-beam lithography (EBL) the Au electrode is defined on the flake. Next, we perform a low voltage 15 s etching step to avoid large damaging of the surface followed by sputtering in-situ a 3 nm Ti layer and a 60 nm Au layer. The Ti layer is grown for better adhesion of the Au on the flake. Next, a second EBL step is performed to define the Nb part of the device. After the EBL step the structure is etched for 15 s at low voltage, followed by in-situ sputtering of 80 nm Nb. BSTS has a small mean free path of 10–40 nm. Therefore, we optimized

*Crystal growth is done by Y. (Yingkai) Huang and D. (Dong) Wu at the Van der Waals-Zeeman Institute in Amsterdam.

Figure 5.2 (a) Microscopic picture of a device to determine the contact resistance between Au and $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$. The contact area is $1 \mu\text{m}^2$. The smallest channel length is $1.5 \mu\text{m}$. The largest is $4.5 \mu\text{m}$ in this picture. Around the leads the original shape of the flake can still be recognized by the colour difference between the middle area of the picture and the surroundings. (b) The resistance of the channels from 300 to 50 K in steps of 50 K.

the EBL step, so that a spacing of 50 nm between the two electrodes exists to make sure that the BSTS is fully proximized by the superconductor (see also Chap. 3). The width of the electrodes is about 300 nm. To avoid damage to the material by physical or chemical etching, we omitted shaping the 3DTI flakes. Therefore, a small contribution to the device conductances results from current spreading laterally on the surface of the flake. Based on the device dimensions, we estimate[†] this contribution to be $\sim 10\%$ for devices 2 and 3 and $\sim 20\%$ for device 1.

Contact resistance

To determine the contribution of the contact resistance between BSTS and the electrodes, we prepared Au/BSTS/Au devices using the same growth parameters as described above with channel lengths between $2 \mu\text{m}$ and $4 \mu\text{m}$ and a width of $2 \mu\text{m}$. The channels are prepared on the same flake that is shaped into different channel lengths by means of Ar ion milling. In this way we also avoid ambiguity in the measured voltage drop [158]. Due to the larger areas of the channels compared to the Au/BSTS/Nb devices we expect that the Ar ion milling step has insignificant influence on the total resistance. The contact area between the electrode and the BSTS is $1 \mu\text{m}^2$. Thereafter, we performed a two point measurement of the resistance as function of temperature for the various channels in a Physical Property Measurement System (PPMS).

In Fig. 5.2(a) a microscopic picture is shown for a device to determine the contact resistance between Au and BSTS. Fig. 5.2(b) shows measurement data obtained from this device. We see that above 200 K the resistance as function

[†]We estimated the total resistance of the surrounding BSTS and the resistance of the BSTS between the electrodes by determining the width and length ratio and assuming a constant resistivity. By using a parallel resistor model we estimated the relative contribution of the surrounding BSTS.

of the channel length is linear, as expected. However, for 200 K and lower, the data points start to deviate from the linear behaviour.

To exclude that a difference in thickness of the different channels is the origin of the resistance behaviour as function of temperature, we measured by means of an atomic force microscope (AFM) the thickness of the various parts. We measured an average thickness of 112 nm with a deviation of 4 nm which is too small to explain the large difference in resistance among the channels.

The deviation can be understood in terms of the inhomogeneity of BSTS. We fitted the RT-curves of the different channels with $\sim e^{-E_g/k_B T}$ where E_g is the distance of the Fermi level to the conduction band. For the channels of 1.5, 2.5 and 3.5 μm (channel 1, 2 and 3 respectively) we obtained respectively for E_g 1.35 meV, 0.85 meV and 1.20 meV. In a semiconductor picture this means that for lower temperatures more carriers are present per unit area for channel 2, followed by channel 3 and then channel 1. Considering Fig. 5.2(b) again this picture is consistent with the resistance distribution of the three channels. This implies then that the difference in carrier densities in the three channels is due to a modest difference in E_g . This effect is stronger than the dependency on the channel length at low T . The modest variation in the position of the Fermi level is probably due to the inhomogeneity of the BSTS samples.

Although this interpretation is consistent with the data, it does not exclude the possibility that the origin of the deviation of the data from a linear behaviour is due to a difference in contact resistance between the Au electrodes and the BSTS. In that case, the contacts can also behave differently as a function of temperature which will lead to scatter in the data as a function of channel length.

In both cases, the contribution of the contact resistances to the conductance measurements remains unknown. Therefore, the contact resistance is treated as an additional parameter in the interpretation of the data.

5.2 Conductance measurements

Two sets of differential conductance measurements were performed with a lock-in amplifier using an AC excitation of 12 nA (device 1) and 50 nA (device 2 and 3). Conductance spectra of device 1 (depicted in the inset of Fig. 5.1(a)) were recorded at several temperatures in the range between 250 mK and 1.5 K (see Fig. 5.3(a)). Devices 2 and 3 were measured at a fixed temperature of 1.7 K (Fig. 5.3(b) and (c)). Although the line shapes of individual devices look distinctly different, several common features are readily identified: All traces display a dip in the conductance at voltages comparable to the gap energy in the superconductor. This is clearly seen in device 1 at the lowest measurement temperature where the recorded dip voltage $V_d = 1.3$ mV is close to the expected gap of the Nb electrode with critical temperature $T_c = 8.4$ K[‡]. As the measurement temperature is increased, the position of the conductance dip moves toward lower voltage. The temperature dependence of the dip position V_d of device 1 is shown

[‡] T_c is measured as an abrupt drop in the device resistance at T_c in an RT measurement in Fig. 5.3(d).

Figure 5.3 Measurements of Au/Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}/Nb devices. (a) Measurements of the conductance of device 1 at different temperatures. For clarity we have given the data corresponding to different temperatures an off-set in steps of $0.1 \cdot 10^{-3} \Omega$. At 1.5 K the off-set is zero and for 253 mK the off-set is the largest. At higher temperatures we see a slight decrease of the gap indicated by the dashed line. The conductance dip at zero energy decreases at higher temperature which is consistent with the behaviour of the proximity effect for normal *s*-wave superconductivity. The dotted line shows the dip position V_d and the red solid line shows the position of a Thouless peak, marked as V_{TH} . The peak positions are also plotted in Fig. 5.4(b). The conductance dips below the gap value are reproduced in all three devices. (b) The blue curve shows the derivative of the conductance as function of voltage to show more clearly that a conductance dip is present at 1.3 meV. Around zero voltage we observe a conductance peak. (c) In device 3 we observe a conductance peak around zero voltage with a small conductance dip modulation on top. (d) An RT measurement of device 1.

in Fig. 5.4(b). Also the dip positions of device 2 and 3 are plotted at 1.7 K. In devices 2 and 3 the dip features appear to have moved significantly below the bulk gap of niobium. However, in device 2 a small depression remains at 1.3 mV which is seen more clearly in the derivative of the conductance spectrum (dashed trace in Fig. 5.3(b)).

The presence of a second, lower characteristic energy scale is evident from the modulation of the conductance spectra at smaller voltages. Devices 1 and 3 show a dip, whereas device 2 exhibits a zero-bias conductance peak. The widths of the features range between 400 and 800 μV and are indicated by V_{TH} in Fig. 5.3(a–c). Unlike the positions of the dips in the conductance spectra of device 1, the voltages at which the peaks appear, do not show a strong temperature dependence, see Fig. 5.4(c).

5.3 Discussion

Superconducting proximity effect

Below, we will argue why the measurement data of Fig. 5.3 can be interpreted as a strong proximity effect between the Nb superconductor electrode and the underlying TI, making this into a superconductor topological insulator (STI) with a sizable induced gap. The STI, then, has a lateral proximity effect with the uncovered TI, giving rise to peaks at the Thouless energy for a diffusive system.

Theoretical studies on the influence of the superconducting proximity effect by means of Green function techniques make use of two important parameters: γ and γ_B , defined as

$$\gamma = \frac{\rho_S \xi_S}{\rho_N \xi_N}, \quad \gamma_B = \frac{R_B}{\rho_N \xi_N}. \quad (5.1)$$

The former is a measure of the strength of the proximity effect and the latter is related to the transparency of the barrier. Here, R_B is the interface resistance of the superconductor/TI boundary, $\rho_{S,N}$ and $\xi_{S,N}$ are the normal resistivities and coherence length of the superconductor (S) and topological insulator (N) material. The induced gap Δ'_{STI} due to the proximity of Nb to the TI (see Fig. 5.4(a) and (b)) is determined by the values of γ and γ_B at the Nb/BSTS interface. Besides this perpendicular proximity effect, there also exists a (lateral) proximity effect (Fig. 5.4(c)) between the STI and the uncovered topological insulator part (TI in Fig. 5.4(a)) [121, 159–162].

