Topological Properties of Helical Shiba Chains

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Majorana quasiparticles are zero-energy modes theorised to exist at the boundaries of topological superconductors. Due to their topological protection and non-Abelian exchange statistics, Majorana quasiparticles have in recent years garnered much interest within the condensed matter community as a promising platform for fault tolerant quantum computing. To this end, theorists constantly attempt to come up with new experimentally feasible models that can host these quasiparticles.

In this thesis, we investigate a recent proposal for realising an effective topological superconductor with Majorana quasiparticles, namely the helical Shiba chain. The system consists of a one-dimensional array of magnetic impurities deposited on a conventional superconductor, such that the overall magnetic texture is helical. A single impurity hosts a bound electron state with an energy within the superconducting gap. For many impurities, these so called Shiba states hybridise and form energy bands, that for a certain range of parameters support topological superconductivity and Majorana bound states at the ends of the chain.

Prior to this work, the Shiba chain has only been studied in the deep-dilute limit where the energies of the individual Shiba states are assumed to be very close to the centre of the gap, and the magnetic impurities are placed sufficiently far away from each other as to keep the resulting bands deep within the gap. By re-expressing the problem in terms of a non-linear eigenvalue equation, we go beyond this limit and extend the study of the topological properties of the Shiba chain to a novel domain of experimental interest – a domain which has until now remained unexplored. We compare our results with previous work and observe an agreement between our more general theory and the deep-dilute limit in the expected parameter regime. However, qualitative differences emerge when the coherence length of the underlying superconductor becomes very large – but only for some special regions in parameter space.
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Chapter 1

Introduction

The universe is to the best of our knowledge most accurately described in terms of mathematics. Physics and mathematics have for a long time enjoyed a symbiotic relationship in which both disciplines have drawn inspiration from each other; many branches of previously considered pure mathematics have found their application in physics, which in turn has stimulated further developments in mathematics. Topology, which will play a central role in this thesis, is no exception to this. The field of topology studies and classifies mathematical spaces according to properties that are preserved under smooth deformations – that is to say transforming without tearing or cutting. Conversely, spaces that cannot be smoothly transformed into each other have different topological properties and are said to be topologically inequivalent. Properties that allow us to distinguish between topologically inequivalent spaces are called topological invariants and typically take on discrete values. For example, an infinite plane with \( n \) holes is topologically distinct from an infinite plane with \( m \) holes as long as \( m \neq n \). Two punctured planes with the same number of holes, on the other hand, can be continuously morphed into one another and are thus topologically equivalent. We see that the number of holes – an integer – is in this case a good topological invariant.

This work is based on the article *Topological properties of helical Shiba chains with general impurity strength and hybridization* [1] and as the name suggests, our main objective is to study the topological properties of the so called helical Shiba chain: a magnetic superconducting system which will be described in more detail later on. The thesis is organized as follows: in Sec. 1.1 we give a brief introduction to the concept of topological order in physics. This is purposely presented in a rather abstract fashion, since we first wish to convey the general idea behind topological order, postponing the more concrete discussion to the succeeding sections. On that note, in Sec. 1.2, we make ourselves acquainted with Majorana bound states (MBS)
and how they relate to the topology we will be dealing with in this work. Here we also discuss why MBS are highly sought after and discuss some of the experimental progress. In Chap. 2, we present important theoretical background, that will serve as a primer to the theory of topological superconductors. In Sec. 2.1 we give a cursory overview on the mean-field theory of superconductivity. Here we develop some of the necessary tools to tackle Sec. 2.2, where we present a pedagogical albeit unrealistic toy model due to Kitaev [2]. This model gives us a more transparent view into how MBS emerge in some superconducting systems. We end the second chapter with Sec. 2.3, where we discuss how we can relate more realistic systems to Kitaev’s toy model.

In Chap. 3 we present our model of the Shiba chain and discuss the possible physical origin of the magnetic texture of the system (Sec. 3.1). We start off in Sec. 3.2 with a discussion on the original model first presented in the article by Pientka et al. [3]. In Sec. 3.3 we move on to our model, valid over larger domains of the parameters of the theory. We formulate this model as a nonlinear eigenvalue (NEV) problem. Having laid all this groundwork, we continue to Chap. 4 where we extract the topological phase boundaries from the NEV equation derived in Chap. 3. The main result, i.e. finding the analytical expressions for the topological phase boundaries for arbitrary values of the superconducting coherence length, is presented in Sec. 4.1. We compare our model to that of Pientka et al. in terms of their topological phase diagrams. We additionally look at how the phase diagram behaves for large values of the coherence length. In the final chapter, we summarize our work and provide an outlook on possible future work using the tools developed here. This thesis has four appendices to which technical details omitted in the main text have been relegated. In App. A the evaluation of some important integrals are performed. In App. B, different kinds of Fourier series are calculated. Some theory for NEV problems is presented in App. C. Finally, in App. D, we derive the energy spectrum from the NEV problem in the limit of an infinite superconducting coherence length.

1.1 Topological order

For the last couple of decades, condensed matter theory has seen big developments on the relatively new field of topological materials. Originally, the concept of topological order was introduced when it became increasingly clear that Landau’s theory of symmetry breaking, which had been successful in explaining a wealth of phases of matter (and the transitions between them), failed to describe many of the new quantum phases that were discovered by theorists and experimentalists alike. These
intrinsically topologically ordered phases were characterized by having a ground state that no local unitary transformation could change into a so called trivial state consisting only of a product of local single-particle states [4]. Any local perturbation of the system can not remove it from its ground state – this is the most intuitive sense in which the mathematical concept of topology reveals itself in the physics. Perhaps the most notable example of such a topologically ordered phase is the fractional quantum Hall effect [5, 6]. As the name suggests, such a phase has a Hall conductance that is a certain fractional multiple of the constant $e^2/h$ and cannot change unless the perturbations become sufficiently large.

In order for a state to be robust against any local perturbations, there must first of all exist an energy gap separating the groundstate from the excited states, i.e. the Hamiltonian of the system is gapped. Second, long-range correlations within the system is also necessary. The energy gap prevents the perturbation from exciting the particles away from the groundstate, while the long-range correlations protect the phase of the system from local perturbations.

1.1.1 Symmetry-protected topological phases

In this thesis, we will only deal with a specific one-dimensonal (1D) system and its topological properties. As mentioned before, the discussion in this section proceeds at an abstract level, since the main objective here is to introduce the reader to the theoretical concepts underpinning our work.

It turns out that the above mentioned intrinsic topological order can only exist in dimensions higher than one [7, 8]. Nevertheless, a weaker topological order – the so called symmetry-protected topological (SPT) order – can be found in one dimension (as well as higher dimensions). As opposed to intrinsic topological order, SPT order mainly deals with many-body systems described by single-particle Hamiltonians.

A system is said to have SPT order if it has a gapped Hamiltonian with some discrete symmetries and satisfies the following properties:

1. Technically, due to the finiteness of physical systems, the energy levels are always discrete so that there will always be some finite gap between the groundstate and the excited states. To reconcile this with our intuitive notions, we first define $H(L)$ to be the Hamiltonian of a system of length $L$ with periodic boundary conditions. We then define a monotonically increasing sequence of $L_i$ such that $i \to \infty \Leftrightarrow L_i \to \infty$. If there exists a fixed gap $\Delta$ in which no eigenvalue of $H(L_i)$ for all $i$ can be found, the Hamiltonian is gapped. Note that this definition is a statement of a family of Hamiltonians and not of any individual Hamiltonian. This is what we really mean when we say that a particular Hamiltonian is gapped (even with open boundary conditions).
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1. Two copies of the system, each in different SPT phases, cannot be smoothly transformed into each other while preserving the symmetries unless the energy gap closes.

2. All phases can be continuously transformed into the same trivial state equivalent to the vacuum by breaking the symmetry.

To rephrase the first point in the language we will use in the rest of the text: two systems with the same symmetries are said to be topologically equivalent if there exists a path between their respective Hamiltonians in the space of all Hamiltonians such that the gap does not close at any point during the transformation. While symmetry-protected topological gapless phases [9–16] that do not lend themselves to this definition of topological equivalence certainly exist, they are beyond the scope of this work.

The reason why we are interested in SPT ordered materials (henceforth we will simply say topological instead of SPT ordered) is that their non-trivial phases can host exotic quasiparticle excitations at their boundaries. In the next section, we present and discuss a specific type of zero-energy quasiparticle that occurs as a localized boundary state (edge states in 1D) in topological materials, namely the Majorana bound state (MBS). To see how MBSs – or other zero-energy modes – appear in topological phases, we will employ the following argument: we recall that according to our definition, two gapped systems are topologically equivalent if we can adiabatically map between the Hamiltonians of the two systems in a manner which does not close the gap. Let us now imagine a system made up of two subsystems in different topological phases with an interpolating region in between. By definition, we can not smoothly go between the two subsystems without closing the gap somewhere between them. This tells us that there must be a zero-energy mode at the surface separating them. Extending this, the vacuum can be thought of as being topologically trivial, so we expect zero-energy states to localize at the edges of any finite topologically non-trivial sample. This is called the bulk-boundary correspondence: a topologically non-trivial bulk comes with edge modes. We emphasise that the argument we used is purely heuristic and fails to take some important technicalities into account, for example, it does not tell us why or when we expect the edge states to be MBSs. Regardless of the nature of these edge states, we can conclude that since they follow from the topology of the system, they are robust and only vanish if the system is driven out of its non-trivial phase.
1.2 Majorana bound states

Before we move on to specific models with MBSs, it is necessary to first recapitulate what MBSs are, and what makes them special. The historical origin of MBSs can be traced back to particle physics, and the Italian physicist Ettore Majorana who in 1937 presented a theory of a neutrally charged particle with the special property that it is its own antiparticle [17]. This particle is known as the Majorana fermion, and while it has been suggested that the neutrino could be a Majorana fermion [18], all the other fermions within the standard model are known to be Dirac fermions. Despite the elusiveness of the Majorana fermions in particle physics, similar concepts have found their way into condensed matter theory. Solid state systems usually consist of ions and electrons, and generally do not contain any fermionic particles being their own antiparticles. Nevertheless, as we for example will see in the case of superconductors, in some systems the natural excitations are quasiparticles that are electron-hole-superpositions (EHSs). A subset of these systems can even have EHS quasiparticles that are their own quasihole partners. The role of holes in condensed matter physics resembles that of antiparticles in high energy physics. In this sense, a quasiparticle being its own hole is similar to that of a Majorana fermion being its own antiparticle.\(^2\)

To put this into a more formal setting, we first introduce the creation and annihilation operators of fermions. We denote these operators by \(a_\nu^\dagger\) and \(a_\nu\)\(^3\) respectively. Here \(\nu\) represents some set of system-specific quantum numbers (e.g. spin and momentum). In condensed matter physics, one can view the annihilation operator not only as an operator representing the annihilation of a particle, but also as the creation operator for the corresponding hole. The creation and annihilation operators satisfy the following commutation relations:

\[
\{a_\nu, a_\mu^\dagger\} = \delta_{\nu\mu}, \quad \{a_\nu, a_\mu\} = \{a_\nu^\dagger, a_\mu^\dagger\} = 0. \tag{1.1}
\]

Here we have used the anticommutator\(^4\) defined by \(\{A, B\} \equiv AB + BA\) and the Kronecker delta, \(\delta_{\nu\mu}\), which equals unity if \(\mu = \nu\), and zero otherwise. With the use

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\(^2\)The term Majorana fermion is often used by condensed matter physicists to refer to Majorana quasiparticles. This, however, gives the wrong impression that they (like their cousins in particle physics theory) are fundamental particles, which is not true.

\(^3\)The notation suggests that the operators are Hermitian conjugates of each other, which is indeed the case.

\(^4\)Similar creation and annihilation operators can also be defined for bosons. The difference being that one needs to replace the anticommutators in Eq. (1.1) with regular commutators, \([A, B] = AB - BA\).
of the fermionic operators, we can construct the Majorana operators

$$\gamma_{\nu,1} = a_{\nu}^\dagger + a_\nu$$
$$\gamma_{\nu,2} = i(a_{\nu}^\dagger - a_\nu).$$

From the above equations, it is evident that $\gamma_{\nu,i} = \gamma_{\nu,i}^\dagger$, $i = 1, 2$. This is the mathematical way of expressing the fact that they are their own antiparticles. Furthermore, because of the relations (1.1), Majorana operators obey

$$\{\gamma_{\nu,i}, \gamma_{\mu,j}\} = 2\delta_{\nu\mu}\delta_{ij}.$$  

(1.3)

Formally, one can always decompose fermionic operators into Majorana operators – in fact, there are multiple ways in which one can perform the decomposition. The question of whether it is useful or not is often a statement about the topology of the system. Moreover, a trade-off of the change of basis is that the occupation number operator is not meaningfully defined in the Majorana basis. For regular fermions $a_{\nu}^\dagger a_\nu$ gives the occupation number for a single-particle state in a given many-body state. For Majorana operators, on the other hand, Eqs. (1.2) and (1.3) imply that we always have $\gamma_{\nu,i}^\dagger \gamma_{\nu,i} = \gamma_{\nu,i} \gamma_{\nu,i} = 1$ regardless of the many-body state. Hence it is not sensible to talk about the occupation number of a single Majorana state – in calculations, one must therefore convert back to conventional fermions to extract physical observables.

### 1.2.1 Anyonic statistics

The main reason why MBSs are sought after in condensed matter physics by both theoreticians and experimentalists alike is that they are known to exhibit non-abelian statistics [19, 20]. Normally, exchanges between identical particles preserve the state up to a possible sign change; in a system with two identical particles, if we were to exchange their positions, the wavefunction of the system gains a complex phase, i.e. $\Psi(r_1, r_2) = e^{i\varphi}\Psi(r_2, r_1)$. Performing this action twice gives us $\Psi(r_1, r_2) = e^{2i\varphi}\Psi(r_1, r_2)$. This constrains the phase to satisfy $e^{2i\varphi} = 1$, which can only be true for two values (modulo $2\pi$) of the phase, namely 0 and $\pi$. We conclude that the wavefunction can thus be either symmetric ($\varphi = 0$) or antisymmetric ($\varphi = \pi$) under particle exchange. In Nature, bosons follow the former, while fermions obey the latter.\(^5\)

\(^5\)Since the particles are identical, we have no way of distinguishing them, and the physics should hence not be altered upon this exchange. The wavefunction can then at most pick up a phase.

\(^6\)This kind of particle statistics is encoded in the algebra defined in Eq. (1.1).
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In Andreev reflection, an incident electron in the normal metal (N) scatters of the boundary to the superconductor (SC), resulting in a Cooper pair in the superconductor and a backwards propagating hole in the normal metal. This transfers a net charge of $-2e$ to the superconductor. An incident electron scattering back as an electron is called normal reflection and obviously transfers no charge. In the pictures, electrons are coloured red and holes green.

Remarkably, this is not the case for quasiparticles in certain two-dimensional systems. From a mathematical perspective, the reason for this has to do with homotopy theory and specifically fundamental groups [21, 22]. The qualitative idea is that the double exchange of two particles can equivalently be seen as one of the particles going along a path around the other one. In three dimensions this path can be continuously deformed to a path which does not circumnavigate the other particle – going around is the same as not going at all. In two dimensions, the path can not be smoothly deformed without the path going through the other particle at some point (in three dimensions we avoid this by simply "lifting" the loop over the stationary particle through the extra dimension); in two dimensions, the winding of one particle around the other is no longer necessarily equivalent to a trivial path. Therefore, two-dimensional systems permit the existence of anyons: quasiparticles whose quantum state upon particle exchange either acquires a phase between 0 and $\pi$ (Abelian), or changes to a whole other state (non-Abelian). Non-Abelian statistics could be used in quantum computing to realize different kinds of logic gates. From a technological standpoint, topological systems hosting MBSs could then prove to be a fruitful venue to consider for certain types of quantum computations.\footnote{The fractional statistics of MBSs is not rich enough for a universal quantum computer, but they}
protected by the topology of the system and are inherently non-local, they are robust against local perturbations due to the environment. This would effectively bypass the decoherence problem – one of the biggest challenges facing the quantum computation community [23].

