Electronic Properties of Domain Walls in Sr$_2$RuO$_4$

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ce fu au tans qu’arbre florissent,
fueillent boschaige, pré verdissent,
et cil oisel an lor latin
dolcement chantent au matin

Perceval ou le Conte du Graal, Chrétien de Troyes, 69-84, AD 1180.

alweinde Parzival dô sprach
“saget mir wâ der gräl hie lige,
op diu gotes giête an mir gesige,
des wirt wol innen disiu schar.”

sîn venje er viel des endes dar
dristunt zôrn der Trinität:
er warp daz müese werden rât
des trûgen mannes herzesêr.
er riht sich ûf und sprach dô mêr
“ceheim, waz wirret dier?”

Parzival, Wolfram von Eschenbach, Buch XVI, 795.20-29, AD 1200.
Abstract

The question of the symmetry of the superconducting state in Sr$_2$RuO$_4$ (Strontium Ruthenate) has been under debate since its discovery in 1994. Up to now the chiral $p$-wave state is the best candidate regarding the numerous experiments that reveal the unconventional behavior of this material. It is a two dimensional odd-parity spin-triplet and time reversal symmetry breaking pairing state. The list of highly specialized experiments that have been accomplished in order to determine the pairing state of Sr$_2$RuO$_4$ is impressive. Listing them doesn’t fail to elicit the attribution of a noble pedigree to this field of science. Let us do so straight away with the major experiments that are making the case for the chiral $p$-wave state’s scenario: first, thermodynamical measurements show a linear temperature dependence of the heat capacity below the critical temperature, $T_c$, as well as a strong dependence of $T_c$ under non-magnetic doping; second, SQUID interferometer experiments reveal a $\pi$-phase shift of the order parameter under inversion of the contacts which is in agreement with the odd-parity pairing; third, NMR Knight shift measurements are consistent with an equal-spin spin-triplet pairing state; fourth, Muon spin relaxation spectroscopy evinces the presence of a spontaneous internal magnetization below $T_c$ that is consistent with the breaking of time reversal symmetry; therewith the optical Kerr effect studies that probe the surfaces lead to the same conclusion; fifth, spin-polarized neutron scattering measurements confirm the spin-triplet pairing state. Last but not least, Josephson interferometry experiments reveal a rich variety of phenomena that are at discrepancy with respect to the conventional s-wave superconductors.

The theoretical properties of the chiral $p$-wave state are found to bear a wealth of exotic phenomena. It is has been early recognized by Volovik that time reversal breaking superconductors can be characterized by the topology of their ground state; and, since the recent infatuation for a broader use of topological concepts in solid state physics, people have been interested in Sr$_2$RuO$_4$ as being possibly the first realization of a non-trivial topological superconductor. The Chern number of the chiral $p$-wave state is a $Z$ topological invariant that can be related to the definite angular momentum quantum number of the Cooper pair, i.e. the chirality. The index theorem then tells us that at a surface between the bulk and the vacuum the jump in angular momentum ($0$ for the vacuum to $1$, or $-1$, for the bulk) is accompanied with the existence of chiral edge states that are topologically protected. Those were early studied on a phenomenological level by Sigrist. An important property of the chiral $p$-wave state is its twofold degeneracy that is linked to the breaking of time reversal symmetry. The index theorem also predicts the existence of topologically protected bound states on a domain wall that separates the two degenerate chiral states. Again Sigrist pioneered the study of the macroscopic structure of domain walls from Ginzburg-Landau theory. We mention for completeness the possibility to form fractional vortices but this aspect will not be treated in this work.

Although the edge states have been observed in STM measurements the statement that those are chiral hasn’t yet won unanimous support among the physics community. Alternatively, a direct observation of domain walls’ spontaneous magnetization through highly sensitive scanning probes at the surface has unfortunately failed so far. An other approach is to probe the internal phase symmetry of the superconducting state through Josephson interferometry experiments. This was achieved by Maeno and collaborators who reported measurements of the critical current as a function of the external magnetic field on Pb/Sr$_2$RuO$_4$ junctions. They observed several important discrepancies of the critical current’s interference pattern in regard to the conventional Fraunhofer pattern: a shift of the maximum critical current off the zero-field with a persistent asymmetry between positive and negative fields; a robust hysteresis effect of the interference pattern as the magnetic field was swept back and forth, accompanied with asymmetric maximum critical currents; last but not least, a random switching of the potential at driven current slightly above $I_c$ (all those for temperatures below $T_c$). The authors of the experimental study proposed the presence of domain walls within Sr$_2$RuO$_4$ as the cause for those unconventional behaviors. However a detailed theoretical study of the influence of domain walls on the Josephson effect in Sr$_2$RuO$_4$ was still missing.