For a 2DEG in contact with a superconductor, γ is small because of the small ratio of the resistivities (as the topological surface states are 2D and the Nb superconductor 3D) and an upper limit of 0.01 can be used [163]. Due to this small value for γ the inverse proximity effect can be neglected and, as a result, the gap size of Nb is unaffected and decoupled from the STI below [121, 159–162]. The temperature dependence of the Nb gap according to BCS theory is shown in Fig. 5.4(b). However, the observed dip feature in device 1 decreases faster as function of temperature. We attribute this feature to the induced gap Δ'_{STI} . In Ref. [121], for example, it is shown that the induced gap decreases faster as function of temperature although it has the same critical temperature shown by the dashed curve in Fig. 5.4(b). The energy corresponding to the dip features in device 2 and 3 are also plotted in the same graph. At low temperatures, the dip feature reaches 1.3 mV which is close to the Nb gap which indicates that the interface between the Nb and BSTS has a high transparency. The dip features of device 2 and 3 are lower in energy than the dip feature of device 1 which can be due to a less transparent interface.

In both the ballistic and the diffusive limit the characteristic energy scale associated with the induced superconductivity is related to the dwell time in the junction and is known as the Thouless energy. For the ballistic limit it is given by $E = \hbar v_f / L$ where v_f is the Fermi velocity in the normal metal and L the system size. In the diffusive limit it is defined as $\hbar D / L^2$ where D

is the diffusion constant [164–166]. The expression for the ballistic limit gives a value of 2.2 meV whereas we obtain for the diffusive limit an energy value between 0.15 and 0.6 meV. We used a Fermi velocity of $3.5 \cdot 10^5$ m/s [104], a mean free path between 10 and 40 nm (Chap. 3) and a junction dimension of 100 nm. The value for the ballistic limit exceeds the energy associated with the gap of Nb so that no features due to ballistic transport are expected below the energy gap. However, the diffusive Thouless energy corresponds very well to the energy scale V_{TH} . This suggests that mainly diffusive transport contributes to the measured conductance spectra and that the observed features can be interpreted as signatures of laterally induced superconductivity in BSTS. To conclude, we see that Δ'_{STI} and the induced superconducting correlations in the normal TI part show similar behaviour in all three devices.

Figure 5.4 (a) Proximity effect in Au/Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}/Nb devices. The Nb induces a superconducting gap into the topological surface states (TSS) directly underneath via a strong proximity effect. The created STI then induces laterally superconducting correlations into the uncovered TI part. (b) The Nb gap according to BCS theory is shown (solid line) and the induced gap Δ'_{STI} in the TSS as function of temperature. The dashed line serves as a guide to eye. (c) The induced gap Δ'_{STI} and the laterally induced Thouless proximity peak in the TI as function of temperature.

The shape of the conductance spectra

We interpreted the modulation of the conductance near zero energy as a signature of induced superconductivity in the normal TI part. The common energy scale associated with the features is at the order of the Thouless energy. Despite the similar energy scale, the shape of the curves look different from each other. In device 1 we see a clear conductance dip, device 2 exhibits a conductance peak and device 3 a broad conductance peak with a small conductance dip modulation on top. The appearance of conductance peaks and dips in the order of the Thouless energy is extensively studied in Refs. [164, 167]. It is shown that for a Thouless energy smaller than the gap value, both conductance peaks and dips near zero-energy can be observed, depending on the ratio of the barrier strengths and the ratio between each barrier and the resistance of the normal part. From the relative magnitude of the conductance modulation near zero voltage we extract that the barriers and the resistance of the normal part are of the same order of magnitude [164]. The combination of a resistance ratio of the order of 1 and a small Thouless energy results in the fact that the conductance peak or dip around zero voltage is very sensitive to small variations in the resistance ratios [167]. So even when the devices are fabricated by the same procedure, a variation in the barrier resistance, that naturally occurs in the growth procedure, can re-

Figure 5.5 (a) Simulations of an SNN' device where N has a length of 3 times the coherence length. For lower barrier height the suppression of the LDOS at the NN' interface become larger. (b) Spectral transmission coefficient of the device. The suppression of the LDOS at the NN' interface is not visible in the transmission coefficient. (c) Schematic sketch of the simulated device. The numbers 1 and 2 indicate the interfaces. The N' layer in the model is in the order of the coherence length.

sult in the observed differences around zero voltage [168]. The existence of both zero conductance peaks and dips is also observed experimentally in semiconductor/superconductor [168, 169], graphene/superconductor [170] and in topological insulator/superconductor devices [171, 172].

The conductance dip at Δ'_{STI} is reproduced in all three the devices. There is an additional small conductance dip at the Nb gap in device 2. We speculate that this feature at the Nb gap energy in device 2 is due to direct proximity between the TI part and the Nb superconductor. Normally a strong coherent peak is expected at the (induced) gap energy resulting in a conductance peak instead of a dip. We will discuss the origin of the conductance dip in the remaining part of this section.

A scenario which results in a conductance dip near the gap energy is the presence of charge imbalance but we rule that out due to the absence of a resistance peak at T_c in the RT-measurement [173–176].

It is known that the proximity effect can change the local density of states (LDOS) in the normal layer drastically. In Refs. [165, 177–182] it is theoretically shown that a suppression of the LDOS is possible. In Ref. [177] this phenomenon is explained by the properties of the contacts and the existence of Andreev bound states at energies just below the gap energy. Those Andreev bound states are related to the tunnel character of the contacts, i.e. contacts with a transmission close to zero. If the contacts have a significantly higher transparency, the contribution of those bound states to the total measured conductance decreases, resulting in a suppression of the LDOS. A small γ can enhance this feature as shown in Ref. [181] and in the next subsection.

Suppression of LDOS

In Fig. 5.5(a) simulations of the LDOS at the NN' interface of an SNN' device are presented. The corresponding device is depicted in Fig. 5.5(c). For this purpose, we used the numerical code from Ref. [183]. We simulated the trilayer model for $\gamma_1 = 0.01$ and different barriers. γ_1 and γ_2 are related to the ratio of the superconductor normal state resistivity and the resistivity of the N layer and to the ratio of the resistivity of the N and N' layer respectively. γ_{B1} and γ_{B2}^* are related to the barrier strength at the SN interface and NN' interface respectively. We see that for a lower value of γ_{B1} , i.e. higher transparent Nb/BSTS interface, the suppression of the LDOS increases. The barrier at the Au/BSTS interface or γ_{B2}^* is less relevant. A decrease in γ_2 means a smaller resistivity of the N layer compared to the N' layer, resulting in an increased proximity effect and therefore a larger induced gap. This enhancement implies that there is a stronger coupling to the superconductor and therefore a decrease in tunneling character of the Nb/BSTS barrier. Therefore we also see next to the larger induced gap a larger suppression at the gap energy (compare for example the solid and the dashed trace in Fig. 5.5(a)).

Figure 5.5(b) shows the spectral transmission coefficient, $T(E)$, of the total device around the gap energy calculated by the same methods as in Ref. [164]. Although a clear suppression is visible in the LDOS at the NN' interface, the

suppression does not appear in the total spectral transmission of the device. At zero temperature the differential conductance is $\sigma(V)$ is equal to $T(V)$.

In the above model we used Kupriyanov-Lukichev boundary conditions. A small total resistance implies therefore automatically that the interface is highly transparent. In the case of a transparent interface, the suppression of the LDOS near the NN' interface is not observable in the conductance as the contribution of this interface to the total conductance can be neglected (see Eq. (15) and (14) in Refs. [164, 167] respectively). Moreover, in the simulations in Ref. [177] a hard wall condition is assumed at the NN' (or TI/Au) interface which is due to the large contact area, not applicable to our devices. Now, a model is needed on an SNN' device to study the regime where the NN' interface can have intermediate transparency values by extending the model in Ref. [167] using circuit theory boundary conditions at the NN' interface. From this model we can extract under which conditions the conductance dips still exist when we move slowly away from the hard wall conditions and hence investigate if such a feature can still be present when the barrier resistance is small but with finite transmission.

If the SNN' theory fails to provide dips at Δ'_{STI} , then these features can be a signature of unconventional induced superconductivity. For example, it is shown by Tkachov and Hankiewicz [141, 142] that the *p*-wave and *s*-wave pairing correlations have different spatial dependencies so that it depends on the channel length of the normal part which superconducting pairing correlation is dominant. We have also seen in Chap. 4 that having conductance dips at the gap energy is one of the features of *p*-wave superconducting correlations.