Figure 1.2: The differential conductance, $dI/dV$, of an indium antimonide semiconductor nanowire in contact with a niobium titanium nitride superconductor as measured at the edge of the where the nanowire and superconductor are in contact. Each line corresponds to a different temperature. From top to bottom we have 300, 250, 225, 200, 175, 150, 125, 100, and 60 mK. The lines have been offset for clarity. For sufficiently low temperature a zero-bias peak is clearly visible, suggesting the presence of a MBS. The picture is taken from Ref. [24]

1.2.2 Observations of Majorana bound states

Even though no conclusive evidence for MBSs\(^8\) have been found, an increasing number of experimental groups [24–28] have gotten promising results that hint towards the existence of MBSs. The experiments have primarily relied on measuring the differential conductance $dI/dV$ due to Andreev reflection. Andreev reflection is a phenomenon

\[^8\]Thus far no conclusive evidence for the existence of any kind of non-abelian anyon has been found, but there has been some progress on abelian anyons [30].

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that occurs at the surface between a normal metal and a superconductor [29]. At the barrier, an incident electron in the normal metal reflects back as a hole, creating a Cooper pair in the superconductor (the scenario is depicted in Fig. 1.1). This transfers a net charge of \(-2e\) into the superconductor. A MBS localized at the barrier will create a resonant peak in the measured conductance at \(V = 0\) [31,32]. The first group to see evidence of a zero-bias peak (ZBP) was Mourik et al. in 2012 [24], who did it in a superconductor-nanowire device (see Fig. 1.2). However, computer simulations have shown that similar conductance plots to what experiments gave can be reproduced by a disordered nanowire [33,34]. Other groups have also shown that the Kondo effect could explain the ZBP [35,36].

Figure 1.3: The measured differential conductance at two different points along a ferromagnetic atomic chain. The left picture shows one end of the chain and the right graph gives the measured conductance for the two points labeled 1 (red) and 2 (blue). The tip has a visible zero-bias peak, which is not present within the bulk of the wire. The picture is taken from Ref. [25]

In the fall of 2014, S. Nadj-Perge et al. [25] presented measurements from a different setup consisting of a single line of magnetic atoms deposited on a superconducting substrate. These atoms then arranged themselves into a ferromagnetic configuration. What set this experiment apart from the previous ones, was that they were able to use scanning tunnelling microscopy to measure the conductance at different points along the chain. They observed that the conductance at the edges of the chain had a ZBP that was not present in the bulk (see Fig. 1.3) as is expected if the ZBP is
due to a MBS. All these experiments together provide us with tentative evidence for 
the existence of MBSs, but are far from a conclusive proof, as this would also require 
probing the quasiparticle exchange statistics and show that it is non-Abelian.

As a final comment on the experiments, we note that they were all based on 
nanowires with strong spin-orbit coupling placed on top of a conventional supercon-
ductor. This similarity is not a coincidence and we will in Sec. 2.3 argue from a 
thoretical standpoint why they are good candidates for hosting MBSs. Our argu-
ments will heavily draw from the conclusions made in Sec. 2.2 where we present 
Kitaev’s celebrated p-wave superconductor [2] as a simple toy model that can host 
topologically protected MBSs. In the next chapter, before examining the p-wave 
superconductor, it is instructive to take a brief look at the theory of conventional 
superconductors, as it will introduce us to several useful notions that are ubiquitous 
throughout the rest of this thesis.
Chapter 2

Theory

2.1 Theory of superconductivity

In 1911 Kamerlingh Onnes showed that in a sample of mercury, the electrical resistance dropped to zero when the sample was cooled below 4.2 K [37] – he had discovered superconductivity. Further experiments showed that superconductors not only supported dissipationless electrical currents, but below a certain threshold of the magnetic field, they were perfect diamagnets [38], i.e. the magnetic field could not penetrate the superconductor (above the threshold, the superconducting phase disappears). Phenomenological theories were developed to understand these effects [39], but it took around 40 years before a microscopic theory was put forth. In 1957 Bardeen, Cooper, and Schrieffer published an article where they presented what is nowadays known as the BCS theory of superconductivity [40,41]. The BCS theory relied on an idea developed by Cooper in an earlier article [42]. Cooper showed that an attractive interaction – no matter how weak – between a pair of electrons with energies close to the Fermi energy of a bulk of non-interacting electrons, would condense together into a so called Cooper pair that has a lower energy than the combined energies of the individual constituent free electrons. The BCS theory essentially extends this idea to all the electrons close to the Fermi energy, such that a gap between the Fermi energy and the highest occupied energy forms. This gap is completely void of electrons, and in order to create excitations in this state, the energy needed must be larger than the superconducting gap. The attractive force between the electrons is conventionally explained by an indirect interaction via phonons in the host crystal, but the formation of Cooper pairs does not specifically require the interaction to be phonon-mediated.
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2.1.1 The Bogoliubov-de Gennes Hamiltonian

The BCS theory can be formulated in the language of second quantization by defining the fermionic creation and annihilation operators $a_{k,\sigma}^\dagger$ and $a_{k,\sigma}$ for an electron with momentum $k$ and spin $\sigma = \uparrow, \downarrow$. These operators obey the commutation relations given in Eq. (1.1). In the absence of interactions, the Hamiltonian of a homogeneous gas of electrons is given by

$$H_0 = \sum_{k,\sigma} \xi_k a_{k,\sigma}^\dagger a_{k,\sigma} \tag{2.1}$$

in Fourier space. Here $\xi_k = \varepsilon_k - \mu$ is the difference between the single-particle energy $\varepsilon_k = k^2 / 2m$ and the chemical potential $\mu$. Roughly speaking, the chemical potential describes the energy cost of occupying a given single-particle state. Incidentally, for a normal (non-superconducting) metal, it is also equal to the Fermi energy when the temperature is zero – hereinafter this is what we will assume the temperature to be.

If we now introduce the two-particle interaction of the BCS theory, the Hamiltonian is no longer diagonal:

$$H = H_0 + \sum_{kk'} V_{kk'} a_{k,\uparrow}^\dagger a_{-k',\downarrow}^\dagger a_{-k',\downarrow} a_{k,\uparrow} \tag{2.2}$$

Since the interaction is mediated by phonons, the coupling $V_{kk'}$ is taken to be non-vanishing only for $|\xi_k|, |\xi_{k'}| < \omega_D$, where the cut-off $\omega_D$ is the Debye frequency (the maximum frequency of the phonons in the underlying lattice). As we already mentioned, in the superconducting state, electrons condense into Cooper pairs resulting in a non-zero groundstate expectation value for $\langle a_{k,\uparrow}^\dagger a_{-k',\downarrow}^\dagger \rangle$. If the fluctuations around this expectation value are small, we can rewrite Eq. (2.2) using a mean-field approximation as

$$H = H_0 - \sum_k (\Delta_k a_{k,\uparrow}^\dagger a_{-k,\downarrow}^\dagger + h.c.) \tag{2.3}$$

where we have defined $\Delta_k \equiv -\sum_{k'} V_{kk'} (a_{-k',\downarrow}^\dagger a_{k',\uparrow})$. The abbreviation $h.c.$ stands for Hermitian conjugate. In the mean-field description, the electron number – with the exception of the total number parity – is evidently no longer conserved. The superconducting terms can now be interpreted as creating ($a^\dagger a^\dagger$) and annihilating ($aa$) Cooper pairs with an associated binding energy given by $|\Delta_k|$.

In contrast to the original Hamiltonian in Eq. (2.2), the mean-field Hamiltonian is readily diagonalizable as we no longer have any two-particle interaction terms. By

1The number operator $\hat{n} = \sum_{k,\sigma} a_{k,\sigma}^\dagger a_{k,\sigma}$ does not commute with the Hamiltonian (2.3). However, parity conservation implies $\{(-1)^\hat{n}, H\} = 0$. 
defining the so called Nambu spinor $\Psi_k = (a_{k,\uparrow}, a_{k,\downarrow})^T$, we can with the aid of the Pauli matrices $\sigma_i$, $i = x, y, z$ rewrite Eq. (2.3) in the form

$$H = \frac{1}{2} \sum_k \Psi_k^\dagger H_k \Psi_k + constant,$$

(2.4)

where $H_k = \sigma_z \xi_k - \sigma_x \text{Re} \Delta_k - \sigma_y \text{Im} \Delta_k$. For an arbitrary Hamiltonian that is written in the form of Eq. (2.4), $H_k$ is commonly referred to as the Bogoliubov-de Gennes (BdG) Hamiltonian for the given system. In this form, we see that while it is not diagonal in Fourier space as in the non-interacting normal phase in Eq. (2.1), it is block diagonal, enabling us to diagonalize each block separately. Using the anticommutativity of the Pauli matrices, we easily see that

$$H_k^2 = (\xi_k^2 + |\Delta_k|^2)1_{2 \times 2} \text{ (i.e. it is proportional to the } 2 \times 2 \text{ identity matrix), which immediately tells us that the eigenvalues of } H_k \text{ are } \pm E_k = \pm \sqrt{\xi_k^2 + |\Delta_k|^2}. \text{ These eigenvalues tell us two important things about the superconductor: first off, as long as } \Delta_k \text{ is non-vanishing, it defines an energy gap separating the valence (negative energies) and conductance (positive energies) bands. Secondly, for each energy level } E, \text{ there is a corresponding energy level at } -E, \text{ which is due to the particle-hole symmetry of the superconductor. To see this from another point of view, consider the BdG equations}

$$H_k \psi_k^\pm = \pm E_k \psi_k^\pm,$$

(2.5)

which are just the eigenvalue equations for the BdG Hamiltonian. Here $\psi_k^\pm$ is a two-component eigenvector. Using the unitary transformation

$$U_k = \begin{pmatrix} \cos \theta_k & - \sin \theta_k \\ \sin \theta_k & \cos \theta_k \end{pmatrix}, \quad \tan 2\theta_k = \frac{\Delta_k}{\xi_k},$$

(2.6)

we can diagonalize Eq. (2.5) and find the eigenmodes.\(^2\) To simplify matters, we assumed $\Delta_k$ to be real instead of complex.\(^3\) The relation between the new creation and annihilation operators, and the original electronic operators is given by

$$\begin{pmatrix} \Gamma_{k,\uparrow} \\ \Gamma_{k,\downarrow}^\dagger \end{pmatrix} = U_k \begin{pmatrix} a_{k,\uparrow} \\ a_{k,\uparrow}^\dagger \end{pmatrix} = \begin{pmatrix} \cos \theta_k a_{k,\uparrow} - \sin \theta_k a_{-k,\downarrow}^\dagger \\ \sin \theta_k a_{k,\uparrow} + \cos \theta_k a_{-k,\downarrow}^\dagger \end{pmatrix}. \quad (2.7)$$

\(^2\)This type of transformation is commonly known as a Bogoliubov transformation and was originally used in the study of superfluidity [43].

\(^3\)Any global complex phase of $\Delta_k = |\Delta_k| e^{i\vartheta}$ can always be removed by the transformation $a_{k,\sigma} \rightarrow e^{i\vartheta/2} a_{k,\sigma}$. 

If we remember that we can regard $a_{k,\sigma}$ as the creation operator for a hole, we see that the natural excitations in a superconductor are EHS. We can furthermore deduce from our analysis that each $\pm E$ energy pair correspond to the same quantum state; adding a quasiparticle with energy $E$ is equivalent to removing a quasihole with opposite spin and momenta at energy $-E$.\footnote{Mathematically, this comes from the fact that the Nambu formalism artificially doubles the degrees of freedom.} This intimate relationship between particles and holes is called particle-hole symmetry (PHS).

This concludes our discussion on the conventional superconductor. Note, however, that we have barely scratched the surface of the BCS theory. The purpose of this section was to acquaint ourselves with superconductivity, its energy gap, EHS, and PHS. In the next section, we will see how these concepts together play a crucial role in topological superconductivity.

### 2.2 Kitaev’s p-wave superconductor

The one-dimensional p-wave superconductor consists of a chain of spinless electrons with unconventional pairing. As we saw in the previous section, the pairing in conventional superconductors is between electrons of opposite spin. This means that the two-electron wavefunction for the Cooper pair is antisymmetric with respect to spin. In Kitaev’s model (we use this term interchangeably with the 1D p-wave superconductor), the electrons are thought to be spinless and the Cooper-pair wavefunctions must therefore be antisymmetric in space. This p-wave pairing is very rare in Nature and the overwhelming majority of superconducting materials are s-wave (previously referred to as conventional superconductors). Nevertheless, the properties of MBSs gleaned from this model prove to be very generic and applicable to more realistic settings.

The Hamiltonian of Kitaev’s p-wave superconductor reads as follows:

$$H = -t \sum_{j=1}^{N-1} (a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j) - \mu \sum_{j=1}^{N} a_j^\dagger a_j + \Delta \sum_{j=1}^{N-1} (a_j a_{j+1} + a_{j+1}^\dagger a_j^\dagger). \quad (2.8)$$

Once again, the operators $a_j^\dagger$ and $a_j$ obey the commutation relations in Eq. (1.1) and can be thought of as creating ($a_j^\dagger$) an electron at position $j \in \{1, \ldots, N\}$ or removing ($a_j$) an electron from the same site. The first term is the hopping term, describing electrons moving between adjacent sites (the energy associated with this is $|t|$). For the sake of simplicity, we assume $t$ to be real. The second term involves the familiar
2.2. KITAEV'S P-WAVE SUPERCONDUCTOR

chemical potential $\mu$. The last term contains the superconducting pairing term energy $\Delta$. We can find the energy spectrum by transforming Eq. (2.8) into Fourier space if we impose periodic boundary conditions $(a_{j+N} = a_j)$. The Fourier transforms are defined by

$$a_k = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{ikd} a_j,$$  \hspace{1cm} (2.9)

where $k \in \{-\pi/d, ..., \pi/d\}$ lies within the first Brillouin zone ($d$ is the lattice constant). The Nambu spinor $\Psi_k = (a_k, a_{-k}^\dagger)^T$ enables us to write the Hamiltonian in the BdG form

$$H = \frac{1}{2} \sum_k \Psi_k^\dagger \left[ (\mu + 2t \cos kd)\sigma_z + 2\Delta \sigma_y \sin kd \right] \Psi_k + \text{const.},$$  \hspace{1cm} (2.10)

where $\sigma_y$ and $\sigma_z$ again are Pauli matrices. This deviates from the s-wave superconductor in that the pairing term now contains antisymmetric momentum dependence. The BdG Hamiltonian $h_k = (\mu + 2t \cos kd)\sigma_z + 2\Delta \sigma_y \sin kd$ is easily diagonalized for every $k$, giving us

$$E(k) = \pm \sqrt{(\mu + 2t \cos kd)^2 + 4\Delta^2 \sin^2 kd}.$$  \hspace{1cm} (2.11)

The gap can then be seen to close for either $k = 0$ or $k = \pm \pi/d$ when $|\mu| = 2|t|$. If this system has non-trivial topology, we then expect this condition to express the boundary between different topological phases. We set $t$ to be positive (the negative case follows next to identical reasoning) and look at each side of the gap closing separately: first for $|\mu| < 2t$, and then for $|\mu| > 2t$. The most explicit way of examining the presence of MBSs in this case is to switch to Majorana operators.