Our aim is, on the one hand, to contribute to the identification and the characterization of the superconducting state of Sr$_2$RuO$_4$ and, on the other hand, to elucidate the microscopic structure of edges and domain walls in the chiral $p$-wave state.

Since a wide range of full microscopic studies treating the three Ru-$t_{2g}$-bands—known to be responsible for the low energy physics of Sr$_2$RuO$_4$—find that the $\gamma$-band is dominant for the superconductivity and favors the chiral $p$-wave state, we restrict our study to the single $\gamma$-band within the mean-field approximation. In particular, we give the numerical self-consistent solution from the Ginzburg-Landau
theory, the quasi-classical theory and the lattice Bogoliubov-de Gennes theory.

The first part of the thesis deals with (i) the study of the macroscopic structure of a domain wall in Sr$_2$RuO$_4$, assuming the chiral $p$-wave state, and (ii) the derivation of a mechanism which aims at reproducing the experimental findings reported by Maeno et al that we mentioned above. For this we derive a Ginzburg-Landau theory—from the microscopic quasi-classical equations in the weak coupling limit—and solve it numerically and self-consistently. We give an exhaustive presentation of the stable and metastable domain walls for the different external parameter ranges. We show that taking the anisotropy of the material—that originates from the electronic band and gap function structures—and the angle of the domain wall—with respect to the main crystal axes—into account, the most stable domain wall configuration spontaneously acquires an non-zero global phase difference between its two sides. This is the key component of our model of the critical Josephson current in which we assume several domain walls reaching the interface. Due to the interaction of the external magnetic field with the domain walls at the interface we find a field-driven polarization of the domain walls’ configuration that straightforwardly leads to the experimental effects observed in the setup studied by Maeno et al. We also reproduce typical interference patterns measured on nano-scale junctions by Bahr. Furthermore we include the influence of the interface’s orientation with respect to the crystal axes. Through the comparison of our simulations and the measured interference patterns we eventually give an estimate of the domain walls’ width.

The second part of this thesis deals with the investigation of the microscopic structure of the domain walls in Sr$_2$RuO$_4$ for the chiral $p$-wave state. We first study the general symmetry and topological properties of the Andreev equation from two simplified non-self-consistent domain wall’s profiles (sharp domain wall and simplified smooth ansatz of the gap function) for which we derive the analytical expression of the domain wall spectrum. We discuss the breaking of the topology in the quasi-classical limit and discuss the limitation of different approaches that were proposed for the proof of the index theorem. This makes the case for the necessity to go beyond the quasi-classical limit. We also discuss the Zaitsev and the Blonder Tinkham Klapwijk wave function’s boundary conditions.

Second, we give the numerical self-consistent solution of the quasi-classical Eilenberger-Riccati equations as a function of the anisotropy and the domain wall’s orientation. On top of showing a very good qualitative agreement with the Ginzburg-Landau results, we explain the domain wall’s spontaneous current and the domain wall’s phase structure in terms of the topological bound states present within it. However we point the attention to the vanishing of a fraction of the bound state’s spectral weight in some domain wall configurations which is due to the breaking of the topology in the quasi-classical limit. Finally we study the transition from a domain wall to an edge through the introduction of a potential barrier at the domain wall.

Third and finally, we study the lattice version of the domain wall problem. This approach constitutes the full quantum version of the problem (at the mean-field level) and it allows us to overcome the limitations of the quasi-classical limit: (i) the anisotropy now enters naturally through the two distinct tight-binding terms: hopping and pairing; (ii) all high order terms beyond the quasi-classical limit are automatically included and it leads to the correct topological structure of the domain wall bound states. We solve numerically and self-consistently the lattice Bogoliubov-de Gennes equations and show a very good qualitative agreement with the other approaches (GL and quasi-classical) regarding the macroscopic structure of the domain walls. The microscopic structure of the topological bound states allows us to give the electronic signature (through the spectral weight) of the chiral edge states and domain wall bound states. Specifically we consider two geometries: (a) when the surfaces of the sample are aligned with one main crystal axis; (b) when the surfaces are rotated by 45°. We also consider the effect of the band filling. In the case of the rotated edges at high filling we find a new feature of the chiral bound states which had not been reported before: the chiral edge states exhibit two extra zero-energy points at $\pm k_y,0 \neq 0$. This provides a clear-cut frame for future STM experiments. This then would pin the question of the chirality of the edge states in Sr$_2$RuO$_4$ and eventually constitute a direct evidence for the chiral $p$-wave state. This finding has also important consequences for the edge currents.