5.4 Noise measurements: initial results

Noise in proximity effect devices is a sensitive probe of induced superconductivity because of the doubling of the noise due to Cooper pairing [184, 185]. We have begun to study the current-noise spectral density of the Au/BSTS/Au and Au/BSTS/Nb devices.[§]

Measurements

The devices have the same dimensions as the devices in the main part of this chapter so that the interpretation of the conductance spectra can be compared to the results of the noise measurements. At low temperatures, energy relaxation is prevented as the sample dimension is smaller than the inelastic scattering length or dephasing length.

The experiments were performed in a ³He insert with 0.6 K base temperature. The temperatures were measured by Johnson-Nyquist noise thermometry. For

[§]We acknowledge Eugene Tikhonov and Vadim S. Khrapai for performing the noise measurements at the Institute of Solid State Physics Russian Academy of Sciences, Chernogolovka, Russia.

Figure 5.6 Noise measurements of Au/BSTS/Au devices at 4.8 K (a), 2.3 K (b) and 0.6 K (c). The red curves are the fits obtained with Eq. (5.2). The Fano factor F is obtained from fitting and decreases with increased temperature.

the shot-noise measurements we measured the voltage fluctuations on a load resistor of 10 k Ω in the frequency range of 15 – 20 MHz. Differential resistance and current noise measurements were performed at the same time.

Figure 5.6 shows the noise measurements on a Au/BSTS/Au sample and Fig. 5.7(a) and (b) for a Au/BSTS/Nb device. Fig. 5.7(c) shows the differential measurement at the same temperature as the noise measurement in Fig. 5.7(b).

Results

The full expression for the power-spectral density S_I of the current fluctuations, due to Johnson-Nyquist and shot noise for low frequencies (i.e. $hf \ll k_B T$) and thermal energies and voltages smaller than the Fermi energy can be written as [185, 186]

$$S_I = 4 \left(\frac{e^2}{h} \right) \sum_n \left[2k_B T \Gamma_n^2 + R_n \Gamma_n q V \coth(qV/2k_B T) \right], \quad (5.2)$$

where n is the number of channels, T the temperature, Γ_n the transmission coefficient of channel n , R_n the reflection coefficient of channel n , q is the charge of the particle and V the voltage. For a constant transmission coefficient Γ Eq.

Figure 5.7 (a) Noise measurement of an Au/BSTS/Nb device at 4.8 K. The effective charge is equal to e . (b) Noise measurement in the sample at 0.6 K. A cross-over in effective charge is observed from $2e$ (red dashed curve) to e (black dashed curve) in the voltage range of between 0.5 mV and 1.0 mV. (c) Differential resistance measurement of the same Au/BSTS/Nb device at 0.6 K. (d) RT-measurement on a Hall bar of $L=6 \mu\text{m}$, $W=3 \mu\text{m}$ and a thickness of 130 nm. The logarithmic dependence below 0.8 K indicates that EEI is dominant at low temperatures.

(5.2) reduces to

$$S_I = \frac{4(1-F)k_B T}{R} + F \cdot 2qI \coth\left(\frac{qV}{2k_B T}\right), \quad (5.3)$$

with R the resistance, I the current, q the effective charge and F the Fano factor. The Fano factor describes the reduction of the noise due to the correlations between the charge carriers compared to an uncorrelated current. The noise measurements on the Au/BSTS/Au devices can be fitted very well with Eq. (5.3) for a charge $q = e$. The Fano factor reaches 0.36 at 0.6 K which is close to $F = 1/3$ for a diffusive wire [187, 188]. This is consistent with our conductance measurements where we concluded (based on the Thouless energy) that diffusive transport is dominant. The Fano factor becomes smaller for higher temperatures. The increase of the noise at $V = 0$ is consistent with the increase of Johnson-Nyquist noise for a constant total resistance and increase in temperature. As the resistance of BSTS is constant within a few percent in this temperature range, this implies that the barrier resistances are also constant in this range. Hence, the change in Fano factor cannot be explained by a change in barrier height. Also processes as the modulation of the carrier density and defects at the barrier

Figure 5.8 (a) Device 1 of the main text. The flake is indicated by the black area. (b) Au/BSTS/Nb device used for the noise measurements of Fig. 5.7(c). An extra contribution from the normal BSTS part is picked up due to the overlap of the larger part of the electrodes and the flake.

and fluctuations in the surface generation-recombination current cannot explain the change in Fano factor [189–192]. All these processes are related to $1/f$ noise which is usually dominant at $f < 100$ kHz and therefore not present in our measurements.

We noticed before that we have to measure at low temperature in order to avoid energy relaxation. According to the measurements shown in Chapter 3 the phase coherence length can already be around 300 nm for several K and hence will lead already at those temperatures to energy relaxation in the BSTS between the Au electrodes. This will reduce the noise and results therefore in a lower Fano factor at higher temperatures.

The noise measurements on Au/BSTS/Nb devices at high temperature (4.8 K) can be fitted with an effective charge $q = e$ and a small Fano factor of 0.07 (Fig. 5.7(a)). Probably this is also due to energy relaxation. At 0.6 K we concluded from the Au/BSTS/Au devices that energy relaxation seems not to be dominant. Therefore, for the Au/BSTS/Nb devices we fix T at 0.6 K. At this same temperature the noise measurement of Fig. 5.7(b) is performed on an Au/BSTS/Nb sample. In the range between -0.5 and 0.5 mV the noise spectra can be fitted with a Fano factor of 0.24 and an effective charge of $q = 2e$. Outside this voltage range the slope changes till it reach a slope corresponding with $q = e$ above 1 mV. This transition between e and $2e$ confirms that transport in these devices is due to the laterally induced proximity effect.

We note that there is a difference between the samples in the main text of this chapter and the samples of the noise measurements. The device layout of the two is shown in Fig. 5.8. An extra current contribution from the non-proximized BSTS can be observed in the noise-measurement-samples. The differential measurement of the Au/BSTS/Nb sample on which the noise measurement in Fig. 5.7(b) is performed, is shown in Fig. 5.7(c). We see again a resistance peak in a voltage range similar to the Thouless energy. However, we observe an additional broader resistance peak ranging from -1 mV to 1 mV. To verify if the pres-

ence of this other broader resistance peak can be explained by electron-electron interaction (EEI) in the surrounding BSTS, we performed additional Hall bar measurements at lower temperatures. The results are shown in Fig. 5.7(d). The quantum correction due to EEI depends on the sample dimension. The thermal diffusion length, $L_T = \pi\sqrt{\hbar D/k_B T}$, determines the crossover between different regimes analogous to the phase coherence length in WAL and WL effects. From Fig. 5.7(d) we see that below 0.8 K the RT-measurement can be fitted well with a logarithmic dependency which is related to EEI in 2D [193–195]

$$\Delta\sigma_{EEI} = \frac{e^2}{4\pi^2\hbar} \left(2 - \frac{3}{2}\tilde{F}_\sigma\right) \ln(T/T_0), \quad (5.4)$$

where $\tilde{F}_\sigma$ is related to the static, screened Coulomb interaction, F , averaged over the Fermi surface by $\tilde{F}_\sigma = -4 + (8/F)(1 + F/2)\ln(1 + F/2)$. We obtain a value $\tilde{F}_\sigma = 0.49$ which is comparable to values found for other topological insulators [195]. The additional feature in the conductance measurement can also be fitted well with a logarithmic dependence where we replaced the thermal energy by the voltage. It suggest that EEI interaction can indeed be the dominant scattering mechanism at low temperatures and be related to the additional feature found in the measurements. The device has a dimension larger than the thermal length indicating that the observed EEI originates from the BSTS around the junction rather than from the BSTS between the electrodes itself. To verify this statement further, measurements are in progress on device 1 in the main text to see if the EEI feature is absent at low temperatures and also to see if a clearer transition in the slope of the noise can then be observed. However, the noise measurements at low T already provide a confirmation of proximity induced superconductivity in our TI.

Follow-up research will focus on the improvement of the statistics and on the noise measurements of Nb/BSTS/Nb samples.

5.5 Outlook beyond this thesis

In this thesis, the first steps towards detecting a Majorana zero-energy mode in superconductor/topological insulator devices are taken. We studied theoretically and experimentally the interaction between Nb and the TI $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$.