The Hamiltonian (2.8) is readily cast into a Majorana basis by the transformation defined in Eq. (1.2), if we replace $\nu$ with $j$:

$$H = -\frac{i}{2} \sum_{j=1}^{N} \mu \gamma_{j,1}\gamma_{j,2} + \frac{i}{2} \sum_{j=1}^{N-1} \left[ (\Delta + t)\gamma_{j,2}\gamma_{j+1,1} + (\Delta - t)\gamma_{j,1}\gamma_{j+1,2} \right].$$  \hspace{1cm} (2.12)

We first consider a point in the region $|\mu| > 2t$, namely the parameters $t = \Delta = 0$ and $\mu \neq 0$. Our Hamiltonian (2.12) now reduces to

$$H = -\frac{i}{2} \sum_{j=1}^{N} \mu \gamma_{j,1}\gamma_{j,2},$$

so the coupling between different Majorana operators is completely local (see Fig. 2.1a). This represents bound electrons with no hopping between different lattice
CHAPTER 2. Theory

points. For the case of \(|\mu| < 2t\), we choose \(t = \Delta\) and \(\mu = 0\). Now our Hamiltonian becomes

\[ H = i\Delta \sum_{j=1}^{N-1} \gamma_{j,2} \gamma_{j+1,1}, \]

where we notice that the coupling suddenly is between Majorana operators at different lattice points (see Fig. 2.1b). More importantly, we see that the two operators \(\gamma_{1,1}\) and \(\gamma_{N,2}\) are not present in the Hamiltonian anymore. This implies that the electronic quasiparticle state corresponding to \(\tilde{a} = (\gamma_{1,1} + \gamma_{N,2})/2\) does not contribute to the total energy of the system, so the ground state of our system now has a degeneracy (the zero-energy state being either occupied or empty). Furthermore, this quasiparticle is highly non-local, since \(\gamma_{1,1}\) and \(\gamma_{N,2}\) are from the beginning and the end of the chain, respectively. In Fig. 2.1c a graph of the wavefunctions of the two MBSs along with the first excited state are plotted for a chain with 30 sites. Note that the two MBSs each correspond to one of the two edges. To have a pair of MBSs is in fact a very general feature of topological superconductors: we need two Majorana operators to form a single fermionic operator, so it is not possible to have an odd number of MBSs in a physical system. The MBSs must therefore come in pairs.\(^5\)

So far no attempt at explaining the robustness of the MBSs has been made. To see how their appearance is not a quirk of the specifically chosen parameters, we need to look to symmetry. We note that the BdG Hamiltonian \((2.8)\) anticommutes with the antiunitary operator \(P = \sigma_x K\), where \(K\) represents the operation of complex conjugation. This is a formal way of showing that the p-wave superconductor possesses PHS,\(^6\) and the energy levels will thus be symmetric around the Fermi energy. This implies that we cannot lift the degeneracy of the groundstate unless we remove the two states from zero\(^7\) simultaneously. This is only achievable if we can couple the two Majorana operators at the ends, but as long as there is a large enough energy gap separating the MBSs from the bulk states, the MBS cannot traverse the bulk. We conclude that the MBS localized at the edges is protected by the bulk gap and PHS; as long the gap does not close, a perturbation that does not break PHS will not remove the degeneracy. This is the essence of SPT order. In Fig. 2.1d we can see that for a finite system the zero-energy states persist up until \(\mu \approx 2t\). At the transition

\(^5\)Some systems even permit several flavours of MBSs – as long as there are an even number of them, see for example Refs. [45–48].

\(^6\)A Hamiltonian \(H\) is said to have PHS, if there exists an antiunitary operator \(P\) such that \(\{H, P\} = 0\) and \(P^2 = \pm 1\).

\(^7\)In this thesis, the energies are usually measured with respect to the Fermi energy, so zero energy is equivalent to the Fermi energy.
2.2. KITAEV’S P-WAVE SUPERCONDUCTOR

Figure 2.1: (a) A schematic picture of the coupling between Majorana operators (blue dots) in the topologically trivial regime. The operators strongly couple within the same site (gray squares). (b) A similar picture as a) except for the topologically non-trivial case. The operators couple between sites, leaving the two operators (purple dots) at the edges uncoupled to any other operators. (c) The amplitude of the wavefunctions in a p-wave superconductor with 30 sites in the topologically non-trivial phase. Parameters $\Delta = t > 0$, and $\mu = 0$ are used. One MBS corresponds to the left peak of the red line, and the other MBS corresponds to the right peak. The black dashed line corresponds to the first excited state. (d) The energy levels for a p-wave system with 30 sites as a function of $\mu$ with $t = \Delta$. The shaded area indicates the topologically non-trivial domain. The two lowest energies are marked in red.

There is another approach, presented in Alicea (2012) [44], which highlights the topological character of Kitaev’s p-wave superconductor from a slightly different, although equivalent, perspective. The starting point is the BdG Hamiltonian from Eq. (2.10), but we will write it in a more generic form as

$$H(k) = h_k \cdot \sigma,$$

where $h_k$ is a vector of $k$ dependent functions, and $\sigma$ is a vectors of Pauli matrices, such that $(\sigma)_i = \sigma_i$. Note that in Fourier space, PHS is expressed through the relation
$H(k) = -\sigma_x H(-k)^* \sigma_x$ or componentwise:

\[ h_x(k) = -h_x(-k), \quad h_y(k) = -h_y(-k), \quad \text{and} \quad h_z(k) = h_z(-k). \]  

These relations relate $k$ to $-k$ so that knowing $H(k)$ for all $k \geq 0$ completely determines the Hamiltonian in the whole Brillouin zone. If $h_k$ is now non-zero for all values of $k$, we can construct a mapping from the Brillouin zone to the unit sphere via

\[ k \mapsto \frac{h_k}{|h_k|}. \]  

Due to the symmetry of the lattice, all values of $k$ that are related to each other by a reciprocal lattice vector, namely an integer number of translations of $2\pi/d$ in our case, are equivalent. This, combined with the relations defined in Eq. (2.14), tells us that

\[ h_x(0) = h_x(\pi) = h_y(0) = h_y(\pi) = 0, \]  

while $h_z(0)$ and $h_z(\pi)$ are non-vanishing ($h_k$ must be non-zero). Depending on the relative sign between $h_z(0)$ and $h_z(\pi)$, as $k$ goes from $0$ to $\pi$, the mapping (2.15) traces out a path starting from one pole that either returns to that pole (same sign) or sweeps across the sphere to the opposite pole (opposing signs). It is not possible to smoothly deform the first path to the second without closing the gap. We can now define a $\mathbb{Z}_2$ topological invariant

\[ \nu \equiv \text{sign}[h_z(0)h_z(\pi)]. \]  

If $\nu = 1$, there will be an even number of pairs of Fermi points in the first Brillouin zone, so that there will be an even number of MBSs at each end of the chain. They will thus combine into local electronic states and the system is trivial. When $\nu = -1$ there must be an odd number of pairs, so that there will be one unpaired MBSs left at each end. We anticipate that $\nu = -1$ indicates a non-trivial phase. For the p-wave superconductor, we have that $h_z(k) = \mu + 2t \cos kd$. From our discussion, we expect the system to be in a topological phase whenever $\text{sign}[h_z(0)h_z(\pi)] = \text{sign}[(\mu + 2t)(\mu - 2t)] = -1$, but this is precisely equivalent to $|\mu| < 2|t|$ that we already obtained earlier. In this argument, we can see that the detailed structure of the bands is not important, since Eq. (2.15) maps the system to a flatband model, where all the eigenvalues are $\pm 1$.

Before we discuss more realistic models, some closing remarks on Kitaev’s model are needed. When we derived the spectrum (2.11) for the p-wave model, we enforced periodic boundary conditions in order to diagonalize the Hamiltonian in Fourier space.
2.3. MAJORANA BOUND STATES IN NANOWIRES

This is equivalent to bringing the two ends of the chain together, forming a ring. Moving to such a geometry would instantly hybridize any MBSs at the edges, leaving a gapped system with no edge modes. This splitting would not affect the bulk spectrum in any significant way, so the gap closings derived from Eq. (2.11) are approximately true for the open chain as well\(^8\). Moreover, for any finite system with open boundary conditions, the groundstate degeneracy is only approximate, as there will always be a non-vanishing coupling between the two ends. In condensed matter physics, the groundstate is said to be degenerate as long as the energy splitting between the two states closest to zero energy vanishes as \( \sim e^{-L/\xi} \) with the length \( L \) of the system for some characteristic length \( \xi \). This is why the transition in Fig. 2.1d is not exactly at \( \mu = 2t \). In the next section, we will discuss more realistic models which will bridge the gap between the toy model presented in this section, and the experiments as well as our model.

2.3 Majorana bound states in nanowires

As we already mentioned in the previous section, Kitaev’s toy model is not realistic, so in order for this discussion to not solely be an academic exercise, we need to come up with more physically feasible systems that could host MBSs. To this end, we will still use the p-wave superconductor as our guiding light.

In the real world, electrons come with spin, which means that a realistic model must contain this degree of freedom as well. However, adding spin trivially to our model will result in a degeneracy, such that if the model without spin hosted MBSs at the edges, the spinful system would have two MBSs fusing into regular finite-energy fermions at both ends. The system would hence always be trivial. To amend this, we need to lift the spin degeneracy. For example a strong Zeeman field allows us to separate the spins, so that the bands in our spectrum are spin-polarized. A magnetic field also comes with the added bonus that it breaks spinful time-reversal symmetry (TRS), which otherwise would make each energy level doubly degenerate, due to Kramer’s theorem. This would eliminate any MBSs, as they would again come in pairs on both edges.

Next, we must change our p-wave pairing to s-wave, as Nature unfortunately overwhelmingly favours the latter over the former. We do not wish to rid ourselves of

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\(^8\)The same energy spectrum could have been established in the case of an infinite chain, since this also makes the system translation invariant. The longer a finite chain is, the more accurately the bulk spectrum is described by Eq. (2.11).
superconductivity altogether, as it gives us an energy gap, as well as PHS to protect the MBSs. This change comes at a cost, however: since s-wave pairing combines electrons of opposing spin, the total spin is conserved. As we already mentioned, a Zeeman field creates spin-polarized bands, so all states come with a definite spin, and s-wave pairing cannot mix them. Since a particle and its hole partner must have opposing spins, it follows that MBSs have to be zero-spin states and as it is now, such states are not possible (if we instead had p-wave pairing, this would not be a problem, as it does not conserve spin). In order to break spin conservation, we must therefore introduce one more thing into our system. This final ingredient is commonly taken to be spin-orbit coupling \cite{49} as it couples spin and momentum. While spin-orbit interaction (much like the Zeeman field) couples to spin, it does not (unlike the Zeeman field) break spinful time-reversal. The Zeeman field is thus not by any means rendered redundant by spin-orbit coupling.

All in all, from our discussions in the previous section as well as in this section, we can conclude that the presence of MBSs necessitates the following features:

- An energy gap in the bulk\(^9\)
- Discrete symmetries (at least PHS)
- Broken spin-conservation.
- No band degeneracies

From the introduction, we know that the first two on the list are nothing but the requirements for any SPT order. The first is automatically satisfied in the presence of a superconductor through the proximity effect \cite{50}. As we saw in the case of the p-wave superconductor, a discrete symmetry is needed to protect the MBSs from splitting. In fact, the presence of PHS in the p-wave system is not a special case, but is required for MBSs to exist. The symmetry must force the spectrum to have energy levels coming in \(\pm E\) pairs. This prevents the MBSs from separately moving away from zero energy, effectively locking them into place. The system can certainly have additional symmetries apart from PHS, but these symmetries (tying in with the last point on the list) must not create any additional band degeneracies.

In this thesis, we will study the Shiba chain: a system consisting of an array of magnetic impurities placed on top of an s-wave superconductor. The impurity mo-

\(^9\)Technically, zero-energy Majorana-like edge states are also present in some topological gapless systems \cite{51}, but for our intents and purposes, we can disregard this.
ments break spinful TRS as well as spin-conservation; local magnetic fields break spinful TRS, and arranging the moments in a helical fashion removes spin-conservation. We will first look at the model in the so called deep-dilute limit (a term which will be explained once we get there), which can be described by an effective two-band BdG Hamiltonian. We then move on to a more general setting (to which no effective BdG description exists), with double the number of bands. We will hence refer to the two models as the two-band model (TBM), and the four-band model (FBM), respectively.\footnote{The doubling of the bands is not due to the model taking more physics into account, but is an artefact of the formalism.}
Chapter 3

The Shiba Chain

In this chapter, our main objective is to present the Shiba chain. We introduce and derive the two models (TBM and FBM) which act as effective low-energy theories for the Shiba chain. A generic Shiba system consists of a conventional superconductor with magnetic impurities placed on top. The impurities are assumed to be static with no direct interaction between different magnetic moments. This kind of setup was originally studied in the 1960s [52–54], when it was shown that the presence of impurities with classical spin could host localized electronic bound states with energies within the gap of the bulk superconductor.

As we already mentioned at the end of the preceding chapter, the Shiba chain offers us a way to satisfy all the criteria needed for MBSs. The presence of a superconductor creates a gap in the spectrum as well as providing us with PHS. The impurities break spinful TRS, by introducing a local magnetic field. Instead of spin-orbit coupling, the helical texture now breaks spin conservation for us. This can be understood from a physical perspective if we imagine one electron moving along the Shiba chain. Since the spin of the electron always tries to align itself with the local magnetic field, the spin direction changes as the electron jumps between impurity sites with non-parallel moments.

Typically, the coherence length of a superconductor is of the order of $\xi \sim 100$ nm, which is fairly large compared to the lattice constant of most materials ($d \sim 0.5$ nm). Given that the magnitude of the wave function of a Shiba state is $\sim e^{-r/\xi} / k_F r$, where $r$ is the distance to the impurity site to which the state is bound, the wavefunction decay is for all practical purposes $1/r$ for most conventional superconductors. In an array of magnetic impurities, the Shiba states will for some systems hence significantly overlap even when the inter-impurity distance $a \gtrsim 10d$.

The overlapping Shiba states will give rise to energy bands, where the effective
superconducting pairing strength together with the hopping terms contain long-range components as a direct consequence of this. However, one often desires exponentially localized MBS, as any overlap between their respective wavefunctions lifts them away from zero energy. This is seemingly at odds with the power-law decay exhibited by the Shiba states. Remarkably, due to the interplay between the pairing and hopping terms, there exists topologically non-trivial regions in parameter space in which the MBS are indeed exponentially localized to the edges of the wire [55]. More generally, the MBS will inherit the power-law decay from the Shiba states with an eventual exponential decay determined by the superconducting coherence length.

In the experiment by Nadj-Perge et al. [25] magnetic atoms were located sufficiently close together for their moments to directly interact, giving rise to a ferromagnetic ordering. The models in this work deviates from this in that the distance between impurities is assumed to be of the order of several lattice constants of the underlying superconductor (and, of course, the magnetic texture). In the following, we take a closer look at the Shiba chain with a helical configuration, where the moment of the impurity at position \( x_n = na \) is given by

\[
S_n = S[\cos(2k_H x_n) \sin \theta, \sin(2k_H x_n) \sin \theta, \cos \theta].
\]

Here we have introduced several important parameters that we will use throughout this work: \( a \) is once more the distance between adjacent impurities, \( S \) is the magnitude of the impurity moment, \( \theta \) is the position-independent polar angle measured with respect to some arbitrarily chosen axis, and \( k_H \) is the helical wavenumber describing the pitch of the helix (\( 2k_H x_n \) is the azimuthal angle for the \( n \)th impurity). For a simple pictorial representation of a helical texture, see Fig. 3.1.
3.1 The Ruderman-Kittel-Kasuya-Yosida interaction

Before we move on to the TBM, some comments on the possible origins of a helical configuration are in order. The impurity moments in the Shiba chain are thought to behave classically, with the impurities placed sufficiently far away as to only couple through an effective Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction \[56\], mediated by the electrons in the bulk superconductor. The RKKY interaction comes from a second-order perturbative treatment and is given by

\[ H_{\text{RKKY}} = \sum_{nm} I_{nm} S_n \cdot S_m, \]

where the exchange coupling \( I_{nm} \sim \chi(r_n - r_m) \) depends on the spin susceptibility \( \chi(r) \) of the system and \( S_n \) does not a priori follow Eq. (3.1). In a normal metal \[50\], the RKKY interaction can be understood from the fact that electrons in the vicinity of a magnetic impurity will become polarized so that their spins align with the impurity moment. These polarized electrons can then come into contact with another impurity, which will then polarize accordingly. This picture is slightly altered in the superconducting state, since the electrons in the ground state form unpolarized Cooper pairs. Furthermore, the gap between the ground state and the excited states prevents the magnetic impurity from polarizing electrons. Since the ratio between the gap \( \Delta \) and the Fermi energy \( \varepsilon_F \) is \( \Delta/\varepsilon_F \ll 1 \), the effect is not large. This argument suggests that the RKKY interaction is to some degree suppressed in the superconducting phase, but remains largely unaffected.

At any rate, for a nanowire on a superconducting bulk, the classical groundstate of the RKKY Hamiltonian (3.2) is helical \[50,57\] with \( k_H \equiv k_F \mod \pi/a \), where \( k_F \) is the Fermi momentum.\(^2\) There is theoretical evidence that these systems naturally self-organize, so that the pitch of the helix gives rise to a topological wire \[57-60\]. Despite this, the helical wavevector is treated as a free parameter in this thesis; in principle other effects in addition to the RKKY interaction can alter the relation between \( k_H \) and \( k_F \), for example spin-orbit coupling or quirks of the band structure.

\(^1\)In 2012, Menzel \textit{et al.} \[61\] observed a helical magnetic ordering, although not in a superconducting system.