In the prospects we present the basis of a theoretical interpretation of the recent measurements of the critical Josephson current on Nb/Ru/Sr$_2$RuO$_4$ junctions by Maeno and collaborators in which they report strong noise effects of the critical current over time at given driven currents slightly above the critical value and for temperatures below $T_c$. Our analysis, which is based on the self-consistent stable and metastable domain wall’s structure, assume the interplay at the interface of two domain walls and a Josephson vortex.
Résumé

La question de la symétrie de l’état supraconducteur du ruthénaïte de strontium, Sr$_2$RuO$_4$, a été débattue depuis sa découverte en 1994. Le meilleur candidat jusqu’à maintenant s’avère être l’état d’onde $p$ chiral au regard des nombreuses expériences qui ont révélé le comportement non conventionnel de ce matériaux. Ceci est un état deux dimensionnel, de parité impaire et de configuration de spin triplet brisant la symétrie d’inversion temporelle. Le nombre d’expériences hautement spécialisées qui ont été réalisées dans le but de déterminer l’état de pairage est impressionnant. En donner la liste ne peut manquer de susciter l’attribution de ses lettres de noblesse à ce domaine de la science. Voici les principales qui plaident pour l’état d’onde $p$ chiral. Premièrement, les mesures thermodynamiques révèlent une dépendance linéaire de la capacité calorifique avec la température en dessous de la température critique, $T_c$, ainsi qu’une forte dépendance de celle-ci en fonction du dopage par des impuretés non-magnétiques. Deuxièmement, les courants tunnels de SQUID subissent un changement de signe après une transfoarmation d’inversion des contacts en accord avec la parité impaire du pairage. Troisièmement, les expériences de RMN pour une magnétisation interne en dessous de $T_c$ qui est consistant avec la brisure de symétrie temporelle. En outre, les études d’effet optic de Kerr qui sondent la surface aboutissent à la même conclusion. Cinquièmement, la diffraction aux neutrons avec polarisation de spin confirme l’état de spin triplet. En outre, les études d’effet optic de Kerr qui sondent la surface aboutissent à la même conclusion.

Les propriétés théoriques de l’état d’onde $p$ chiral permettent une multitude de phénomènes exotiques. Il a été reconnu par Volovik que les supraconducteurs qui brisent la symétrie temporelle peuvent être caractérisés par la topologie de leur état fondamental; ainsi, depuis le récent enthousiasme pour l’utilisation plus large des concepts topologiques dans la physique des états solides, l’intérêt s’est porté sur Sr$_2$RuO$_4$ comme potentiellement le premier supraconducteur topologique non-trivial. Le nombre de Chern de l’état d’onde $p$ chiral est un invariant $Z$ qui peut être associé à un nombre quantique de moment angulaire définit, $id est$ la chiralité. Ainsi, le théorème d’index nous dit qu’à la surface entre le matériaux et le vide, le saut du nombre quantique de moment angulaire qui s’y produit ($0$ pourle vide et $1$, ou $-1$, pour le matériaux) est accompagné par la présence d’états liés de surface chiraux qui sont protégés par la topologie. Ces états liés de surface dans le Sr$_2$RuO$_4$ ont été étudiés précocement sur un plan phénoménologique par Sigrist. Une propriété importante de l’état d’onde $p$ chiral est sa double dégénérescence liée à la brisure de symétrie temporelle. Ainsi, le théorème d’index prédit également l’existence d’états liés topologiques au sein d’une paroi de domaines qui sépare dans l’espace les deux états chiraux dégénérés. Par souci d’exhaustivité, nous mentionnons également la possibilité de former des vortex fractionnels, mais nous ne discuterons pas plus avant cet aspect dans cette thèse.

Bien que les états liés de surface ont été observés par des mesures par microscope à effet tunnel (STM) la question de leur chiralité ne fait pas l’unanimité parmi la communauté scientifique. Alternativement, le balayage hautement sensible à la surface dans le but d’apercevoir la magnétisation spontanée générée par des parois de domaines n’a donné aucun résultat concluant. Une autre approche est de sonder la symétrie interne de phase de l’état supraconducteur par interférométrie de Josephson. Maeno et ses collaborateurs qui en ont été les pionniers, ont réalisé des mesures du courant critique de jonctions Pb/Sr$_2$RuO$_4$ en fonction du champ magnétique extérieur. Ils ont observé des écarts importants dans le motif d’interférence du courant critique comparé au motif conventionnel de Fraunhofer : un déplacement du courant critique maximum en dehors du champ zéro avec une asymétrie persistante entre les champs positifs et négatifs, un effet d’hystérie du motif d’interférence selon que le champ est changé continuellement d’un sens à l’autre, enfin un effet de bruit et de saut du potentiel mesuré sous l’application d’un courant dirigé avec une valeur supérieure à $I_c$. Les auteurs ont proposé la présence de parois de domaines comme la cause de ces comportements non conventionnels. Cependant il n’existait pas encore d’étude théorique détaillée de l’influence des parois de domaines sur l’effet Josephson dans le Sr$_2$RuO$_4$.