The Josephson junction described in Chap. 3 has already a width of 40 nm so that combined with gating experiments we can tune the device into a single channel regime[¶]. The absence of backscattering for the zero angle of incidence state allows then for the observation of a quantized supercurrent in steps of $e\Delta/\hbar$ [107]. In previous experiments the quantized steps observed are smaller than $e\Delta/\hbar$ due to the finite transparency of the interface [196, 197]. Also the 4π periodicity in the Andreev bound states becomes dominant in the single channel regime as the zero-angle of incidence channel causes only the 4π periodic state as discussed in

[¶]We estimated in Chap. 3 that for a 40 nm wide junction and a Dirac velocity of 4.5×10^5 m/s, the Fermi level have to be tuned within 50 meV from the Dirac point.

Figure 5.9 (a) Device for the realization of the braiding of Majorana fermions. Each trijunction can contain one Majorana fermion. By extending the device by more of hexagonal shaped superconductors (or trijunctions) a systems where multiple qubits can be braided is realized. (b) A top view of device (a). δ in the expression of the phase of the upper superconductor is a small phase change compared to the phase π . If δ is changed from a small positive value to a small negative value, the Majorana fermion indicated by the black sphere is transported from the left trijunction to the right trijunction. (After [8])

Chap. 2. However, due to interaction of the Andreev bound states to the phonon bath or to the continuum, the occupation of the 4π -state can change during the measurement and therewith fades out the signature of the doubled periodicity. In order to overcome this problem, there have been different kinds of proposals made to study the doubled periodicity in AC-measurements. Shapiro steps and current noise spectrum measurements are examples of such measurements. In Shapiro step-measurements the doubled periodicity would result in only even steps in current-voltage measurements, i.e. steps at $eV = k\Omega$ [41, 198–200]. Ω is the frequency of a small ac bias and $k \in \mathbb{Z}$. In noise measurements, a peak at half the Josephson frequency would be visible [201].

In Chap. 4 we have seen that signatures of unconventional superconductivity should already be visible outside the “Majorana regime”. The measurements presented in this chapter shows the result of the device discussed in Chap. 4 without a ferromagnet. Although, we are not in the ballistic limit as assumed in Chap. 4, clear signatures of proximized BSTS are observed. Next to the noise measurements, future measurements will include the study of the proximity effect with a ferromagnet on top of the uncovered part of the topological insulator. By means of gating, the enhancement of unconventional superconductivity should then become visible. Optimizing the coupling between the ferromagnet and the topological insulator can, in combination with gating, also result in a chemical potential smaller than the magnetization energy and hence entering the “Majorana regime”. As proposed by Linder *et al.*[66], similar measurements as performed in this chapter, can then be used for the observation of the Majorana fermion.

The 4π periodicity in a topological insulator Josephson junction can also be explained by the interchanging of two Majorana fermions [8]. Due to the anyonic statistic the Majorana’s have to be interchanged twice before the junction returns to its original state. This leads to a doubling of periodicity but corresponds only to a change of phase of the state $|0\rangle$ or $|1\rangle$. This is also the only possibility in a system where only one qubit is present because parity is conserved. Therefore the total number of electrons that occupy the qubit state has always to be even or odd. With one qubit there is only one possible state for each parity. If we start with two qubits so that the possible states are $|00\rangle$, $|11\rangle$, $|01\rangle$ and

$|10\rangle$, the number of possible operations increases. Starting in the state $|00\rangle$ it is now possible to end in the state $|11\rangle$ or a combination of $|00\rangle$ and $|11\rangle$ as both have an even parity. A way to realize the braiding of multiple qubits is shown in Fig. 5.9(a) and a top view of the same device in Fig. 5.9(b). By changing the phase of the corresponding superconductors relative to each other, a Majorana fermion can appear at the tri-junction and be transported to another tri-junction by adiabatically changing the phase of one of the superconductor from just below π to a value above π while keeping the phases of the other superconductors fixed [8]. The energy gap between the Majorana state and the first non-zero energy state in these devices is $1.5\hbar\tilde{v}/L$ [8], where L is the distance between the two Majorana states and $\tilde{v}$ is a function of the Fermi velocity and the chemical potential. The smaller the chemical potential, the larger $\tilde{v}$. For fixed length L also here gating towards the Dirac point increases the visibility of the braiding between two Majorana states. The challenge for this proposal is to develop a SQUID or other device that is able to tune the phase difference of the superconductors during measurements.

All the research so far is performed on TI flakes. In the appendix we will discuss TI thin films as an alternative path towards realizing a stable qubit.

CHAPTER 6

Appendix: Tight binding model for a three dimensional topological insulator

We calculated the dispersion relation and location of the wavefunction for different amounts of quintuple layers in three-dimensional topological insulators by means of a tight binding model. We also study the influence of magnetization on the gap. Below five quintuple layers where a hybridization gap already exists, the gap first closes due to the shift of the spin bands and then re-opens again. The magnitude of the gap is therefore not the hybridization gap plus the magnetization but rather the magnetization minus the hybridization gap. Thereafter, we discuss the appearance of the quantum anomalous Hall effect for a film thickness of 5 quintuple layers and lower. We see that the tight binding model presented reproduces the special features of a three-dimension topological insulator thin film as known from literature and can therefore be used in future research to estimate the required film thickness and magnetization to observe the quantum anomalous Hall effect and the appearance of a two-dimensional topological insulator state. Finally, we apply the model to scanning tunneling spectroscopy data obtained from a topological insulator thin film.

6.1 Introduction

The use of topological insulator thin films has advantages above the use of flakes. First of all one is not restricted to the size of the flake when it comes to devices, such as the complex multiple tri-junctions [8] to braid Majorana fermion zero-modes. Furthermore, when growing thin films one has control over the thickness of the topological insulator which is useful when considering back-gating [150, 202] and the observation of exciton condensation [203, 204]. When the thickness is below 5 quintuple layers (QLs) there are no surface states and the structure is fully gapped [205]. This regime is especially interesting for the expected possibility to create 2D topological insulators from the Bi-compound 3D topological insulators. An applied magnetic field can also serve as an extra tool to enter different topological regimes.

In this chapter we present the simulations performed on an effective model of the band structure of a 3D topological insulator with a thickness of a few QLs. In the literature it is already shown that in this limit an oscillatory crossover exists from a 2D to a 3D topological insulator [205]. Moreover, under an applied magnetic field one can even enter different regimes of the quantum anomalous

Hall effect (QAH). In this chapter, we start with presenting the effective model used and the resulting dispersion relations with and without a magnetic field. We show then how the existence of different topological regimes follows from this model. Thereafter, we discuss shortly the use of the developed model to interpret the scanning tunnel spectroscopy data obtained from a Bi_2Te_3 thin film.

6.2 Tight binding model

We use the effective model of Ref. [17] in the base $(|+, \uparrow\rangle, |+, \downarrow\rangle, |-, \uparrow\rangle, |-, \downarrow\rangle)$. Here $\pm$ indicates the parity of the band and $\uparrow, \downarrow$ denotes the spin:

$$H(k) = \epsilon \mathbb{1} + \begin{pmatrix} M(k) & 0 & B_0 k_z & A_0 k_- \\ 0 & M(k) & A_0 k_+ & -B_0 k_z \\ B_0 k_z & A_0 k_- & -M(k) & 0 \\ A_0 k_+ & -B_0 k_z & 0 & -M(k) \end{pmatrix}, \quad (6.1)$$

with

$$\epsilon = C_0 + C_1 k_z^2 + C_2 (k_x^2 + k_y^2), \quad (6.2)$$

$$M(k) = M_0 + M_1 k_z^2 + M_2 (k_x^2 + k_y^2), \quad (6.3)$$

where $k_{\pm} = k_x \pm i k_y$ and $\mathbb{1}$ is the unity matrix. $C_0, C_1, C_2, M_0, M_1, M_2, A_0$ and B_0 are constants which are determined by fitting the model to a measured dispersion relation.