\(^2\)Even though the use of \( k \) is primarily reserved for wavenumbers in this thesis, we work in units where \( h = 1 \), so wavenumbers and momenta are equivalent.
3.2 The deep-dilute two-band model

In this section, we present the Two-band model of the helical Shiba chain, put forth by Pientka et al. (2013) [3]. The theory of the TBM rests on two key assumptions: first, the magnetic impurities are said to be dilute. This means that the spacing between neighbouring impurities is large enough for pairs of Shiba states to form at each individual impurity and that the hybridization due to wavefunction overlap is small enough ($\Delta / k_F a \ll \Delta$) so that the resulting energy bands remain within the gap. The second assumption we make is that the energy $\epsilon$ of an individual Shiba state lies deep within the gap, $\epsilon \ll \Delta$. This keeps the bands from joining the bulk spectrum outside the gap, and additionally allows us to construct an effective Hamiltonian describing only the subgap Shiba bands.

The starting point is the tight-binding BdG Hamiltonian

$$H = \xi_p \tau_z - J \sum_n (\mathbf{S}_n \cdot \mathbf{\sigma}) \delta (\mathbf{r} - \mathbf{r}_n) + \Delta \tau_x,$$

which is written in the Nambu space defined by $\Psi = (\psi_\uparrow, \psi_\downarrow, \psi_\downarrow^\dagger, -\psi_\uparrow^\dagger)^T$ (we have for the sake of clarity omitted the spatial $\mathbf{r}$ arguments from the field operators $\psi_\sigma$). We denote the Pauli matrices in the particle-hole and spin subspaces with $\tau$ and $\sigma \equiv (\sigma_x, \sigma_y, \sigma_z)$ respectively.\(^3\) The Dirac-delta function $\delta (\mathbf{r} - \mathbf{r}_n)$ localises the coupling between the impurity moment and the electron spin to the impurity site $\mathbf{r}_n$. The coupling strength is given by the factor $J$. As before, $\xi_p$ and $\Delta$ are the single-particle energy measured relative to the chemical potential, and the superconducting gap (which we assume to be real and positive).

Before we proceed, we will first make a couple of remarks regarding the Hamiltonian (3.3) and its symmetries. We can see that the Hamiltonian anticommutes with the antiunitary operator $\mathcal{P} = \tau_y \sigma_y K$. As expected, the Hamiltonian possesses PHS. In our chosen basis, the antiunitary operator representing spinful TRS is $\mathcal{T} = i \sigma_y K$, which commutes with both the first and the third term in the Hamiltonian, but not the term coupling the electrons to the magnetic impurities. Additionally, this term is also responsible for removing the commutation between the Hamiltonian and any spin operator $s = \sum_i \alpha_i \sigma_i \hat{x}_i^i$ as long as the chain consists of several non-aligned $S_n$. This means that spin conservation is broken in a helically ordered chain, formalising what we already argued from a physical standpoint.

\(^3\)In this thesis, we avoid writing out the cross product explicitly. Instead, we write $\tau_i \sigma_j \equiv \tau_i \otimes \sigma_j$. Similarly, $\tau_i$ and $\sigma_j$ standing alone really mean $\tau_i \otimes 1$ and $1 \otimes \sigma_j$, where $1$ is the $2 \times 2$ identity matrix.

\(^4\)\(\alpha_i\) are complex constants, and $\hat{x}_i$ is the unit vector in the direction $i = x, y, z$. 
3.2. THE DEEP-DILUTE TWO-BAND MODEL

In the next subsections, we present and lay the groundwork for the TBM. These discussions will closely follow the arguments in Ref. [3].

3.2.1 The single-impurity energy

An important energy scale in the Shiba chain is the single-impurity energy, which can be obtained from the BdG equations

\[(\xi_p \tau_z \mp JS \sigma_z \delta(r) + \Delta \tau_z) \Psi(r) = E \Psi(r),\] (3.4)

This is the Hamiltonian (3.3) reduced to a single impurity placed at the origin. Without loss of generality, we set the impurity moment to point in the \(z\)-direction, so that the BdG equations decouple in spin (spin up corresponds to the negative sign and spin down to the positive sign). We now isolate the impurity term

\[(E - \xi_p \tau_z - \Delta \tau_z) \Psi(r) = \mp JS \sigma_z \delta(r) \Psi(0),\] (3.5)

and Fourier transform both sides so that we end up with

\[(E - \xi_p \tau_z - \Delta \tau_z) \Psi_p = \mp JS \sigma_z \Psi(0).\] (3.6)

From this we can immediately solve for \(\Psi_p\) and perform an inverse transform back to real space. We end up with the expression

\[\left[1 \mp \frac{\alpha}{\sqrt{\Delta^2 - E^2}}(E + \Delta \tau_z)\right] \Psi(0) = 0.\] (3.7)

In accordance with the prevailing notational conventions, we have defined \(\alpha \equiv JS \nu_0 \pi\), where \(\nu_0\) is the density of states at the Fermi energy in the normal-ordered phase. The intermediate steps between Eqs. (3.6) and (3.7) can be found in App. A.

The subgap single-impurity energies can now easily be obtained from Eq. (3.7):

\[\varepsilon_\alpha = \Delta \frac{1 - \alpha^2}{1 + \alpha^2}.\] (3.8)

The eigenvectors can be derived from Eq. (3.7) by noting that everything except for the term with \(\tau_x\) is proportional to the unit matrix. The eigenvectors must then be those of \(\tau_x\). Written in our Nambu basis, they are

\[\Psi_+(0) = \frac{1}{\sqrt{N}} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad \Psi_-(0) = \frac{1}{\sqrt{N}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix},\] (3.9)
where \( N = (1 + \alpha^2) / 2\pi \nu_0 \Delta \alpha \) can be obtained from the normalization condition

\[
\int dr |\Psi_\pm(r)|^2 = \int \frac{dk}{(2\pi)^3} |\Psi_\pm(k)|^2 = 1. \tag{3.10}
\]

Note that because of PHS, the eigenvectors are related by \( \Psi_-(0) = P \Psi_+(0) \).

In anticipation of what is soon to come, we note that we can rewrite the eigenvectors in general coordinates as

\[
\Psi_+(r) = \frac{1}{\sqrt{N}} \begin{pmatrix} |\uparrow\rangle \\ |\uparrow\rangle \\ \end{pmatrix}, \quad \Psi_-(r) = \frac{1}{\sqrt{N}} \begin{pmatrix} |\downarrow\rangle \\ -|\downarrow\rangle \\ \end{pmatrix}, \tag{3.11}
\]

where \(|\sigma\rangle\) is the eigenvector for a spin \( \sigma \) with arbitrary direction; for an eigenstate of a spin aligned with a magnetic moment defined by Eq. (3.1), we have \(|\uparrow, n\rangle\) = \((\cos(\theta/2), \sin(\theta/2)e^{2ikx_n})^T\) and \(|\downarrow, n\rangle\) = \(T|\uparrow, n\rangle\) = \((\sin(\theta/2)e^{-2ikx_n}, -\cos(\theta/2))^T\). This will become important in the coming subsection, when we introduce more impurities to our system.

### 3.2.2 Many impurities

We are now equipped to tackle the problem of many impurities. Following the steps from the singly-impurity problem, we separate the impurity terms from the rest in the BdG equation

\[
(E - \xi_p \tau_z - \Delta \tau_x) \Psi(r) = -J \sum_n (S_n \cdot \sigma) \delta(r - r_n) \Psi(r_n). \tag{3.12}
\]

We then Fourier transform and multiply both sides with the inverse of the matrix on the left-hand side:

\[
\Psi_p = -J \sum_n e^{-ip \cdot r_n} (S_n \cdot \sigma) (E - \xi_p \tau_z - \Delta \tau_x)^{-1} \Psi(r_n), \tag{3.13}
\]

where we made use of the commutation between matrices operating in different subspaces to move the inverse past \((S_n \cdot \sigma)\). Moving back to real space, we end up with

\[
\Psi(r_n) = -\sum_m J_E (r_n - r_m) (\hat{S}_m \cdot \sigma) \Psi(r_m), \tag{3.14}
\]

which is a set of coupled equations relating the Shiba states at different impurities. We have absorbed the magnitude of the impurity moment into the coupling term (and
ultimately $\alpha$), and used the notation $\hat{S}_m \equiv S_m/|S_m| = S_m/S$. The coupling matrix is derived in App. A and is for $r \equiv |r| \neq 0$ shown to be

$$J_E(r) = -\frac{\alpha}{\sqrt{\Delta^2 - E^2}} \frac{e^{-r/\xi_E}}{k_F r} \times$$

$$\begin{pmatrix}
  E \sin k_F r + \sqrt{\Delta^2 - E^2} \cos k_F r & \Delta \sin k_F r \\
  \Delta \sin k_F r & E \sin k_F r - \sqrt{\Delta^2 - E^2} \cos k_F r
\end{pmatrix}$$

(3.15)

and

$$J_E(0) = -\frac{\alpha}{\sqrt{\Delta^2 - E^2}} [E1 + \Delta \tau_x]$$

(3.16)

for vanishing argument. In Eq. (3.15), we have introduced the coherence length $\xi_E = v_F/\sqrt{\Delta^2 - E^2}$ containing the Fermi velocity $v_F$. Note that $\xi_0$ is the coherence length of the underlying superconductor as described by the BCS theory.

At this point we invoke our assumptions that the single-impurity energy lies deep within the gap, i.e. $\Delta \gg |\varepsilon_\alpha| \approx \Delta(1 - \alpha)$ or equivalently that $\alpha \approx 1$, and that the Shiba states are sufficiently dilute as to also keep the energy bands well within the gap. This allows us to find an approximate solution by expanding Eq. (3.14) in terms of $(1 - \alpha), E/\Delta$ and $1/k_F r_nm$, keeping only terms up to linear order in all three. Note that all the terms in the sum in Eq. (3.14) except for $m = n$ are already linear in $1/k_F r_nm$, so it suffices to set $E = 0$ and $\alpha = 1$ in all terms for which $m \neq n$. Rearranging the result gives us

$$\left( 1 - \frac{E}{\Delta} + \alpha \tau_x \right) (\hat{S}_n \cdot \sigma) \Psi(r_n) =$$

$$\sum_{m \neq n} \frac{e^{-r_{nm}/\xi_0}}{k_F r_{nm}} (\tau_z \cos k_F r_{nm} + \tau_x \sin k_F r_{nm}) (\hat{S}_m \cdot \sigma) \Psi(r_m),$$

(3.17)

where $r_{nm} \equiv r_n - r_m$. We now wish to remove $(\hat{S}_n \cdot \sigma)$ from the term proportional to $E$ to permit us to transform Eq. (3.17) into the form of an energy eigenvalue equation from which we can extract an effective Hamiltonian. We then wish to project the resulting equation to the low-energy Shiba states in Eq. (3.11). The first step is achieved by noting that $(\hat{S}_n \cdot \sigma)^2 = 1$, so multiplying Eq. (3.17) by $(\hat{S}_n \cdot \sigma)$ gives us

$$\left( (\hat{S}_n \cdot \sigma) - \frac{E}{\Delta} + \alpha \tau_x \right) \Psi(r_n) =$$

$$\sum_{m \neq n} \frac{e^{-r_{nm}/\xi_0}}{k_F r_{nm}} (\tau_z \cos k_F r_{nm} + \tau_x \sin k_F r_{nm}) (\hat{S}_n \cdot \sigma)(\hat{S}_m \cdot \sigma) \Psi(r_m).$$

(3.18)
CHAPTER 3. THE SHIBA CHAIN

Projecting this equation onto the subgap Shiba states and isolating the term proportional to \( E \) finally yields the equation

\[
H_{\text{eff}} \psi = E \psi, \tag{3.19}
\]

where the effective Hamiltonian is given by

\[
H_{\text{eff}} = \begin{pmatrix} \hat{h} & \Delta \\ \Delta^\dagger & -\hat{h}^T \end{pmatrix}. \tag{3.20}
\]

The elements of the subblock matrices are

\[
\hat{h}_{nm} = \begin{cases} \varepsilon_n & n = m \\ -\Delta \sin \frac{k_F r_{nm}}{\xi_0} e^{-r_{nm}/\xi_0} \langle \uparrow, n | \uparrow, m \rangle & n \neq m \end{cases}, \tag{3.21}
\]

\[
\Delta_{nm} = \begin{cases} 0 & n = m \\ \Delta \cos \frac{k_F r_{nm}}{\xi_0} e^{-r_{nm}/\xi_0} \langle \uparrow, n | \downarrow, m \rangle & n \neq m. \end{cases}
\]

So far our arguments have not made any reference to the spatial dimensions (as long as it can be embedded in 3D as the Fourier transforms are calculated in 3D) or magnetic texture of the Shiba array. From now on, however, we will assume a 1D chain with a helical texture. This means that we change \( r_{nm} \to x_n - x_m = a(n - m) \) and the local spin states \( |\sigma, n\rangle \) have associated spins aligned with \( S_n \) as defined in Eq. (3.1). The inner products between different spin states can now be written out explicitly as

\[
\langle \uparrow, n | \uparrow, m \rangle = \cos^2 \frac{\theta}{2} e^{i k_H (x_n - x_m)} \\
\langle \uparrow, n | \downarrow, m \rangle = i e^{-i k_H (x_n + x_m)} \sin \theta \sin[k_H (x_n - x_m)]. \tag{3.22}
\]

Due to the complex exponent on the latter expression, the Hamiltonian is not translation invariant.\(^5\) This can be remedied by a unitary transformation defined by

\[ \mathcal{U} = \exp(i k_H \sigma_z \otimes X/2), \]

where \( X \) is a matrix with entries \( X_{nm} = \delta_{nm} x_n \). The transformed Hamiltonian \( \mathcal{H} = \mathcal{U} H_{\text{eff}} \mathcal{U}^\dagger \) has the structure of Eq. (3.20), but with matrix elements

\[
\hat{h}_{nm} = \begin{cases} \varepsilon_n & n = m \\ -\Delta \sin \frac{k_F r_{nm}}{\xi_0} e^{-r_{nm}/\xi_0} \left( \cos^2 \frac{\theta}{2} e^{i k_H (x_n - x_m)} + \sin^2 \frac{\theta}{2} e^{-i k_H (x_n - x_m)} \right) & n \neq m, \end{cases} \tag{3.23}
\]

\(^5\)By translation invariant, we of course mean an infinite chain or closed boundary conditions; a finite system with open boundary conditions cannot have translation symmetry under any circumstances.
and
\[ \tilde{\Delta}_{nm} = \begin{cases} 0 & n = m \\ i \frac{k_F r_{nm}}{\xi_0} e^{-r_{nm}/\xi_0} \sin \theta \sin[k_F(x_n - x_m)] & n \neq m, \end{cases} \quad (3.24) \]
which are both translation invariant.

A peculiarity of the new Hamiltonian is that for \( \theta = \pi/2 \) it commutes with the antunitary operator \( \tilde{T} = i \sigma_z K \), where the Pauli matrix now acts in the particle-hole like space explicitly written out in Eq. (3.20). In other words, \( \tilde{T} \) is formally a time-reversal operator. While there is no Kramer’s degeneracy since \( \tilde{T}^2 = 1 \), this additional symmetry would alter the topological classification from \( \mathbb{Z}_2 \) (having at most one pair of MBSs) to \( \mathbb{Z} \) \([62–64]\) (potentially having several different flavours of MBSs) due to the additional chiral symmetry; a system possessing both PHS and TRS automatically gives it a third symmetry commonly referred to as a chiral symmetry.\(^6\) Even though this symmetry might be relevant for an exhaustive description of the helical Shiba chain, we do not concern ourselves with it in this thesis.

### 3.2.3 The connection to Kitaev’s toy model

To make contact with the toy model from Sec. 2.2, and simultaneously pinpoint the differences between the TBM and Kitaev’s p-wave superconductor, we consider the experimentally less relevant situation of a system with short coherence length \( \xi_E \leq a \). In this limit, it is reasonable to approximate the off-diagonal matrix elements in Eqs. (3.23) and (3.24) to be zero whenever \( |n - m| > 1 \), or put differently: only hopping and pairing between nearest neighbours are taken into account.

Using Eq. (3.20) and setting \( \theta = \pi/2 \), we can write a second quantized Hamiltonian
\[ H = \varepsilon_a \sum_n c_n^\dagger c_n - t \sum_n (c_{n+1}^\dagger c_n + h.c.) + i \tilde{\Delta} \sum_n (c_{n+1}^\dagger c_n^\dagger - h.c.), \quad (3.25) \]
with the identifications \( t \equiv \Delta \frac{\sin k_F a}{k_F a} e^{-a/\xi_0} \cos k_H a \) and \( \tilde{\Delta} \equiv i \Delta \frac{\cos k_F a}{k_F a} e^{-a/\xi_0} \sin k_H a \).