Following Ref. [206] the Hamiltonian in the limit of only nearest neighbor hopping becomes

$$H(k) = \tilde{\epsilon} \mathbb{1} + \begin{pmatrix} \widetilde{M}(k) & 0 & B_0 \sin k_z c & A_- \\ 0 & \widetilde{M}(k) & A_+ & -B_0 \sin k_z c \\ B_0 \sin k_z c & A_- & -\widetilde{M}(k) & 0 \\ A_+ & -B_0 \sin k_z c & 0 & -\widetilde{M}(k) \end{pmatrix}, \quad (6.4)$$

where

$$\tilde{\epsilon} = \overline{C}_0 + 2\overline{C}_1 (1 - \cos k_z c) + 2\overline{C}_2 (2 - \cos k_x a - \cos k_y a), \quad (6.5)$$

$$\widetilde{M}(k) = \overline{M}_0 + 2\overline{M}_1 (1 - \cos k_z c) + 2\overline{M}_2 (2 - \cos k_x a - \cos k_y a), \quad (6.6)$$

$$\overline{A}_{\pm}(k_x, k_y) = \overline{A}_0 (\sin k_x a \pm i \sin k_y a). \quad (6.7)$$

Here, a is the unit cell (UC) constant in the xy -plane and c the UC lattice constant along the z -direction. Note that here for simplicity the model assumes that the topological insulator has a tetragonal lattice structure, i.e. the angle between the lattice vectors in the xy -plane is 90° and the angle between the xy -plane and c -lattice constant is 90° (see Fig. 6.1). The model is therefore only useful to study low energy and long wavelength features of the topological insulator. Also, if one wants to include the warping term, the modelling has to be done in the rhombohedral structure due to the three-fold symmetry. Because we are only

Figure 6.1 (a) Crystal structure of Bi_2Se_3 . c is the height of unit cell (or quintuple layer) in the z -direction. In the lowest Se layer the unit cell in the xy -plane is shown with solid lines between the atoms. (b) Top view of the unit cell in the xy -plane. (c) The Brillouin zone corresponding with the unit cell in the xy -plane. Three high symmetry, $\bar{\Gamma}$, $\bar{M}$ and $\bar{K}$, points are indicated. (d) The unit cell in the xy -plane considered in the model. “ a ” is the lattice constant. (e) Corresponding Brillouin zone for the tetragonal lattice structure. Also here three high symmetry points are indicated, $\bar{\Gamma} = (0, 0)$, $\bar{M} = (\pi/a, \pi/a)$ and $\bar{X} = (0, \pi/a)$.

interested in the behaviour of the gap under the application of a magnetic field, we use the simplified model in the tetragonal lattice structure.

The parameters with an overline are related to the parameters in Eq. (6.1) by [206]

$$\begin{aligned} \overline{M}_0 &= M_0, \overline{C}_0 = C_0, \overline{M}_1 = M_1/c^2, \overline{C}_1 = C_1/c^2, \\ \overline{M}_2 &= M_2/a^2, \overline{C}_2 = C_2/a^2, \overline{A}_0 = A_0/a, \overline{B}_0 = B_0/c. \end{aligned} \quad (6.8)$$

The cleavage of the crystals is the easiest along the (111) direction which corresponds to the z -direction. Therefore we assume that the z -direction is finite and the x and y -dimensions are infinite so that k_x and k_y are still good quantum numbers. Assuming hopping along the z -direction only along neighboring layers

the Hamiltonian is then given by [206]

$$H(k_x, k_y) = \sum_{n=1}^N c_n^\dagger(k_x, k_y) H_0(k_x, k_y) c_n(k_x, k_y) + \sum_{n=1}^{N-1} [c_n^\dagger(k_x, k_y) H_1(k_x, k_y) c_{n+1}(k_x, k_y) + h.c.], \quad (6.9)$$

where N is the number of QLs. The Hamiltonians H_0 and H_1 are given by

$$H_0(k_x, k_y) = \begin{pmatrix} \overline{M} + \overline{\epsilon} & 0 & 0 & A_- \\ 0 & \overline{M} + \overline{\epsilon} & A_+ & 0 \\ 0 & A_- & -\overline{M} + \overline{\epsilon} & 0 \\ A_+ & 0 & 0 & -\overline{M} + \overline{\epsilon} \end{pmatrix}, \quad (6.10)$$

where

$$\overline{\epsilon} = \overline{C}_0 + 2\overline{C}_1 + 2\overline{C}_2 (2 - \cos k_x a - \cos k_y a), \quad (6.11)$$

$$\overline{M} = \overline{M}_0 + 2\overline{M}_1 + 2\overline{M}_2 (2 - \cos k_x a - \cos k_y a), \quad (6.12)$$

and

$$H_1 = \begin{pmatrix} -\overline{M}_1 - \overline{C}_1 & 0 & i\overline{B}_0/2 & 0 \\ 0 & -\overline{M}_1 - \overline{C}_1 & 0 & -i\overline{B}_0/2 \\ i\overline{B}_0/2 & 0 & \overline{M}_1 - \overline{C}_1 & 0 \\ 0 & -i\overline{B}_0/2 & 0 & \overline{M}_1 - \overline{C}_1 \end{pmatrix}. \quad (6.13)$$

H_1 is the Fourier transform of the elements of the total Hamiltonian Eq. 6.4 including k_z .

6.3 Energy dispersion relations

The eigen values and vectors are numerically solved. The values for the parameters can be extracted from Ref. [207]. We used $\overline{M}_0 = -0.28$ eV, $\overline{M}_1 = 0.216$ eV, $\overline{M}_2 = 2.60$ eV, $\overline{A}_0 = 0.80$ eV, $\overline{B}_0 = 0.32$ eV, $\overline{C}_0 = -0.0083$ eV, $\overline{C}_1 = 0.024$ eV, $\overline{C}_2 = 1.77$ eV. Fig. 6.2(a) and (b) shows the dispersion relation for 4 and 6 QLs. At 4 QLs the wavefunctions of the top and bottom surface states overlap and a gap is opened.

To include magnetization, we neglect the orbital contribution since we assume that Landau levels cannot form yet, but we keep the Zeeman spin term. We add therefore a $+m_z$ on the diagonal of the first and third row (corresponding with spin up bands) and $-m_z$ on the diagonal of the other rows (corresponding with spin down bands).

In Fig. 6.2(c) and (d) the dispersion relation for a magnetization of 0.05 eV for a 6 QLs and 4 QLs respectively is shown. To study the gap in more detail, we simulated the gap as function of magnetization. In Fig. 6.2(e) the

Figure 6.2 (a) Dispersion relation of 6 QL. (b) Dispersion relation of 4 QLs. A gap is opening. (c) Dispersion relation for 6 QLs and a magnetization of 0.05 eV. (d) Dispersion relation for 4 QLs and a magnetization of 0.05 eV. (e) Evaluation of the gap for 6 QLs as function of magnetization. (f) Evaluation of the gap for 3 and 4 QLs as function of magnetization.

evaluation of the gap is seen for 6 QLs. First, the gap exists, but around 0.1 eV of magnetization the gap closes. That is because the spin down bands above the gap are pushed towards lower energy and the spin up bands below the gap are pushed up in energy. For a certain magnetization they cross around zero energy and the gap is closing. The magnitude of the gap below 0.1 eV is equal to two times the magnetization.

Next, we simulated the effect on the magnetization when a gap due to hybridization of the surface states is already present. Fig. 6.2(f) shows the gap evaluation for 4 QLs and for 3 QLs. The gap is first closing due to the same reason as

Figure 6.3 (a) Influence of the magnetization for the band crossing at 3 QLs thickness. (b) Chern number as a function of film thickness for a magnetization of 0.2 eV. Parameters are taken from Ref. [17].

mentioned above for the closing of the gap in the case of 6 QLs. Note that from the simulations it appears that the gap is not completely closing at a certain magnetization. This is, however, due to a numerical error caused by finite step size in momentum space. We fitted the gap value in the range the gap is opening again, i.e. above a magnetization of 0.0075 eV till 0.15 eV. For the 4 QLs as well as for the 3 QLs the slope of the fit is two times the magnetization and intersects the y -axis at minus the hybridization gap.

In Ref. [205] it is shown that in the limit the band is not closed yet, an oscillatory crossover exist from a normal insulator to a 2D topological insulator depending on the number of quintuple layers.

As a function of magnetization we have shown that below 5 QLs the gap is in first instance closing whereafter it re-opens again. In Fig. 6.3 we show the splitting of the E_1 (solid curve) and H_1 (dashed curve) band given by

$$\begin{aligned} E_1 &= C_0 + M_0 + (C_1 + M_1) \left(\frac{n\pi}{d} \right)^2 \pm m_z \\ H_1 &= C_0 - M_0 + (C_1 - M_1) \left(\frac{n\pi}{d} \right)^2 \pm m_z \end{aligned} \quad (6.14)$$

in analogy to Ref. [205] where we neglected the spin-orbit coupling term B_0 for a moment. We see that only one of the spin bands reverses order, suggesting that one can enter a topological regime where edge states are present with only one spin direction. This idea is also noted in Refs. [208–210] for magnetically doped 3DTI thin films and also experimentally confirmed in Ref. [211] by Chang *et al.* In Ref. [210] it is shown that the Chern number is simply given by

$$C = N_+ - N_-, \quad (6.15)$$

where N_+ is the number of crossing between $E_n \downarrow$ and $H_n \uparrow$ and N_- the number of crossings between $E_n \uparrow$ and $H_n \downarrow$. n is the number of the subband. Fig. 6.3(b) shows the Chern number as a function of film thickness for a magnetization of

0.2 eV. The influence of the spin orbit coupling along k_z is the coupling between the $E_n(H_n)$ and the $H_{n\pm 1}(E_{n\pm 1})$ as can be seen from the hopping model at the beginning of this chapter. The transition from one Chern number to the other can therefore be positioned at a slightly different value of film thickness and magnetic field magnitude. To estimate the parameters corresponding to a topological phase transition, the tight binding model in this chapter can be used after tuning the tight binding parameters such that it fits the dispersion of the used thin film. This topological regime has a high potential to be used for low-power-consumption electronics [212].

6.4 The distribution of the wavefunction

In Fig. 6.4(a) and (b) we plotted the absolute value of the wavefunction at $k_x=0.001\pi/a$ and $k_y=0$ for different QLs. $|\psi|$ is defined as the sum of $|+, \uparrow\rangle$, $|+, \downarrow\rangle$, $|-, \uparrow\rangle$ and $|-, \downarrow\rangle$ and normalized to the total of the sum of those four components over all QLs.

For 10 QLs we see for high energy that the wavefunction is mainly located in the bulk. We also plotted the wavefunctions of the degenerate Dirac cone. One of the eigen values corresponds to a wavefunction on the top surface and the other to the bottom surface. However, when we go lower in k_x value or towards the Dirac point, the waves become delocalized over both surfaces. Considering that the fermi wave length goes to infinity in this regime, this result can be understood.

For 3 QLs and a magnetization of 0.018 eV the gap is opened. The wavefunctions corresponding to energies just below and above the gap are now mainly located on both top and bottom surface instead of being located on one surface. For higher energy the absolute value of the wavefunction peaks in the second layer.

Figure 6.4 (a) The location of the wavefunction around zero momentum for different energies for 10 QLs (b) and for 3 QLs with a magnetization of 0.018 eV.

Figure 6.5 (a) The conductance obtained from a measurement on a 30 nm thick Bi_2Te_3 thin film. The data is fitted by means of a linear dispersion relation plus a warping term (dotted blue curve) and by means of the tight binding model plus the warping term (red dashed curve). The best fit with the former model is obtained for $v_f = 2.55 \text{ eV}\cdot\text{\AA}$ and $\lambda = 250 \text{ eV}\cdot\text{\AA}^3$. (b) In the $\bar{\Gamma} - \bar{M}$ direction the dispersion relation of the surface states bends outwards. The warmer colors represents a higher DOS. From [17].

6.5 Fitting STM data

Fig. 6.5(a) shows data from a scanning tunneling spectroscopy (STS) measurement at 77 K of a 30 nm thick Bi_2Te_3 grown by means of e-beam evaporation.* The background pressure in the STS chamber was in the range of 10^{-12} mbar. The data are obtained from an average of 3000 I-V curves whereafter they are numerically differentiated. In Fig. 6.5(a) the bottom of the conduction band (E_{BCB}) and the top of the valence band (E_{T-BVB}) are indicated. The Dirac cone is positioned in between and is often described by

$$E = v_F|k| + \lambda k^3 \cos(3\theta), \quad (6.16)$$

where v_F is the Fermi velocity, λ the strength of the warping effect and θ the angle between k_x and k_y . The observed kink feature in the data of Fig. 6.5(a) is often attributed to this cubic warping term. Therefore, this extended dispersion relation of the Dirac cone is fitted to the data. The best fit is shown by the blue-dotted curve in Fig. 6.5(a). We did not manage to fit both the slope and the strong kink at the same time by means of the density of states (DOS) obtained from this dispersion relation.

In Ref. [17] it is shown by Zhang *et al.* by means of *ab initio* calculations that in the $\bar{\Gamma} - \bar{M}$ direction the Dirac cone of Bi_2Te_3 has a strong outward bending close to the bulk conduction band (Fig. 6.5(b)) which is not included in Eq. (6.16). To understand the origin of the kink, we used the tight binding model as presented in this chapter to fit the dispersion relation around this kink in the $\bar{\Gamma} - \bar{M}$ direction as good as possible. As a starting point we used $M_0 = -0.30 \text{ eV}$, $M_1 = 10 \text{ eV}\cdot\text{\AA}^2$, $M_2 = 57.38 \text{ eV}\cdot\text{\AA}^2$, $C_0 = -0.18 \text{ eV}$, $C_1 = 6.55 \text{ eV}\cdot\text{\AA}^2$, $C_2 = 29.68 \text{ eV}\cdot\text{\AA}^2$, $A_0 = 2.87 \text{ eV}\cdot\text{\AA}$ and $B_0 = 2.26 \text{ eV}\cdot\text{\AA}$ as reported in Ref. [207]. The total

*Growth of the samples and measurements are performed by P. Ngabonziza.

number of QLs was set to 30 to match the thickness of the grown Bi_2Te_3 . As this tight binding model does not take into account the warping term we used a combination of Eq. (6.16) and the tight binding model to fit the data. Equation (6.16) is used for the DOS at energies below and above the kink feature. We replaced the DOS obtained from Eq. (6.16) around this outward bending by the DOS obtained from fitting the tight binding model to Fig. 6.5(b). We also took into account that the outwards bending only occurs for specific crystal directions. The best fit was obtained by replacing the DOS obtained from Eq. (6.16) in a 78° range by the tight binding model DOS. The resulting fit is shown by the red-dashed curve in Fig. 6.5(a). We note that the addition of DOS will not give a quantitative value of the DOS but it can be used for the interpretation of the shape of the topological insulator surface states in this system.

6.6 Discussion and conclusions

We discussed in this chapter the dispersion relation and wavefunctions of a topological insulator calculated from an effective model with and without an applied magnetic field. It is shown that the magnetization causes in the first place a closing of the gap for thicknesses below 5 QLs. This is due to the shifting of the spin up and down bands to higher and lower energies respectively when a magnetic field is applied. The effective model used, deviates from the true crystal structure of a topological insulator by assuming a tetragonal structure. Despite this simplicity it can catch the main results also observed from more advanced tight binding models as described in the references in this chapter. Therefore, this model can be used to estimate experimental regimes necessary to observe the various topological regimes in our own thin films and to interpret the data. However, as we have seen in the fitting of the STM data one has to develop the hopping model in the rhombohedral structure in order to also include the warping term and do therefore also quantitative fittings to the data at higher energy.

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Summary

The main focus of this thesis is to understand the correlations present at the *s*-wave/three-dimensional topological insulator interface both theoretically and experimentally. In the future, devices containing these kind of interfaces can be used to create and manipulate a Majorana zero-energy mode which serves as a building block for a topological quantum bit.

In Chapter 1 the basics around quantum computation is considered and we show that the observation of a 4π periodicity in a superconductor/topological insulator Josephson junction is the hallmark for the detection of a Majorana fermion mode. Chapter 2 studies in more detail the properties and conditions of the existence of this 4π periodicity in a superconductor/three-dimensional topological insulator Josephson junction. We consider the system in an experimentally relevant regime, i.e. a chemical potential higher than the superconducting gap and a magnetization much smaller than the chemical potential. A 4π periodicity is still visible in the Andreev bound state spectrum. However, it is only present for the channel at normal incidence. The other channels have a 2π periodicity and should therefore be eliminated in order to be able to observe this single 4π periodicity channel. We show that by exploiting the effect of magnetization, caused by a ferromagnet on top of the topological insulator, the number of channels contributing to a 4π period can be increased. It enhances the chance of Zener tunneling for the 2π periodic channels resulting in an artificial 4π periodic signal.

In Chapter 3 measurements are presented on $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ (BSTS) flakes. From Hall bar measurements on these flakes we conclude that the bulk conduction is negligible at low temperatures and that the transport is dominated by the topological surface states. Due to the small mean free path of those surface states (around 30 nm), superconducting leads are fabricated on top of the surface with a small separation of just 50 nm between the leads. We succeeded to realize a Josephson supercurrent which is confirmed by the observed supercurrent and Fraunhofer pattern. The dominant transport by the surface states and coherence length of 28 nm obtained from fitting our data, make it plausible that the supercurrent goes through the topological surface states without a bulk shunt. The data can be explained by normal *s*-wave theory which is expected due to the ‘normal’ behaviour of the 2π periodic channels.