The operators \( c_n \) are as usual fermionic. Comparing Eq. (3.25) to Eq. (2.8), we can conclude that Eq. (3.25) is nothing but the familiar p-wave model.\(^7\)

The above argument gives us a relation between the Shiba chain and a model we know hosts MBSs. However, the arguments also implicitly tell us about some of the qualitative differences between Kitaev’s model and the general case: for example, the

\(^6\)If \( \mathcal{C} \) is a unitary operator and \( \mathcal{T} \) is an antunitary operator satisfying \( \{ \mathcal{C} \mathcal{T}, H \} = [\mathcal{T}, H] = 0 \), it follows that \( \{ \mathcal{C}, H \} = 0 \).

\(^7\)The connection can be made even more explicit by performing a unitary transformation \( c_n \rightarrow e^{i \pi/4} c_n \).
superconducting pairing is indeed p-wave, but the pairing (and hopping) inherits the algebraic decay from the Shiba states.

3.2.4 The two-band model in momentum space

For the analysis of the topological properties in the subsequent chapter, it will be useful to transform our effective Hamiltonian into Fourier space. The Fourier transformation of the effective Hamiltonian with matrix elements (3.23) and (3.24), is obtained from

\[ \tilde{h}_k = \sum_m \tilde{h}_{nm} e^{ik(x_n - x_m)} \]
\[ \tilde{\Delta}_k = \sum_m \tilde{\Delta}_{nm} e^{ik(x_n - x_m)}. \] (3.26)

In App. B, we show that these Fourier transformations can be written in terms of elementary functions as

\[ \tilde{h}_k = \varepsilon - \frac{\Delta}{k_Fa} \left( \cos^2 \frac{\theta}{2} [A(k_F + k + k_H) + A(k_F - k - k_H)] + \sin^2 \frac{\theta}{2} [A(k_F - k + k_H) + A(k_F + k - k_H)] \right) \]
\[ \tilde{\Delta}_k = \frac{\sin \theta}{4k_Fa} \left[ f(k_F + k + k_H) + f(k_F - k - k_H) - f(k_F - k + k_H) - f(k_F + k - k_H) \right], \] (3.27)

where we have introduced the two functions

\[ A(k) = \arctan \left( \frac{\sin ka}{e^{a/\xi_0} - \cos ka} \right) \]
\[ f(k) = -\ln \left( 1 + e^{-2a/\xi_0} - 2e^{-a/\xi_0} \cos ka \right). \] (3.29)

The effective Hamiltonian is block diagonal in momentum space, with the 2 \times 2 sub-blocks

\[ \mathcal{H}_k = \begin{pmatrix} \tilde{h}_k & \tilde{\Delta}_k \\ \tilde{\Delta}_k & -\tilde{h}_{-k} \end{pmatrix} \] (3.30)
giving us two energy bands.

This concludes our presentation of the TBM. We return to it in the next chapter, when we take a closer look at its topological properties. Next, we take a closer look at the FBM, where we relax the assumptions made when deriving the TBM.
3.3 General impurity strength and hybridization

In the previous section, we saw that through a series of clever manipulations, we could rewrite the original BdG equation from Eq. (3.3) describing a chain of magnetic impurities on a conventional superconductor as an effective BdG Hamiltonian with p-wave pairing. In order for us to make analytical progress, we imposed two assumptions, viz. the single-impurity energy lies deep within the gap, and the impurities are far from each other. Together, the assumptions gave rise to the deep-dilute limit. In this section our objective is to move away from this limit and consider the system in a more general setting. Since much of the discussion regarding the physical aspects of the model has already been done prior to this, this section comes with more emphasis on the mathematical framework of the FBM.

3.3.1 The non-linear eigenvalue problem

The main point of departure is Eq. (3.17), as the linearisation scheme is not valid anymore. Without approximations, the equation corresponding to Eq. (3.17) is

\[
\left( 1 + J_E(0) \langle \hat{S}_n \cdot \sigma \rangle \right) \Psi(r_n) = - \sum_m J_E(r_{nm}) \langle \hat{S}_n \cdot \sigma \rangle \langle \hat{S}_m \cdot \sigma \rangle \Psi(r_m),
\]

where both sides now depend non-linearly on \( E \) and \( 1 - \alpha \). Since we no longer assume that the energy bands are located deep within the gap, we cannot simply project our equation to the low-energy bands.\(^8\) Instead, in addition to the states in Eq. (3.11), we must also take the two states

\[
\tilde{\Psi}_+(r) = \frac{1}{\sqrt{N}} \begin{pmatrix} |\downarrow\rangle \\ |\downarrow\rangle \end{pmatrix}, \quad \tilde{\Psi}_-(r) = \frac{1}{\sqrt{N}} \begin{pmatrix} |\uparrow\rangle \\ -|\uparrow\rangle \end{pmatrix}
\]

(3.32)

into account. We can write our complete basis in the compact form

\[
|\pm \uparrow\rangle = \frac{1}{\sqrt{N}} \begin{pmatrix} |\uparrow\rangle \\ \pm |\uparrow\rangle \end{pmatrix}, \quad |\pm \downarrow\rangle = \frac{1}{\sqrt{N}} \begin{pmatrix} |\downarrow\rangle \\ \pm |\downarrow\rangle \end{pmatrix}.
\]

(3.33)

The basis vectors are direct products of Pauli spin-matrix eigenvectors spanning the particle-hole and spin space; the leftmost argument in \( |\tau \sigma\rangle = |\tau\rangle \otimes |\sigma\rangle \) thus represents

\(^8\)At the beginning of this chapter, we said that we would derive low-energy theories of our two models. In the present context, this simply refers to the subgap physics.
the eigenvector of $\tau_x$ with eigenvalue $\tau = \pm 1$ and the rightmost argument corresponds to the spin eigenvector with eigenvalue $\sigma = \pm 1$.

We can now project Eq. (3.32) onto the basis defined by

$$\langle \Psi \rangle_n = \begin{pmatrix} \langle + \uparrow | \Psi(r_n) \rangle \\ \langle - \downarrow | \Psi(r_n) \rangle \\ \langle + \downarrow | \Psi(r_n) \rangle \\ \langle - \uparrow | \Psi(r_n) \rangle \end{pmatrix}. \quad (3.34)$$

To this end, we define the matrices

$$h_{\sigma\sigma'}^{nm} \equiv \begin{cases} 0 & n = m \\ e^{-r_{nm}/\xi}k_{F}\sin k_{F}r_{nm}\langle \sigma, n|\sigma', m \rangle & n \neq m \end{cases} \quad (3.35)$$

$$d_{\sigma\sigma'}^{nm} \equiv \begin{cases} 0 & n = m \\ e^{-r_{nm}/\xi}k_{F}\cos k_{F}r_{nm}\langle \sigma, n|\sigma', m \rangle & n \neq m \end{cases}$$

and the parameter

$$\lambda_E = \frac{\Delta + E}{\sqrt{\Delta^2 - E^2}}. \quad (3.36)$$

Observe that in this notation, $\tilde{h} = -\Delta \hat{h}^{\uparrow \uparrow} + \epsilon \alpha 1$ and $\tilde{\Delta} = \Delta \hat{d}^{\uparrow \downarrow}$. From the projection to Eq. (3.34), we obtain

$$\lambda_E^2 A_2 \Psi + \lambda_E A_1 \Psi + A_0 \Psi = 0, \quad (3.37)$$
where

\[
A_2 = \begin{pmatrix}
1 + h^{\uparrow\uparrow} & 0 & -h^{\uparrow\downarrow} & 0 \\
0 & 0 & 0 & 0 \\
-h^{\downarrow\uparrow} & 0 & 1 + h^{\downarrow\uparrow} & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}
\]

\[
A_1 = \begin{pmatrix}
\frac{-1}{\alpha} & -d^{\downarrow\downarrow} & 0 & d^{\uparrow\uparrow} \\
-d^{\uparrow\uparrow} & \frac{1}{\alpha} & 0 & d^{\downarrow\downarrow} \\
0 & d^{\downarrow\downarrow} & \frac{1}{\alpha} & 0 \\
d^{\uparrow\uparrow} & 0 & -d^{\downarrow\downarrow} & -\frac{1}{\alpha}
\end{pmatrix}
\]

(3.38)

\[
A_0 = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 1 + h^{\downarrow\downarrow} & 0 & -h^{\uparrow\uparrow} \\
0 & 0 & 0 & 0 \\
0 & -h^{\uparrow\downarrow} & 0 & 1 + h^{\uparrow\uparrow}
\end{pmatrix}
\]

In contrast with Eq. (3.17) of the TBM, Eq. (3.37) is a $4N \times 4N$ NEV equation for a finite chain of length $N$. A somewhat more in-depth treatment of NEV problems can be found in App. C but roughly speaking, they can be viewed as generalisations of the familiar linear eigenvalue equations. We have thus managed to rewrite our original linear problem with eigenvalue $E$ in the form of a NEV equation with eigenvalues $\lambda_E$. The basis (3.34) was chosen so that the TBM can be obtained from the upper left $2N \times 2N$ block of Eq. (3.37) after performing the necessary linearisations. In this basis, the terms omitted in the projection to the lowest energy bands for the TBM are all located in the $2N \times 2N$ off-diagonal blocks.

As our final deed for this chapter, we write the NEV equation (3.37) in momentum space. The momentum representation can be calculated through similar expressions.
as Eq. (3.26). The result is

\[
\begin{pmatrix}
\lambda^2(1 + h_k^{↑↑}) - \lambda/\alpha & -\lambda d_k^{↑↓} & -\lambda^2 h_k^{↑↓} & \lambda d_k^{↑↑} \\
-\lambda d_k^{↑↓} & -1 - h_{-k}^{↑↑} + \lambda/\alpha & \lambda d_{-k}^{↑↑} & h_{-k}^{↑↓} \\
-\lambda^2 h_k^{↑↓} & \lambda d_{-k}^{↑↑} & \lambda^2(1 + h_{-k}^{↑↑}) + \lambda/\alpha & -\lambda d_{-k}^{↑↓} \\
\lambda d_k^{↑↑} & h_{-k}^{↑↓} & -\lambda d_{-k}^{↑↓} & -1 - h_{-k}^{↑↑} - \lambda/\alpha
\end{pmatrix} \Psi_k = 0,
\]

where we have omitted the index \( E \) on the \( \lambda \)'s. The definitions of \( h_k^{\sigma\sigma'} \) and \( d_k^{\sigma\sigma'} \) in terms of elementary functions along with their derivations are found in App. B.

At first glance it seems as if we have gone against the usual approach to solving problems in physics: we have in a way started from a simpler problem and turned it into a larger, more complex problem. Nevertheless, in this case it will turn out to be useful, when we in the next chapter analyse the topological properties of our models.
Chapter 4

Topological properties of helical Shiba chains

We saw in the previous chapter how our model of the Shiba chain can be expressed as a NEV problem. In this chapter, we present the main results of this thesis. From the NEV equation, we derive analytical expressions for the topological phase diagrams of both the TBM and FBM for arbitrary coherence lengths. Using our analytical solutions, our first objective in this chapter is to reproduce the topological phase diagrams in Ref. [3]. We must emphasize that the phase diagrams in Ref. [3] were obtained within the framework of the TBM presented in Sec. 3.2 by numerically calculating the lowest energy for different parameter values. In contrast, our results for the topological phase boundaries are purely analytical. Our second objective is to compare the FBM for different superconducting coherence lengths and see how well the topological phase diagrams of finite coherence lengths agree with the phase diagram for infinite coherence length.

Naively, the NEV equation (3.39) seems to be too convoluted to permit any non-numerical progress. The important observation here is that it is superficially polynomial in \( \lambda E \), in which the energy \( E \) is hidden. For polynomial eigenvalue problems of order \( p \), i.e. \( \sum_{n=0}^{p} \lambda^n A_j = 0 \), there exists a method by which one can transform the equation into a generalized linear eigenvalue equation of dimension \( pN \times pN \) when the dimensions of the matrices \( A_j \) are \( N \times N \) (for a concrete example, see App. C). To complicate matters, the energy is also present in the exponential factors containing the coherence length. So Eq. (3.39) is strictly speaking not a polynomial eigenvalue problem. To circumvent this, we basically have two options: either we look at the limit \( \xi_E \rightarrow \infty \), which would remove all energy dependence from the exponents, or we look for \( E = 0 \) solutions (which would remove all energy dependence).
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To derive the topological phase diagram the obvious choice is the latter option. Topological phase transitions are characterized by the closing of the energy gap, so what we need to look for are solutions of our NEV problem for \( E = 0 \). We also expect gap closings between different topological regions to only occur at momenta \( ka = 0 \) and \( ka = \pm \pi \). The motivation for this is that due to Kitaev [2], we know that the topological phase of our TBM (3.30) is determined by the value of the topological invariant \( \nu = \text{sign}(\tilde{h}_0 \tilde{h}_{\pi/\alpha}) \) (an argument for this was already given in Sec. 2.2, see Eq. (2.17)). The invariant can therefore only change when the energy gap closes at \( ka = 0, \pm \pi \). Since the FBM and TBM ought to have the same topological classification with similar phases, we can extract the topological phase boundaries for the FBM (3.39) by setting \( E = 0 \) (\( \lambda_0 = 1 \)) and \( ka \) to either 0 or \( \pi \). Any non-trivial solution then requires that

\[
\begin{vmatrix}
1 + h_{\uparrow \uparrow}^{\uparrow \uparrow} - 1/\alpha & 0 & 0 & d_{\downarrow}^{\uparrow} \\
0 & -1 - h_{\uparrow}^{\uparrow \uparrow} + 1/\alpha & d_{\downarrow}^{\uparrow \uparrow} & 0 \\
0 & d_{\downarrow}^{\uparrow \uparrow} & 1 + h_{\downarrow}^{\uparrow \uparrow} + 1/\alpha & 0 \\
d_{\downarrow}^{\uparrow \uparrow} & 0 & 0 & -1 - h_{\downarrow}^{\uparrow \uparrow} - 1/\alpha
\end{vmatrix} = 0, \quad (4.1)
\]

where \( q \) is taken to be either 0 or \( \pi/\alpha \). As can be seen from the explicit forms of the Fourier transformations in App. B, all the terms indexed with opposing spins\(^1\) vanish for these specific values. An important point to note is that neither \( h_{\uparrow \uparrow}^{\uparrow \uparrow} = [A(k_F + q + k_H) + A(k_F - q - k_H)]/k_F a \) nor \( d_{\downarrow}^{\uparrow \uparrow} = [f(k_F + q + k_H) + f(k_F - q - k_H)]/2k_F a \) depend on the polar angle \( \theta \). The caveat is that for non-planar angles \( \theta \neq \pi/2 \) the parameter space contains regions where the system is gapless, and by construction our trick cannot tell us anything about these; to properly capture the gapless regions we would either need to look for \( E = 0 \) solutions at generic momenta, or numerically calculate the lowest energy for different parameters (a method which we will employ shortly). That being said, in places where the gapless regions do not overlap with the topological boundaries, our method still gives us the correct topological phase boundaries between regions where the system is gapped.\(^2\) The link between non-planar helices and the existence of gapless regions is perhaps not so obvious, but we

\(^1\)In real space, the spins were associated with different impurity sites and were not in general aligned. In this sense it is not sensible to talk about opposite and parallel spins. However, this is unlikely to be a source of confusion.

\(^2\)It is not a priori clear where the gapless regions overlap with the phase boundaries and must thus be checked separately.
4.1. COMPARISON OF THE TWO MODELS

postpone such discussions to Subsec. 4.1.2. Nonetheless, the solution of Eq. (4.1) can be expressed in terms of $\alpha$ as a function of the remaining parameters $k_Fa$ and $\xi_0$:

$$\alpha_{FBM}^q = \frac{1}{\sqrt{(1 + h_q^\uparrow)^2 + (d_q^\uparrow)^2}}, \quad (4.2)$$

from which $\alpha_{FBM}^0$ and $\alpha_{FBM}^{\pi/a}$ provide us with one boundary surface each.

The topological phase boundaries for the TBM are easily calculated from the leftmost upper subblock of Eq. (4.1)

$$\operatorname{det} \begin{vmatrix} 1 + h_q^\uparrow - 1/\alpha & 0 \\ 0 & -1 - h_q^\uparrow + 1/\alpha \end{vmatrix} = 0 \quad (4.3)$$

where we also need to linearise the expressions with respect to $1 - \alpha$. In the deep-dilute limit we then have

$$\alpha_{TBM}^q = 1 - h_q^\uparrow. \quad (4.4)$$

4.1 Comparison of the two models

In the previous chapter, we obtained the TBM by linearising not only with respect to $E/\Delta \approx (1 - \alpha)$ but also with respect to $1/k_Fa$. Since $h_q^\uparrow$ (and also $d_q^\uparrow$) is already $\mathcal{O}(1/k_Fa)$ there was no need for an expansion in terms of this parameter. The difference between the two models is then $\mathcal{O}((1 - \alpha)^2, (1/k_Fa)^2)$. The expressions for the topological boundaries maintain this relationship, which can be seen from expanding $\alpha_{FBM}^q$ in terms of $h_q^\uparrow$ and $d_q^\uparrow$:

$$\alpha_{FBM}^q = \frac{1}{[1 + 2h_q^\uparrow + (h_q^\uparrow)^2 + (d_q^\uparrow)^2]^{1/2}} = 1 - h_q^\uparrow - \frac{(h_q^\uparrow)^2 + (d_q^\uparrow)^2}{2} + \mathcal{O}\left(\frac{1}{k_Fa}\right)^3$$

$$\alpha_{TBM}^q = \alpha_{FBM}^q + \mathcal{O}\left(\frac{1}{k_Fa}\right)^2. \quad (4.5)$$

In the above expression we used Eq. (4.4) in conjunction with the aforementioned fact that both $h_q^\uparrow$ and $d_q^\uparrow$ are $\mathcal{O}(1/k_Fa)$.

4.1.1 The planar helix

A comparison between the phase diagrams of the two models for a planar helix along with Fig. 6a in Ref. [3] can be seen in Fig. 4.1. The figure clearly shows that the
Figure 4.1: The topological phase diagram for a planar helix. The topological and trivial regions are labeled by T and N respectively. The gray borders corresponds to the numerically obtained diagram Fig. 6a in Ref. [3]. The dashed line is the analytical solution for the TBM. As is apparent from the figure, the two methods match each other very well. The main difference being that the non-topological gap-closing dividing the topological sector is absent for the analytical solution. The red line shows the phase boundaries for the FBM. The parameters used are $\theta = \pi/2$, $k_{Ha} = \pi/4$, and $\xi_0 = 50a$. For the numerical solution, the energies were measured relative to $\Delta$.

The analytical TBM is in perfect agreement with the diagram of Ref. [3] and the FBM only seems to deviate from the TBM to a greater extent when $|1 - \alpha| \geq 0.1$. Curiously, there seems to be some disagreement in the vicinity of $\alpha = 1$ as well, even though we would expect the resemblance to be the greatest in that region. This is most likely attributed to the relatively small $k_{Fa}$. In fact, the diagram in Fig. 4.1 is restricted to a narrow interval of $k_{Fa}$ values and, as such, does not illustrate the convergence of the models in terms of this parameter. In Fig. 4.2, we see the topological phase diagram for a wider range of values. When $k_{Fa} \lesssim 4\pi$ the discrepancies between the two models become significant. This behaviour is to be expected, since the TBM should only be valid when $k_{Fa} \gg 1$. If we now look at the specific point $(k_{Fa}, \alpha) = (2.7\pi, 1.3)$ in Fig. 4.2, the FBM should have MBSs while the TBM is trivial. In Fig. 4.3 we have plotted the amplitude of the wavefunction of the two lowest positive-energy states for
4.1. COMPARISON OF THE TWO MODELS

Figure 4.2: A comparison between the topological phase diagrams of the TBM (dashed line) and FBM (solid line) for a system with the same parameters as in Fig. 4.1. The non-trivial regions should be obvious from Fig. 4.1 (which in the current figure can be found between $k_Fa = 4\pi$ and $k_Fa = 5\pi$). The difference between the two models decreases as the value of $k_Fa$ increases.

Both models. As we surmised, the lowest state is a MBS localized to the edges of the chain for the FBM and has an energy of the order of $\sim 10^{-5}\Delta$ for a chain of 100 impurities. The first excited state has an energy roughly $10^3$ times larger. The lowest energy for the TBM has the same order of magnitude as the first excited state in the FBM and shares the shape of the wavefunction.

The first equality in Eq. (4.5) seems to suggest that the boundaries of the FBM should be offset to lower values of $\alpha$ in comparison to the TBM, because of the first correction being strictly negative. Instead we see the opposite happen at some swaths of parameter space. While the expansion parameter $1 + 2h_q^{\uparrow\uparrow} + (h_q^{\uparrow\uparrow})^2 + (d_q^{\uparrow\uparrow})^2$ has a magnitude less than 1, it is not usually the case that $|1 + 2h_q^{\uparrow\uparrow} + (h_q^{\uparrow\uparrow})^2 + (d_q^{\uparrow\uparrow})^2| \ll 1$, so higher order corrections can to some degree influence the results. Nonetheless, the qualitative similarities to the FBM makes the TBM a reasonable approximation even in the case of a relatively dense impurity chain.
CHAPTER 4. TOPOLOGICAL PROPERTIES OF HELICAL SHIBA CHAINS

4.1.2 Non-planar configurations

So far we have restricted much of our discussion to planar helices. Moving away from the planar case opens up regions within the parameter space where the spectrum becomes gapless. To understand why $\theta \neq \pi/2$ always has gapless regions in the parameter space, it is beneficial to see why the spectrum is otherwise always gapped except for at the topological phase transitions. For simplicity, we only consider the TBM, as the spectrum for the FBM (see App. D) is too convoluted to work with. The conclusions ought to be the same for both models, since the TBM represents the deep-dilute limit. It is then reasonable to expect that energies close to $E = 0$ (like gap closings) are similar in both models – at least for dilute chains. The TBM spectrum for $\theta = \pi/2$ is easily obtained from the TBM Hamiltonian (3.30):

$$E_k^\pm = \pm \sqrt{\tilde{h}_k^2 + \tilde{\Delta}_k^2},$$

(4.6)

using the fact that now $\tilde{h}_k = \tilde{h}_{-k}$. We end up with two bands mirrored about $E = 0$ that only vanish if $\tilde{h}_k$ and $\tilde{\Delta}_k$ are simultaneously zero. This is only possible at the special points $ka = 0, \pm \pi$, which are the gap closings associated with the topological phase transitions.

When the system is tuned away from $\theta = \pi/2$, the helix sweeps out a cone. The non-vanishing net magnetisation introduces an antisymmetric term $\tilde{h}_k^A(\theta)$ to $\tilde{h}_k(\theta) =$
4.2. LONG COHERENCE LENGTHS

\[ \hat{h}_k^S + \hat{h}_k^A(\theta), \] where \( \hat{h}_k^S \equiv \hat{h}_k(\theta = \pi/2) \). The spectrum now becomes

\[ E_k^\pm = \hat{h}_k^A \pm \sqrt{(\hat{h}_k^S)^2 + \Delta_k^2}. \] (4.7)

The antisymmetry guarantees that \( \hat{h}_k^A \) and \( \pm \sqrt{(\hat{h}_k^S)^2 + \Delta_k^2} \) must have different signs at half of all values of \( k \). It is not hard to see that the system becomes gapless if the magnitude of \( \hat{h}_k^A \) is greater than \( \sqrt{(\hat{h}_k^S)^2 + \Delta_k^2} \). Physically, the introduction of antisymmetric terms reduces the resonance between time-reversed electrons, suppressing the Cooper pairing between fermions with anti-parallel momentum.

To reliably plot the topological phase diagram, we are forced to use the energy spectrum to find all the gap closings – such a plot can be seen in Fig. 4.4. A noticeable difference between the FBM and the TBM is that the gapless regions of the FBM leak out, making them larger than in the TBM case, while simultaneously reducing the size of the topological regions (the underlying reason for this is addressed in the next section).

The full expressions for the energy bands used to plot Fig. 4.4 are derived in App. D. As we mentioned before, they can only be found analytically in the infinite coherence length limit, so the obvious next (and last) step is to examine how this limit compares to finite coherence lengths.

4.2 Long coherence lengths

Generally, the coherence length \( \xi_0 = \hbar v_F/\Delta \) (we have explicitly included \( \hbar \) here) is large compared to the lattice constant \( a \). To make contact with reality, we consider a lead superconductor as a concrete example. It has a Fermi velocity of \( v_F \approx 1.8 \times 10^6 \) m/s [65], a gap (at zero temperature) of about \( 27.3 \times 10^{-4} \) eV [66] and a bulk lattice constant at the order of \( \sim 500 \) pm [67]. Together, this gives us that \( \xi_0 \sim 150a \) if we conservatively assume that the lattice constant \( a \) of the impurity chain is around six times that of \( a \) the underlying bulk. We can thus see that at least for lead, the coherence length is large compared to \( a \).

In any realistic experimental setup, the length of the chain is most likely at the order of 10s of impurities with a coherence length several multiples of that. The decay of the Shiba states is then predominantly algebraic – effectively behaving as if \( \xi_0 = \infty \). From this perspective, it is natural to examine to what extent one can approximate \( \xi_0 \) to be infinite. In Fig. 4.5 we see that the phase boundaries of the FBM for \( \xi_0 = 50a \) and \( \xi_0 = \infty \) coincide relatively well with the exception that the lower
Figure 4.4: (a) A topological phase diagram for a non-planar helix described by the FBM. The gapless region is labeled with G, and N and T denote the trivial and topological regions as before. The parameters used were $\theta = \pi/5$, $k_H = \pi/8$, and $\xi_E = \infty$. We used $\Delta$ as the energy scale. (b) The same topological diagram, but instead for the TBM. This is similar to Fig. 6b in Ref. [3] except for the infinite coherence length.

Figure 4.5: (a) The topological phase diagram for the FBM for different coherence length. The solid line corresponds to an infinite coherence length, while the dashed line shows the diagram for $\xi_0 = 50a$. The planar helix from Fig. 4.1 is also used here. The inset depicts the same situation for the TBM. Once again we denote the trivial and topological regions by N and T. (b) A wider diagram for the same system.
corners of the diagram acquire tails in the long coherence length limit, but otherwise the boundaries remain smooth. This is different from the TBM (inset of Fig 4.5a), whose diagram gains sharp corners. The differences accumulate at the corners, so as long as our system remains sufficiently far away from them, the infinite limit should be applicable.

The coherence length enters through an exponential factor and as such it is hardly surprising that the phase diagrams in Fig. 4.5a are mostly very similar. An illustration of the convergence with increasing coherence length is seen in Fig. 4.6, where the phase diagrams corresponding to three finite coherence lengths are plotted along with the infinite case. For $\xi_0 > 100a$, the system effectively behaves as if $\xi_0 = \infty$.

![Figure 4.6: The topological phase diagram of the same system as in the previous figures, but for different coherence lengths.](image)

### 4.2.1 Singular behaviour at $\xi_E = \infty$

There are some qualitative differences between the FBM and TBM when $\xi_E \rightarrow \infty$. We already saw in Fig. 4.4 (which was obtained in the long coherence length limit) a certain leakage in the phase diagram. The origin of this effect along with the tails present in the planar helix requires us to briefly discuss the contents of App. B.

If we set $\xi_E = \infty$, the derivations done in App. B are mathematically not as
straightforward (although the end result is the same) as for finite $\xi_E$. For example, suppose we were to take the limit before Fourier transforming $h_{nm}^{\uparrow\uparrow}$. In that case, the Fourier series (B.8) is not strictly convergent as the expansion parameter has unit magnitude.\(^3\) However, if we instead take the final result in Eq. (B.15), and let $\xi_E \to \infty$, the answer is finite. To be more explicit, from Eq. (B.14) we get that

$$\lim_{\xi_E \to \infty} A(k) = \arctan(\tan(ka)), \quad (4.8)$$

where $\arctan x$ maps its argument to the principal branch $[-\pi/2, \pi/2]$. We get that $A(k)$ maps $k$ to $k \mod \pi/a$ such that the translated $ka$ ends up within the principal branch. At any rate, the value of $A(k)$ remains finite.

The function $f(k)$, on the other hand, acquires logarithmic singularities at $ka = 2\pi n$, $n \in \mathbb{Z}$ in this limit – something which is evident:

$$\lim_{\xi_E \to \infty} f(k) = -\ln 2 - \ln(1 - \cos(ka)). \quad (4.9)$$

The singularities are the reason for the tails and the leaking effect observed in the diagrams for infinite coherence length. For example, the tails in Fig. 4.5a occur at $k_F a - k_H a = 4\pi$ and $k_F a + k_H a = 5\pi$. The former corresponds to $q = 0$, while the latter to $q = \pi/a$. Why these points are special is clear from Eqs. (B.24) and (B.23): $k_F$ and $k_H$ come in combinations of $k_F \pm k_H$ and depending on whether $q = 0$ or $q = \pi/a$, the singularities occur at either $(k_F a \pm k_H a) \mod 2\pi = 0$ or $(k_F a \pm k_H a) \mod 2\pi = \pi$. All the tails are hence found at $k_F a = n\pi \pm k_H a$, $n \in \mathbb{N}$, which we can confirm to hold true in Fig. 4.5b.

The tails only exist for the FBM due to the presence of $d_q^{\uparrow\uparrow}$ in Eq. (4.5) describing the phase boundaries for the FBM. In contrast, the expression (4.4) for the phase boundaries in the TBM only had $h_q^{\uparrow\uparrow}$, which is bounded. Of course, the expressions for the FBM boundaries are finite regardless of the magnitude of $d_q^{\uparrow\uparrow}$, since it enters through the denominator. If we had exact precision, the tails of the computed diagrams would go down to $\alpha = 0$. On the other hand, tails are present for both models in the energy spectrum, since here none of the singular terms cancel.

As a final remark, we wish to emphasise that even though the parameters used in the figures and in the text are all from a very narrow scope of the full parameter regime, our main results have been numerically verified for other parameters as well. The reason for only showing the results for parameters analogous to those used in Ref. [3] is to more clearly illustrate the differences and similarities between the models.

---

\(^3\)For some values of $k, k_F,$ and $k_H$ harmonic series even seemingly pop up.
Chapter 5

Conclusions

In this thesis, we have studied the topological properties of the helical Shiba chain. Our main result, published in Ref. [1], is the successful generalization of previous work done in Ref. [3] in the deep-dilute limit to a larger parameter regime. This was achieved by a novel approach in which the problem was completely reformulated in terms of a nonlinear eigenvalue problem.

We began with a brief introduction to the concept of topological order and more specifically symmetry-protected topological order. We saw how the presence of certain symmetries and an energy gap between the conductance and valence band of a non-interacting fermionic system give rise to robust zero-energy edge modes referred to as Majorana bound states. These Majorana bound states furthermore had the special property of being their own hole states. All this was illustrated using the example of Kitaev’s toy model of a 1D p-wave superconductor. We argued how one can define a topological invariant for a two-band model using the diagonal elements of the Hamiltonian in momentum space.

Using the toy model as a stepping stone to more realistic nanowire systems, we discussed what ingredients are required in order for a system to host Majorana bound states. We then introduced the helical Shiba chain and showed that it indeed satisfies all the requirements to host Majorana bound states.

Starting from a tight-binding Bogoliubov-de Gennes Hamiltonian, we transformed our problem into a non-linear eigenvalue problem. This resulted in a four-band description with a larger domain of applicability for this system, which had previously only been studied with a two-band model in the low-energy limit for a dilute chain of impurities. From the non-linear eigenvalue problem, we were able to extract analytical expressions for the topological phase diagrams for the two- as well as the four-band model. We then compared this to previous numerical results and confirmed that they
indeed agreed with each other in the correct limit.

For finite coherence lengths, we saw that the diagrams of the models were qualitatively the same, although there were quantitative differences. Comparing finite and infinite coherence lengths showed qualitative differences in the form of tails (wedges of topological sectors in the otherwise trivial domain) at \( k_Fa = \pm k_H \mod \pi \) for \( \xi_E = \infty \) for the four-band models. The origin of these tails could be attributed to singularities in Fourier space. The tails were not present in the topological phase diagram of the two-band model. We also saw that the topological phase diagrams for the four-band model with finite coherence length were practically identical to the infinite coherence length case when \( \xi_E \geq 100a \).