Chapter 4 describes the calculations on the superconducting correlations present at the *s*-wave proximized topological insulator surface states. We show that in the time-reversal symmetry case there is an equal admixture of *s* and *p*-wave correlations. As soon as time-reversal symmetry is broken, the *p*-wave correlations become dominant because spin-triplet pairing is favoured due to the alignment

of the spins. By means of Green function techniques we show that the Majorana zero-energy mode is a full odd-frequency state. Thereafter, we study the conductance spectra of a topological insulator with one half covered by a ferromagnet and the other half covered by an s -wave superconductor. Also, when a Majorana fermion is not present, the required presence of dominant p -wave correlations can already be observed for magnetization values around half the chemical potential. The appearance of a conductance dip at the gap energy together with a zero-energy peak are the distinguishing features for a dominant p -wave pairing correlation.

In Chapter 5 we use the known properties of BSTS described in Chapter 3 together with the theory in Chapter 4 to fabricate Au/BSTS/Nb devices in order to study the superconductor correlations at the s -wave superconductor proximized topological insulator surface states. The electrodes have a lateral spacing in the order of the mean free path of BSTS so that the BSTS is fully proximized. There is a clear conductance modulation visible between 0 and 700 μV which corresponds well with the Thouless energy as is expected for induced superconducting correlations in a diffusive system. The shape of the modulations can be explained by existing s -wave theory in SNN' devices. Appearance of both conductance dips and peaks around zero energy naturally occurs in the regime where the resistances of the barriers are of the same order of magnitude as the resistance of the BSTS. The reproducibility of the conductance dip at the induced superconducting gap in BSTS is, however, less trivial. We excluded charge imbalance as a possible origin by the absence of a resistance peak in RT-measurement around the critical temperature. If these dips can be explained by conventional s -wave superconductivity or unconventional induced superconductivity is left as an open question. We discuss the necessity of a model that can describe an SNN' device with an NN' interface for intermediate transmission values and small total resistance to distinguish between the two.

In the final chapter, Chapter 6, we have presented a tight binding model of a three-dimensional topological insulator to model the properties of a few quintuple layers. With this model we can reproduce the results already reported in the literature such as the quantum anomalous Hall effect. It shows that this model can be used to estimate the number of quintuple layers and the required magnetic field to enter different topological regimes. At the end of Chapter 6 we applied the model to scanning tunneling spectroscopy data performed on a 30 nm thick Bi_2Te_3 thin film. The observed kink feature in the density of states of the Dirac cone could not fully be explained by means of warping. Fitting the tight binding model to existing *ab initio* calculations done on Bi_2Te_3 shows that the strong outward bending of the Dirac cone in the $\bar{\Gamma} - \bar{M}$ direction near the conduction band can provide a qualitative explanation of the kink feature.

Samenvatting

Het hoofddoel van dit proefschrift is het zowel theoretisch als experimenteel begrijpen van de aanwezige correlaties op het grensvlak tussen een s -symmetrie supergeleider en een drie-dimensionale topologische isolator. Toekomstige structuren die dit soort grensvlakken bevatten, kunnen gebruikt worden om een Majorana multistoestand te creëren en te manipuleren. Met twee Majorana multistostanden is uiteindelijk een topologische kwantumbit te realiseren.

In hoofdstuk 1 wordt de basis rond kwantumberekeningen beschouwd en we laten zien dat het observeren van een 4π periode in een supergeleider/topologische isolator Josephson junctie karakteristiek is voor de detectie van een Majorana multistoestand. In Hoofdstuk 2 bestuderen we in meer detail de eigenschappen en condities voor het bestaan van deze 4π periode in een supergeleider/drie-dimensionale topologische isolator Josephson junctie. We bestuderen het systeem in een experimenteel relevant regime, d.w.z. een chemische potentiaal groter dan de supergeleidende *gap* en een magnetisatie veel kleiner dan de chemische potentiaal. In dit regime is in het Andreev gebonden toestandenspectrum nog steeds een 4π periode zichtbaar. Echter, dit geldt alleen voor het kanaal met loodrechte inval. De andere kanalen hebben een 2π periode en moeten daarom vermeden worden om de 4π periode te kunnen waarnemen. We laten zien dat door het effect van magnetisatie, veroorzaakt door een ferromagneet bovenop de topologische isolator, optimaal te benutten het aantal kanalen dat bijdraagt aan de 4π periode vergroot kan worden. Het vergroot de kans op Zener tunneling voor de 2π periodieke kanalen en resulteert zodoende in een artificieel 4π periodiek signaal.

In hoofdstuk 3 presenteren we metingen op $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ (BSTS) *flakes* (kleine schilfers BSTS afkomstig van het BSTS kristal). Uit Hall bar metingen op deze flakes kunnen we concluderen dat de bijdrage van toestanden anders dan de topologische oppervlakte toestanden, verwaarloosbaar is op lage temperaturen en dat het transport gedomineerd wordt door de topologische oppervlakte toestanden. Door de kleine vrije weglengte van deze oppervlakte toestanden (rond 30 nm), hebben de gefabriceerde supergeleidende elektrodes bovenop het oppervlak een tussenafstand van 50 nm. We zijn er in geslaagd om een Josephson superstroom te realiseren wat bevestigd wordt door de observatie van een superstroom en Fraunhofer patroon. De dominantie van de oppervlakte toestanden in transport en de coherentielengte van 28 nm verkregen uit het fitten van onze data, maken het plausibel dat de superstroom door de topologische oppervlakte toestanden gaat zonder transport door andere (niet-topologische) toestanden. De data kan verklaard worden met normale s -symmetrie supergeleidende theorie wat te verwachten is door het ‘normale’ gedrag van de 2π periodieke kanalen.

Hoofdstuk 4 beschrijft de berekeningen aan de aanwezige supergeleidende correlaties op het s -symmetrie supergeleider/topologische isolator grensvlak. We laten zien dat in het geval van tijdsymmetrie er een gelijke bijdrage is van s en p -symmetrie correlaties. Zodra tijdsymmetrie verbroken wordt, worden de p -symmetrie correlaties dominant, omdat spin-triplet paring begunstigd wordt door de uitlijning van de spins. Door middel van Green functie technieken laten we zien dat de aanwezige Majorana multioestand een volledig oneven-frequentie toestand is. Vervolgens bestuderen we de geleidingsspectra van een topologische isolator waar een helft is bedekt met een ferromagneet en de andere helft met een s -symmetrie supergeleider. Zelfs als een Majorana fermion niet aanwezig is, kan de vereiste aanwezigheid van dominante p -symmetrie correlaties al waargenomen worden voor een magnetisatiewaarde ongeveer twee keer zo klein als de chemische potentiaal. Een lagere geleidingswaarde op de supergeleidende *gap* energie samen met een toename van geleiding rond een spanning van nul, zijn de onderscheidende kenmerken voor deze dominante p -symmetrie correlatie.

In hoofdstuk 5 gebruiken we de bekende eigenschappen van BSTS, beschreven in hoofdstuk 3, samen met de theorie uit hoofdstuk 4 om Au/BSTS/Nb structuren te fabriceren om de supergeleidende correlaties te bestuderen aan het s -symmetrie supergeleider/topologische isolator grensvlak. De elektrodes hebben een onderlinge afstand in de orde van de vrije weglengte van BSTS zodat het BSTS volledig door de supergeleidende correlaties beïnvloed wordt. Er is een duidelijke geleidingsmodulatie zichtbaar tussen 0 en 700 μV wat goed overeenkomt met de Thouless energie zoals verwacht voor geïnduceerde supergeleidende correlaties in een diffuus systeem. De vorm van de modulatie kan verklaard worden met bestaande s -symmetrie theorie in SNN' structuren. De aanwezigheid van zowel een afname als toename in geleiding rond een energie van nul gebeurt van nature in het regime waar de weerstanden van de barrières in dezelfde orde zijn als de weerstand van BSTS. De lagere geleidingswaarde, reproduceerbaar voor alle drie de structuren, rond de geïnduceerde supergeleidende gap in BSTS, is minder triviaal. We sluiten een disbalans in lading uit als een mogelijke oorzaak door de afwezigheid van een weerstandspiek in een RT-meting rond de kritische temperatuur. Of deze afname in geleiding dan verklaard kan worden met conventionele s -symmetrie supergeleiding of dat geïnduceerde, onconventionele supergeleiding de oorzaak is, blijft een open vraag. Om tussen de twee te onderscheiden is er een model nodig die een SNN' structuur kan beschrijven met een NN' grensvlak waarbij de transmissiewaarde tussen de nul en een kan liggen terwijl de totale weerstand klein kan zijn.

In het laatste hoofdstuk, hoofdstuk 6, presenteren we een "tight binding" model voor een drie-dimensionale topologische isolator om de eigenschappen van een topologische isolator met een dikte van een paar eenheidscellen te modelleren. Met dit model kunnen we de gerapporteerde resultaten in de literatuur reproduceren zoals het kwantum anomale Hall effect. Het laat zien dat dit model gebruikt kan worden om het aantal eenheidscellen en magnetisch veld te schatten die nodig zijn om in verschillende topologische regimes te komen. Aan het einde van dit hoofdstuk passen we het model toe op scanning tunneling spectroscopie data uitgevoerd op een 30 nm dikke Bi_2Te_3 film. De waargenomen

knik in de toestandsdichtheid van de Dirac kegel kan niet volledig beschreven worden met *warping*. De variabelen in het “tight binding” model zijn aangepast zodat het overeenkomt met bestaande *ab initio* berekeningen gedaan op Bi_2Te_3 . De sterke uitbuiging van de Dirac kegel dicht tegen de geleidingsband aan in de $\bar{\Gamma} - \bar{M}$ richting, kan een kwalitatieve verklaring geven voor de knik in de STM data.

Dankwoord

Met het dankwoord leg ik dan de laatste hand aan mijn proefschrift. Met veel plezier kijk ik terug op de afgelopen periode. Een periode van hard werken, maar tevens was er binnen de vakgroep genoeg ruimte om te lachen, te schaatsen, te zeilen, te curlen en ons ICE voetbalteam toe te juichen.

Als eerste wil ik Alexander en Hans bedanken voor het vertrouwen om mij in het snel ontwikkelende veld van topologische isolatoren te laten werken. Met name Alexander wil ik bedanken voor de vele begeleiding. Het was erg prettig dat ik altijd naar binnen kon lopen voor een discussie of voor overleg. Ook de ruimte en de stimulans om mezelf verder te ontwikkelen op andere vlakken zoals de Centrale Ondernemingsraad bij het FOM en het volgen van de lerarenopleiding, heb ik erg gewaardeerd.

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Regarding the outside-university collaboration I am also eager to thank Mark Golden and his research group at the UvA for the collaboration on the $\text{Cu}_x\text{Bi}_2\text{Se}_3$ and BSTS crystals. My sincerest thanks to you too, Vadim Khrapai and Eugene Tikhonov, for the collaboration on the Nb/BSTS/Au devices. The first results are very promising and I am very curious what kind of noise spectra the Nb/BSTS/Nb devices will produce!

Twee tweetallen waren onmisbaar om de motor draaiend te houden: Frank & Dick en Ans & Inke. Bedankt voor jullie grote hulp bij het maken van devices door alles in het lab goed draaiend te houden. Ook de verlichting van alle administratie zorgde ervoor dat je je volledig kon concentreren op het project.

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Most of my PhD time I shared the room with Denise, Prosper and Martin. I had the most fun with all of you both in discussions and in small talk. Also my other former room mates I owe a “thank you” for the nice time: Bernard, Menno and Agnes.

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Publications

Conductance spectroscopy of a proximity induced superconducting topological insulator

M. Snelder, M. P. Stehno, A. A. Golubov, C. G. Molenaar, T. Scholten, Y. K. Huang, W. G. van der Wiel, M. S. Golden, A. Brinkman
In preparation.

Observability of surface Andreev bound states in a topological insulator in proximity to an s -wave superconductor

M. Snelder, A. A. Golubov, Y. Asano, A. Brinkman
Submitted to Journal of Physics: Condensed Matter (2015).

In-situ spectroscopy of intrinsic Bi_2Te_3 topological insulator thin films and impact of extrinsic defects

P. Ngabonziza, R. Heimbuch, N. de Jong, R. A. Klaassen, M. P. Stehno, M. Snelder, A. Solmaz, S. V. Ramankutty, E. van Heumen, G. Koster, M. S. Golden, H. J. W. Zandvliet, A. Brinkman
Submitted to Physical Review B (2015).

High school students' understanding of magnetism

M. Snelder, J. T. van der Veen
Submitted to American Journal of Physics (2014).

Low carrier concentration crystals of the topological insulator

$\text{Bi}_{2-x}\text{Sb}_x\text{Te}_{3-y}\text{Se}_y$: a magnetotransport study

Y. Pan, D. Wu, J. R. Angevaere, H. Luigjes, E. Frantzeskakis, N. de Jong, E. van Heumen, B. Zwartsenberg, Y. K. Huang, M. Snelder, A. Brinkman, M. S. Golden, A. de Visser
New Journal of Physics **16**, 123035 (2014).

Josephson supercurrent in a topological insulator without a bulk shunt

M. Snelder, C. G. Molenaar, Y. Pan, D. Wu, Y. K. Huang, A. de Visser, A. A. Golubov, W. G. van der Wiel, H. Hilgenkamp, M. S. Golden, A. Brinkman
Superconductor Science and Technology **27**, 104001 (2014).

Nonlocal spin-entangled Andreev reflection, fractional charge, and current-phase relations in topological bilayer-exciton-condensate junctions

M. Veldhorst, M. Hoek, M. Snelder, H. Hilgenkamp, A. A. Golubov, A. Brinkman

Physical Review B **90**, 035428 (2014).

Andreev bound states and current-phase relations in three-dimensional topological insulators

M. Snelder, M. Veldhorst, A. A. Golubov, A. Brinkman

Physical Review B **87**, 104507 (2013).

Magnetotransport and induced superconductivity in Bi based three-dimensional topological insulators

M. Veldhorst, M. Snelder, M. Hoek, C. G. Molenaar, D. P. Leusink, A. A. Golubov, H. Hilgenkamp, A. Brinkman

Physica Status Solidi (RRL) **7**, 26 (2013).

Josephson supercurrent through a topological insulator surface state

M. Veldhorst, M. Snelder, M. Hoek, T. Gang, X. L. Wang, V. K. Guduru, U. Zeitler, W. G. van der Wiel, A. A. Golubov, H. Hilgenkamp, A. Brinkman

Nature Materials **11**, 417-421 (2012).

Propositions

accompanying the thesis

Non-triviality matters

Examining the interplay between s-wave superconductivity and topological surface states

Marieke Snelder

Proposition 1: Breaking of time-symmetry has an important role in the observation of p-wave superconductivity in topological insulator/s-wave superconductor devices. (Chapter 2 and 4)

Proposition 2: The multiple channels and the interaction of a topological Josephson junction with the environment, hampers the observation of a doubled periodicity in DC transport measurements. (Chapter 3 and 5)

Proposition 3: The use of thin films instead of flakes is an important step towards the realization of topological spintronic and Majorana devices. (Chapter 6)

Proposition 4: There can be a considerable difference between a good and successful researcher, which indicates that the assessment system is wrong.

Proposition 5: It is counterproductive to award prizes and to offer job positions just for women.

Proposition 6: The mountaineers ethics “leave no trace” should also be the ethics for every experimentalist.

Proposition 7: The best shelves (Dutch: stellingen) are solid and have a lot of storage space.

Proposition 8: For the understanding of the current western culture, education in Norse mythology and culture is as important as education in Greek and Roman mythology and culture.

Stellingen

behorende bij het proefschrift

Non-triviality matters

Examining the interplay between s-wave superconductivity and topological surface states

Marieke Snelder

Stelling 1: Het verbreken van tijd-symmetrie speelt een belangrijke rol in het observeren van p-symmetrie supergeleiding in topologische isolatoren/s-symmetrie supergeleider grensvlakken. (Hoofdstuk 2 en 4)

Stelling 2: De vele kanalen en de interactie van een topologische Josephson junctie met de buitenwereld, verhindert het waarnemen van een dubbele periodiciteit in DC transportmetingen. (Hoofdstuk 3 en 5)

Stelling 3: Het gebruik van dunne films in plaats van kristallen is een belangrijke stap in de realisatie van topologische spintronica en Majorana toestanden. (Hoofdstuk 6)

Stelling 4: Dat er een groot verschil kan bestaan tussen een goede en een succesvolle onderzoeker geeft aan dat het beoordelingssysteem verkeerd is.

Stelling 5: Het werkt averechts om prijzen uit te reiken en posities aan te bieden speciaal voor vrouwen.

Stelling 6: De bergbeklimmers code “laat geen spoor achter” zou ook de code moeten zijn voor elke experimentator.

Stelling 7: De beste stellingen zijn stevig en hebben veel opberg-ruimte.

Stelling 8: Voor het begrijpen van de huidige, westerse cultuur is onderwijs in Noorse mythologie en cultuur net zo belangrijk als in de Griekse en Romeinse mythologie en cultuur.