A derivation and treatment of a two-band model was recently presented by Brydon et al. (2015) [68] for a Shiba chain with ferromagnetic order. The derivation and analysis was done in the spirit of Ref. [3]. The study of ferromagnetic order in Shiba systems is primarily motivated by the recent experiments performed by Nadj-Perge et al. who saw hints of the presence of Majorana bound states in a ferromagnetic Fe wire placed on top of a Pb superconductor with strong spin-orbit Rashba coupling. As the experiment was conducted in the strong hybridization and large coherence length limit, a modification of our nonlinear eigenvalue problem approach can provide a way to go beyond the deep-dilute regime [69] and bridge the gap between the experiments and recent theoretical work [45, 46, 48, 68, 70].
Bibliography


[54] A.I. Rusinov, JETP Lett. 9, 85 (1969)


[67] Wolfram Alpha LLC., http://www.wolframalpha.com/input/?i=ElementData%5B%22Lead%22%2C+%22LatticeConstant%22%5D
(accessed July 17, 2015)


Appendix A

Integrals

In this appendix, we carry out a detailed calculation of integrals of the form

\[ J(\mathbf{r}) = \int \frac{d\mathbf{p}}{(2\pi)^3} e^{-i\mathbf{p} \cdot \mathbf{r}} (E - \xi_p \tau_z - \Delta \tau_x)^{-1}. \]  

(A.1)

The evaluation of this type of integral is central to bridge the gap between Eqs. (3.6) and (3.7) when deriving the single-impurity energy, as well as finding the form of the coupling matrix (3.15) for many impurities.

In order to proceed, we must first find the inverse of the matrix \( E - \xi_p \tau_z - \Delta \tau_x \). This is quite straightforwardly achieved since we are dealing with a 2 \( \times \) 2 matrix. As can be easily verified, the inverse is simply

\[ (E - \xi_p \tau_z - \Delta \tau_x)^{-1} = \frac{E + \xi_p \tau_z + \Delta \tau_x}{E^2 - \xi_p^2 - \Delta^2}. \]  

(A.2)

The form of the inverse tells us that in order to successfully evaluate the integral in Eq. (A.1), we must first evaluate the two auxiliary integrals

\[ J_1(\mathbf{r}) = \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{e^{-i\mathbf{p} \cdot \mathbf{r}}}{E^2 - \xi_p^2 - \Delta^2} \]  

(A.3)

and

\[ J_2(\mathbf{r}) = \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{\xi_p e^{-i\mathbf{p} \cdot \mathbf{r}}}{E^2 - \xi_p^2 - \Delta^2}. \]  

(A.4)

Since \( \xi_p = p^2/2m - \mu \) the second integral is not strictly convergent. To accommodate this, we introduce a convergence factor \( \omega_D^2/(\xi_p^2 + \omega_D^2) \) such that

\[ J_2(\mathbf{r}) = \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{\xi_p e^{-i\mathbf{p} \cdot \mathbf{r}} \omega_D^2}{E^2 - \xi_p^2 - \Delta^2 \xi_p^2 + \omega_D^2}. \]  

(A.5)

This cut-off is motivated by the fact that the BCS theory is only valid up to energies at the scale of the Debye frequency \( \omega_D \). Now, due to the denominators, both integrals are
peaked around $\xi_p = 0$, or equivalently (since we are working in the zero-temperature limit) $p \approx k_F$. It is then reasonable to expand $\xi_p$ to linear order in $p - k_F$ so that we end up with $p = k_F + \xi_p/v_F$. Our integrals can then be approximated as

$$J_1(r) \approx -\frac{\nu_0}{2} \int_{-1}^{1} d\cos \theta \int_{-\infty}^{\infty} d\xi \frac{e^{-i(k_p + \xi/v_F)r \cos \theta}}{E^2 - \xi^2 - \Delta^2}, \quad \text{(A.6)}$$

and

$$J_2(r) \approx -\frac{\nu_0}{2} \int_{-1}^{1} d\cos \theta \int_{-\infty}^{\infty} d\xi \frac{\xi e^{-i(k_p + \xi/v_F)r \cos \theta}}{E^2 - \xi^2 - \Delta^2} \frac{\omega_D^2}{\xi^2 + \omega_D^2}, \quad \text{(A.7)}$$

where the density of states at the Fermi surface $\nu_0$ comes from

$$\frac{d\nu}{d\xi} \left( \frac{dn}{dp} \right)^{-1} \nu_{\xi_p} = \left( \frac{4\pi p^2}{(2\pi)^3} \right)^{-1} \nu_{\xi_p} \approx \frac{(2\pi)^3}{4\pi p^2} \nu_0.$$  

By definition the density of states at energy $\xi_p$ (momentum $p$) is given by $dn/d\xi$ (where $n$ is the density of electrons).

We restrict the analysis to subgap energies, i.e. $|E| < \Delta$, so the $\xi$ integrals are readily calculated through standard contour integration in the complex plane. For $J_1(r)$, we then have

$$J_1(r) = -\frac{\nu_0}{2} \left[ \int_{-1}^{0} d\cos \theta \frac{e^{-i(k_F + i\sqrt{\Delta^2 - E^2}/v_F)r \cos \theta}}{\sqrt{\Delta^2 - E^2}} + \int_{0}^{1} d\cos \theta \frac{e^{-i(k_F - i\sqrt{\Delta^2 - E^2}/v_F)r \cos \theta}}{\sqrt{\Delta^2 - E^2}} \right], \quad \text{(A.8)}$$

which reduces to

$$J_1(r) = -\frac{\pi \nu_0}{\sqrt{\Delta^2 - E^2}} \frac{\sin k_F r}{k_F} e^{-r/\xi_E}, \quad \text{(A.9)}$$

where we have introduced $\xi_E = v_F/\sqrt{\Delta^2 - E^2}$ (not to be confused with the energy $\xi_p$), which is nothing but the coherence length of the bulk superconductor.\(^1\) We furthermore assumed that $\xi_E k_F \gg 1$.

For $J_2(r)$ the steps are similar, except that we now how to take into account the additional poles due to the cut-off factor. Having done all the integrals, all that remains is to eliminate the cut-off by taking the limit $v_F k_F, \omega_D \to \infty$ such that the ratio $v_F k_F/\omega_D$ is constant. This limit is valid if we restrict ourselves to the situation where $r \gg v_F/\omega_D$. We finally end up with

$$J_2(r) = -\frac{\pi \nu_0}{k_F} \cos k_F r e^{-r/\xi_E}. \quad \text{(A.10)}$$

With these two, we can construct $J_E(r)$ as long as $r$ is sufficiently far away from zero. In the case of $r = 0$, however, we must return to Eqs. (A.6) and (A.7) and

\(^1\) Usually there is an additional factor of $\pi$ in the denominator.
set $r = 0$ before calculating the integrals. For $J_1(0)$ we can once more use contour integration to obtain

$$J_1(0) = \frac{\pi \nu_0}{\sqrt{\Delta^2 - E^2}},$$

(A.11)

and for $J_2(0)$ we simply conclude that the integral vanishes due to the antisymmetry of the integrand.
Appendix B

Fourier transformations

In this appendix we derive the explicit expressions for the Fourier transformations of the entries in the NEV problem (3.39).

We begin by considering the real-space terms $h_{nm}^{\sigma\sigma'}$ and $d_{nm}^{\sigma\sigma'}$. Before we look at the Fourier transformations, we must first address an issue already brought up in the main text in the context of the TBM, namely that some of the matrix elements are not translation invariant. With the implicit assumption that we only deal with the off-diagonal terms (since $h_{nm}^{\sigma\sigma'} = d_{nm}^{\sigma\sigma'} = 0$ in any case), the elements are given by

$$
\begin{align*}
    h_{nm}^{\sigma\sigma'} &= e^{-r_{nm}/\xi E_{k_F r_{nm}}} \sin k_{F r_{nm}} \langle \sigma, n | \sigma', m \rangle \\
    d_{nm}^{\sigma\sigma'} &= e^{-r_{nm}/\xi E_{k_F r_{nm}}} \cos k_{F r_{nm}} \langle \sigma, n | \sigma', m \rangle 
\end{align*}
$$

(B.1)

where the inner products of spin eigenstates follow directly from

$$
\begin{align*}
    | \uparrow, n \rangle = \begin{pmatrix}
        \cos(\theta/2) \\
        \sin(\theta/2)e^{2ik_H x_n}
    \end{pmatrix},
    | \downarrow, n \rangle = \begin{pmatrix}
        \sin(\theta/2)e^{-2ik_H x_n} \\
        -\cos(\theta/2)
    \end{pmatrix}.
\end{align*}
$$

(B.2)

As we can see in the table below, showing all the different possible inner-product combinations, two of the products are not translation invariant as they carry a factor of $e^{\pm ik_H(x_n+x_m)}$.

| $\langle \uparrow, n \rangle$ | $| \uparrow, m \rangle$ | $| \downarrow, m \rangle$ |
|--------------------------|------------------|------------------|
| $\langle \uparrow, n \rangle$ | $\cos^2 \frac{\theta}{2} + \sin^2 \frac{\theta}{2} e^{-2ik_H(x_n-x_m)}$ | $ie^{-ik_H(x_n+x_m)} \sin \theta \sin[k_H(x_n - x_m)]$ |
| $\langle \downarrow, n \rangle$ | $ie^{ik_H(x_n+x_m)} \sin \theta \sin[k_H(x_n - x_m)]$ | $\cos^2 \frac{\theta}{2} + \sin^2 \frac{\theta}{2} e^{2ik_H(x_n-x_m)}$ |
Similarly to what we did with the TBM, we can remove these factors with a unitary transformation of the Hamiltonian. For the FBM the desired transformation matrix is
\[ U = \exp(ik_H \sigma_z \otimes \sigma_z \otimes X/2), \]
with \( X_{nm} = x_n \delta_{nm} \). This gives us the following matrices

\[ h_{nm}^{\uparrow \uparrow} = e^{-r_{nm}/\xi_E} \sin k_{F} r_{nm} \left( \cos \frac{\theta}{2} e^{ik_H(x_n-x_m)} + \sin \frac{\theta}{2} e^{-ik_H(x_n-x_m)} \right) \tag{B.3} \]
\[ h_{nm}^{\uparrow \downarrow} = i e^{-r_{nm}/\xi_E} \sin k_{F} r_{nm} \sin \theta \sin[k_H(x_n-x_m)] \tag{B.4} \]
\[ d_{nm}^{\uparrow \uparrow} = e^{-r_{nm}/\xi_E} \cos k_{F} r_{nm} \left( \cos \frac{\theta}{2} e^{ik_H(x_n-x_m)} + \sin \frac{\theta}{2} e^{-ik_H(x_n-x_m)} \right) \tag{B.5} \]
\[ d_{nm}^{\uparrow \downarrow} = i e^{-r_{nm}/\xi_E} \cos k_{F} r_{nm} \sin \theta \sin[k_H(x_n-x_m)], \tag{B.6} \]

and the rest can be obtained via the identities \( h_{nm}^{\uparrow \uparrow} = (h_{nm}^{\uparrow \downarrow})^* \) and \( h_{nm}^{\uparrow \downarrow} = h_{nm}^{\uparrow \uparrow} \) (same for \( d_{nm}^{\sigma\sigma'} \)).

In this representation, the matrix elements are manifestly translation invariant.

We are now in position to make the Fourier transformations

\[ h_k^{\sigma\sigma'} = \sum_n e^{ik(x_n-x_m)} h_{nm}^{\sigma\sigma'}, \]
\[ d_k^{\sigma\sigma'} = \sum_n e^{ik(x_n-x_m)} d_{nm}^{\sigma\sigma'}, \tag{B.7} \]

where \( x_n = an, \ n \in \mathbb{Z} \). We first deal with the \( h \) terms and then with the \( d \) terms. It is sufficient to only consider the two spin combinations \( \uparrow \uparrow \) and \( \uparrow \downarrow \); from \( h_{nm}^{\uparrow \uparrow} = (h_{nm}^{\uparrow \downarrow})^* \) we get \( h_k^{\uparrow \uparrow} = h_k^{\downarrow \downarrow} \), and from \( h_{nm}^{\uparrow \downarrow} = h_{nm}^{\uparrow \uparrow} \) we obviously get \( h_k^{\uparrow \downarrow} = h_k^{\uparrow \downarrow} \).

For \( h_k^{\uparrow \uparrow} \) we now have

\[ h_k^{\uparrow \uparrow} = \sum_n e^{ik(x_n-x_m)} h_{nm}^{\uparrow \uparrow} = \sum_{n \neq m} e^{ik(x_n-x_m)} e^{-r_{nm}/\xi_E} \sin k_{F} r_{nm} \left( \cos \frac{\theta}{2} e^{ik_H(x_n-x_m)} + \sin \frac{\theta}{2} e^{-ik_H(x_n-x_m)} \right) = \sum_{n \neq 0} e^{ikan - a|n|/\xi_E} \sin k_{F} a|n| \left( \cos \frac{\theta}{2} e^{ik_H a|n|} + \sin \frac{\theta}{2} e^{-ik_H a|n|} \right). \tag{B.8} \]

To simplify matters, we consider a sum of the form

\[ S(k) = \sum_{n \neq 0} e^{ikan - a|n|/\xi_E} \sin k_{F} a|n| = \Re \sum_{n \neq 0} e^{ikan - a|n|/\xi_E} \sin k_{F} a|n|, \tag{B.9} \]

where the last step follows from \( S(k) = S(k)^* \). To get rid of the norms, we split the
sum into \( n < 0 \) and \( n > 0 \):

\[
S(k) = \Re \sum_{n=1}^{\infty} \frac{e^{-an/\xi_E}}{k_F a} \sin k_F an \left( e^{ian} + e^{-ian} \right)
\]

\[
= \Re \frac{1}{2i} \sum_{n=1}^{\infty} \frac{e^{-an/\xi_E}}{k_F a} \left( e^{ian} - e^{-ian} \right) \left( e^{ian} + e^{-ian} \right)
\]

\[
= \Re \frac{1}{2i} \sum_{n=1}^{\infty} \frac{e^{-an/\xi_E}}{k_F a} \left( e^{ian} + e^{ian(k_F-k)} - e^{ian(-k_F+k)} - e^{ian(-k_F-k)} \right).
\]

Now, noting that the Taylor expansion for \(- \ln(1-x)\) is

\[
- \ln(1-x) = \sum_{n=1}^{\infty} \frac{x^n}{n}, \quad |x| < 1
\]

it follows that

\[
S(k) = - \Re \frac{1}{2ik_F a} \left( \ln(1 - e^{a(i(k_F+k)-1/\xi_E)}) + \ln(1 - e^{a(i(k_F-k)-1/\xi_E)}) \right)
\]

\[
- \ln(1 - e^{a(i(-k_F+k)-1/\xi_E)}) - \ln(1 - e^{a(i(-k_F-k)-1/\xi_E)}) \right)
\]

\[
= - \frac{1}{2k_F a} \Im \left( \ln(1 - e^{a(i(k_F+k)-1/\xi_E)}) + \ln(1 - e^{a(i(k_F-k)-1/\xi_E)}) \right)
\]

\[
- \ln(1 - e^{a(i(-k_F+k)-1/\xi_E)}) - \ln(1 - e^{a(i(-k_F-k)-1/\xi_E)}) \right)
\]

\[
= - \frac{1}{2k_F a} \left( \arg(1 - e^{a(i(k_F+k)-1/\xi_E)}) + \arg(1 - e^{a(i(k_F-k)-1/\xi_E)}) \right)
\]

\[
- \arg(1 - e^{a(i(-k_F+k)-1/\xi_E)}) - \arg(1 - e^{a(i(-k_F-k)-1/\xi_E)}) \right).
\]

The argument of a complex number with a positive real part is given by \( \arg(z) = \arctan(\Im z / \Re z) \). For any finite \( \xi_E \) we always have that \( 1 > e^{-a/\xi_E \cos ka} \), so all arguments in Eq. (B.12) follow this recipe:

\[
S(k) = \frac{1}{2k_F a} \left[ A(k_F + k) + A(k_F - k) - A(-k_F + k) - A(-k_F - k) \right]
\]

\[
= \frac{1}{k_F a} \left[ A(k_F + k) + A(k_F - k) \right],
\]

where we have used the function

\[
A(k) = \arctan \left( \frac{e^{-a/\xi_E \sin ka}}{1 - e^{-a/\xi_E \cos ka}} \right),
\]

with the last line coming from the fact that \( A(k) = -A(-k) \). Putting all this together, we have that

\[
h_k^\dagger = \frac{\cos^2 \frac{\theta}{2}}{k_F a} \left[ A(k_F + k + k_H) + A(k_F - k - k_H) \right]
\]

\[
+ \frac{\sin^2 \frac{\theta}{2}}{k_F a} \left[ A(k_F + k - k_H) + A(k_F - k + k_H) \right].
\]
For \( h_{k}^{\uparrow \downarrow} \) we have

\[
\begin{align*}
 h_{k}^{\uparrow \downarrow} &= \sum_{n} e^{i k(x_n - x_m)} h_{nm}^{\uparrow \downarrow} \\
 &= i \sum_{n \neq 0} e^{ikan} \frac{e^{-a|n|/\xi_E}}{k_F a |n|} \sin(k_F a |n|) \sin \theta \sin(k_H a n).
\end{align*}
\] (B.16)

Clearly, \( h_{k}^{\uparrow \downarrow} = (h_{k}^{\uparrow \downarrow})^{*} \), so we can then write

\[
\begin{align*}
 h_{k}^{\uparrow \downarrow} &= \text{Re} i \sum_{n \neq 0} e^{ikan} \frac{e^{-a|n|/\xi_E}}{k_F a |n|} \sin(k_F a |n|) \sin \theta \sin(k_H a n) \\
 &= -\text{Im} \sum_{n \neq 0} e^{ikan} \frac{e^{-a|n|/\xi_E}}{k_F a |n|} \sin(k_F a |n|) \sin \theta \sin(k_H a n) \\
 &= -\sin \theta \text{Im} \frac{S(k + k_H) - S(k - k_H)}{2i} = \frac{\sin \theta}{2} [S(k + k_H) - S(k - k_H)].
\end{align*}
\] (B.17)

The \( d \) terms follow from similar reasoning, but instead with the sum

\[
\begin{align*}
 s(k) &= \sum_{n \neq 0} \frac{e^{ikan} \cos k_F a |n|}{k_F a |n|} = \text{Re} \sum_{n \neq 0} \frac{e^{ikan - a|n|/\xi_E}}{k_F a |n|} \cos k_F a |n|.
\end{align*}
\] (B.18)

The principles are the same, so after separating the sum into \( n < 0 \) and \( n > 0 \), and expanding \( \cos k_F a n \) in complex exponents, we get

\[
\begin{align*}
 s(k) &= -\text{Re} \frac{1}{2k_F a} \left( \ln(1 - e^{a(i(k_F + k) - 1/\xi_E)}) \right. \\
 &\quad + \left. \ln(1 - e^{a(i(k_F - k) + 1/\xi_E)}) \right) + \ln(1 - e^{a(i(-k_F + k) - 1/\xi_E)}) + \ln(1 - e^{a(-i(k_F + k) - 1/\xi_E)}) \\
 &= -\frac{1}{2k_F a} \left( \ln |1 - e^{a(i(k_F + k) - 1/\xi_E)}| + \ln |1 - e^{a(i(k_F - k) + 1/\xi_E)}| \\
 &\quad + \ln |1 - e^{a(i(-k_F + k) - 1/\xi_E)}| + \ln |1 - e^{a(-i(k_F + k) - 1/\xi_E)}| \right) \\
 &= \frac{1}{4k_F a} \left( f(k_F + k) + f(k_F - k) + f(-k_F + k) + f(-k_F - k) \right) \\
 &= \frac{1}{2k_F a} \left( f(k_F + k) + f(k_F - k) \right),
\end{align*}
\] (B.19)

where

\[
f(k) = -\ln(1 - 2e^{-a/\xi_E} \cos ka + e^{-2a/\xi_E}).
\] (B.20)
The Fourier transformations of all the different matrices are summarized below:

\[
h_{k}^{\uparrow\uparrow} = \frac{\cos^{2}\frac{\theta}{2}}{k_{F}a} [A(k_{F} + k + k_{H}) + A(k_{F} - k - k_{H})]
+ \frac{\sin^{2}\frac{\theta}{2}}{k_{F}a} [A(k_{F} + k - k_{H}) + A(k_{F} - k + k_{H})]
\]

(B.21)

\[
h_{k}^{\uparrow\downarrow} = \frac{\sin(\theta)}{2k_{F}a} [A(k_{F} + k + k_{H}) + A(k_{F} - k - k_{H})
- A(k_{F} + k - k_{H}) - A(k_{F} - k + k_{H})]
\]

(B.22)

\[
d_{k}^{\uparrow\uparrow} = \frac{\cos^{2}\frac{\theta}{2}}{2k_{F}a} [f(k_{F} + k + k_{H}) + f(k_{F} - k - k_{H})]
+ \frac{\sin^{2}\frac{\theta}{2}}{2k_{F}a} [f(k_{F} + k - k_{H}) + f(k_{F} - k + k_{H})]
\]

(B.23)

\[
d_{k}^{\uparrow\downarrow} = \frac{\sin\theta}{4k_{F}a} [f(k_{F} + k + k_{H}) - f(k_{F} + k - k_{H})
+ f(k_{F} - k - k_{H}) - f(k_{F} - k + k_{H})]
\]

(B.24)

\[
h_{k}^{\downarrow\downarrow} = h_{-k}^{\uparrow\uparrow}, \quad d_{k}^{\downarrow\downarrow} = d_{-k}^{\uparrow\uparrow}, \quad h_{k}^{\downarrow\uparrow} = h_{k}^{\uparrow\downarrow}, \quad d_{k}^{\downarrow\uparrow} = d_{k}^{\uparrow\downarrow}.
\]

(B.25)
Appendix C

Nonlinear eigenvalue problems

The purpose of this appendix is to present the mathematical concept of non-linear eigenvalue problems. To provide some necessary background from which to build on, we start off by briefly discussing linear eigenvalue problems. All of what we say about linear algebra should already be known to the reader, but our aim with this discussion is to highlight certain properties and facts that are transferable to the nonlinear eigenvalue problem.

C.0.2 Linear eigenvalue problems

In linear algebra, an eigenvalue equation means an equation of the form

\[ Ax = \lambda x, \quad (C.1) \]

where \( A \) is a square matrix and \( x \) a column vector. If \( x \) satisfies the above relation for some scalar \( \lambda \), we say that \( x \) is an eigenvector of the matrix \( A \). Correspondingly, \( \lambda \) is called the eigenvalue. The recipe for finding the eigenvalues in these types of equations is to first rearrange the equation so that we have

\[ (A - \lambda 1)x = 0, \quad (C.2) \]

where \( 1 \) now is the identity matrix. This equation is automatically satisfied by a vector whose every component is zero regardless of \( \lambda \) or \( A \). This is why the zero vector is not generally considered an eigenvector of any matrix, since we cannot ascribe a unique eigenvalue to it. If we now suppose that the matrix \( A - \lambda 1 \) is invertible, we can multiply both sides of Eq. (C.2) by \( (A - \lambda 1)^{-1} \) yielding

\[ (A - \lambda 1)^{-1}(A - \lambda 1)x = 0 \quad \rightarrow \quad x = 0. \quad (C.3) \]
In other words, the solutions are trivial. Now, a well-known theorem in linear algebra tells us that a matrix is invertible if and only if its determinant is non-vanishing. Conversely, a non-invertible matrix must have zero determinant. We can then only find non-trivial solutions when

$$\det(A - \lambda I) = 0.$$  \hspace{1cm} (C.4)

This so called characteristic equation is polynomial in $\lambda$ with the order determined by the dimension of the matrix. In general, for an $N \times N$ matrix $A$, there are $N$ unique eigenvalues (unless they happen to be degenerate) due to the fact that an $N$:th degree polynomial has $N$ roots.

## C.1 Nonlinear eigenvalue problems

A non-linear eigenvalue equation is a generalisation of the linear eigenvalue problem defined by Eq. (C.2). In this case, the equations come in the form

$$A(\lambda)x = 0,$$ \hspace{1cm} (C.5)

where $A(\lambda)$ is now a matrix depending non-linearly on $\lambda$, which is still considered as an eigenvalue of sorts. Similarly to the linear case, the eigenvalues are obtained by the non-invertibility constraint

$$\det A(\lambda) = 0.$$ \hspace{1cm} (C.6)

Now, in contrast to the linear case, the characteristic equation is no longer a polynomial in general and we cannot say anything about the number of roots to this equation. As a trivial example, consider the equation

$$\begin{pmatrix} e^{-\lambda} & \lambda^N \\ 1 & e^\lambda \end{pmatrix} x = 0, \quad N \in \mathbb{Z}.$$ \hspace{1cm} (C.7)

Setting the determinant to zero yields the equation $\lambda^N = 1$, whose eigenvalues are the $N$th roots of unity ($N$ in total), so even though our matrix is $2 \times 2$, we can get an arbitrary number of eigenvalues.\footnote{For $N = 0$, we even get uncountably many solutions.}
C.1. NONLINEAR EIGENVALUE PROBLEMS

C.1.1 The polynomial eigenvalue problem

A common type of non-linear eigenvalue problem (that is also an integral part of this thesis) is the polynomial eigenvalue problem. This refers to equations of the form

\[ \sum_{n=1}^{p} \lambda^n A_n x = 0, \]  

(C.8)

where \( A_n \) are constant matrices.\(^2\) It turns out that polynomial eigenvalue equations can be mapped to generalized linear eigenvalue problems. For example, a quadratic eigenvalue equation

\[(\lambda^2 A_2 + \lambda A_1 + A_0) x = 0 \]  

(C.9)

can be rewritten as

\[
\begin{pmatrix}
-A_0 & 0 \\
0 & 1
\end{pmatrix}
\begin{pmatrix}
x \\
y
\end{pmatrix}
= \lambda
\begin{pmatrix}
A_1 & A_2 \\
1 & 0
\end{pmatrix}
\begin{pmatrix}
x \\
y
\end{pmatrix}.
\]  

(C.10)

Here we have defined an additional vector \( y = \lambda x \). If any of the matrices on either side is invertible,\(^3\) we can apply the usual machinery for linear eigenvalue problems. Notice however, that linearising the equation came with the cost of doubling the dimensions of the problem. In general, a polynomial eigenvalue problem of order \( p \) with matrices of size \( N \times N \) can be rewritten as a generalized linear eigenvalue problem of size \( pN \times pN \). Despite this trick, one cannot usually make any analytical progress with regards to the eigenvectors in polynomial eigenvalue problems save for a few special cases. This method can, however, be used for numerically finding the eigenvectors.

---

\(^2\)as a special case of a first-order polynomial equation, we have the regular linear eigenvalue equation.

\(^3\)Some extra care should be taken if the only invertible matrix is \( A_0 \) as this would yield a linear equation in \( 1/\lambda \). This can be problematic if one of the eigenvalues is \( \lambda = 0 \).
Appendix D

The energy spectrum

This appendix is dedicated to the derivation of the explicit expressions for the energy bands in the infinite coherence length limit for the FBM.

Our starting point is the NEV problem in Eq. (3.39) in which we right away set \( \xi_E = \infty \). Now the energy only enters through \( \lambda_E \). For non-trivial solutions, we require that the determinant of the matrix must be zero. Since our matrix is \( 4 \times 4 \), we expect it to be an eighth degree polynomial in \( \lambda_E \) (our matrix contains terms that are quadratic in \( \lambda_E \)), which is not a desirable result. However, explicitly calculating the determinant and rearranging terms gives us an equation of the form

\[
a_k \lambda^4 + b_k \lambda^3 + c_k \lambda^2 - b_k \lambda + a_k = 0,
\]

where the coefficients are given by

\[
a_k = \alpha^2 \left[ (h_k^{\uparrow \downarrow})^2 - (1 + h_k^{\uparrow \uparrow})(1 + h_{-k}^{\uparrow \uparrow}) \right]
\]

\[
b_k = \alpha^3 \left[ (1 + h_k^{\uparrow \uparrow})(D_{-k}^{\uparrow \uparrow})^2 - (1 + h_k^{\downarrow \downarrow})(D_k^{\downarrow \downarrow})^2 + 2D_k^{\uparrow \downarrow}h_k^{\downarrow \downarrow}(D_k^{\uparrow \uparrow} - D_{-k}^{\uparrow \uparrow}) \right]
+ \alpha^3(h_{-k}^{\uparrow \uparrow} - h_k^{\uparrow \uparrow}) \left[ (1 + h_k^{\downarrow \uparrow})(1 + h_{-k}^{\uparrow \uparrow}) + (D_k^{\downarrow \uparrow})^2 - (h_k^{\downarrow \uparrow})^2 + \alpha^{-2} \right]
\]

\[
c_k = \alpha^4 \left[ (D_k^{\uparrow \downarrow})^2 - (h_k^{\uparrow \downarrow})^2 + (1 + h_k^{\uparrow \uparrow})(1 + h_{-k}^{\uparrow \uparrow}) - D_k^{\uparrow \uparrow}D_{-k}^{\uparrow \uparrow} \right]^2
+ \alpha^4 \left[ 2D_k^{\uparrow \downarrow}h_k^{\downarrow \downarrow} - (1 + h_k^{\uparrow \uparrow})D_{-k}^{\uparrow \uparrow} - D_k^{\uparrow \uparrow}(1 + h_{-k}^{\uparrow \uparrow}) \right]^2
+ \alpha^2 \left[ 2(D_k^{\uparrow \downarrow})^2 - (D_k^{\uparrow \uparrow})^2 - (D_{-k}^{\uparrow \uparrow})^2 - (h_k^{\uparrow \uparrow} - h_{-k}^{\uparrow \uparrow})^2 \right] + 1.
\]

While a fourth degree polynomial is certainly better than a eighth degree polynomial in that there exists a general solution for these, it is not necessarily practical. However,
the symmetry between the coefficients reduces the solution to

$$\lambda_{\beta\gamma}(k) = \beta \sqrt{\frac{b_k^2 - 4a_k c_k - 8a_k^2}{4a_k^2}} + \gamma \left( \frac{\phantom{\sqrt{b_k^2}}}{2} \right) \frac{\phantom{\sqrt{b_k^2}}}{2} \frac{\phantom{\sqrt{b_k^2}}}{\sqrt{b_k^2}} \frac{\phantom{\sqrt{b_k^2}}}{2} \frac{\phantom{\sqrt{b_k^2}}}{4a_k^2} \frac{\phantom{\sqrt{b_k^2}}}{\sqrt{b_k^2}} \frac{\phantom{\sqrt{b_k^2}}}{2} \frac{\phantom{\sqrt{b_k^2}}}{4a_k^2} \frac{\phantom{\sqrt{b_k^2}}}{\sqrt{b_k^2}}\right)$$

(D.3)

where $\gamma$ and $\beta$ are independent sign factors giving us four different solutions. The solution presupposes that $a_k \neq 0$, which is the case for the parameters used in this thesis. The symmetry of Eq. (D.1) implies that if $\lambda_E \neq 0$ is a solution, so is $-1/\lambda_E = -\lambda_{-E}$. This is nothing but PHS at play, since $\lambda$ and $-\lambda$ correspond to the same energy, which is evident from inverting $\lambda = \lambda_E$:

$$E = E(\lambda) = \Delta \frac{\lambda^2 - 1}{\lambda^2 + 1}.$$  

(D.4)

When we insert Eq. (D.3) into $E(\lambda)$\(^1\) we get four energy bands in total. The symmetries of these bands require us to only calculate one of the bands, as the others can be obtained by mirroring the first band about $k = 0$ and $E = 0$ in all possible ways. In fact, due to the redundancy in our mathematical formalism, only the two bands that reduce to the deep-dilute limit are physical. As it turns out, the physical bands are $E(\lambda_{++}(k))$ and $E(\lambda_{-+}(k))$ (which are related to each other by reflecting about both $k = 0$ and $E = 0$).

For planar helices, the solution is even less cumbersome; when $\theta = \pi/2$, we get that $b_k = 0$. Now the solution in terms of $\lambda$ is

$$\lambda^2 = -\frac{c_k}{2a_k} \pm \sqrt{\frac{c_k^2}{4a_k^2} - 1}.$$  

(D.5)

The expressions for $a_k$ and $c_k$ (D.2) also slightly simplify, owing to the fact that for planar configurations $h_{++}^k = h_{-+}^k$ and $d_{++}^k = d_{-+}^k$.

\(^1\)Had we not taken the limit $\xi E \rightarrow \infty$, the insertion of Eq. (D.3) into Eq. (D.4) would have given us a transcendental equation for $E$. 