Notre objectif est, d’une part, de contribuer à l’identification et à la caractérisation de l’état supraconducteur de Sr$_2$RuO$_4$, et, d’autre part, de déterminer la structure électronique des états liés de surface et des états liés de parois de domaines dans l’état d’onde $p$ chiral.

Les études microscopiques qui traitent les trois bandes $t_{2g}$ provenants des électrons $4d$ des ions Ru, connues comme étant responsables des propriétés électroniques aux basses températures de Sr$_2$RuO$_4$, convergent largement pour montrer que la bande $\gamma$ est dominante pour la supraconductivité et réalise
l’état d’onde \( p \) chiral. C’est pourquoi nous nous limiterons ici à des modèles de champs moyens pour la seule bande \( \gamma \) : nous abordons successivement la théorie de Ginzburg-Landau, la théorie quasi-classique et la théorie de Bogoliubov-de Gennes sur un réseau cristallin.

La première partie de cette thèse s’occupe (i) de l’étude de la structure macroscopique des parois de domaines dans \( \text{Sr}_2\text{RuO}_4 \) en assumant l’état d’onde \( p \) chiral, et (ii) de la dérivation d’un mécanisme qui a pour but de reproduire les résultats expérimentaux qui ont été reportés pour Maeno et al et que nous avons mentionné plus haut. À cette fin, nous avons dérivé une théorie de Ginzburg-Landau à partir des équations microscopiques dans la limite de couplage faible et nous l’avons résolue numériquement de façon auto-consistante. Nous donnons une présentation exhaustive des parois de domaines stables et métastables pour différentes tranches de paramètres. Nous montrons qu’en prenant en compte l’anisotropie du matériaux—qui tient son origine de la structure électronique de bande, ainsi que de la structure de la fonction de gap—et l’angle de la paroi de domaines—par rapport aux orientations principales du réseau cristallin—, la paroi de domaines la plus stable développe spontanément une différence de phase entre ses deux côtés. Ceci constitue le facteur clé de notre modèle du courant critique de Josephson pour lequel nous supposons que plusieurs paroi de domaines atteignent l’interface. À cause de l’interaction du champ magnétique extérieur avec les parois de domaines, nous obtenons une polarisation forçée par le champ de la configuration de celles-ci qui engendre consécutivement les effets observés dans l’expérience. Nous reproduisons également le motif d’interférence reportés par Bahr à partir de mesures sur des jonctions de taille nano. Nous incluons également l’effet de l’orientation de l’interface par rapport aux axes cristallins. À travers la comparaison de nos simulations et des motifs d’interférence mesurés nous donnons l’estimation de la largeur d’une paroi de domaines.

La deuxième partie de cette thèse se concentre sur l’étude de la structure microscopique des paroi de domaines dans \( \text{Sr}_2\text{RuO}_4 \) pour l’état d’onde \( p \) chiral. Nous étudions dans un premier temps les propriétés générales de l’équation d’Andreev pour deux profils simplifiés non-auto-consistants de la paroi de domaines (paroi de domaines angleuse et lisse) à partir desquelles nous dérivons l’expression analytique du spectre. Cela nous permet de discuter de la brisure de la topologie d’origine (pour le problème quantique complet) suite à la prise de la limite quasi-classique : ceci explique la suppression d’une fraction du poids spectral des états liés dans la paroi de domaines stable supposant le matériaux isotrope et démontre la nécessité de résoudre le problème au-delà de la limite quasi-classique. En outre, nous comparons les conditions aux limites pour la fonction d’onde de Zaitsev et celles de Blonder Tinkham et Klapwijk.

Dans un deuxième temps, nous donnons la solution auto-consistante des équations quasi-classiques de Eilenberger et Riccati, celle-ci avec pour paramètres l’anisotropie et l’angle de la paroi de domaines. En plus d’une très bonne équivalence qualitative avec les résultats de Ginzburg-Landau, nous sommes en mesure d’expliquer le courant spontané qui se propage le long de la paroi de domaines, ainsi que la structure de phase de celle-ci, en terme d’états liés présents dans la paroi de domaines. À cela s’ajoute l’étude de la transition d’une paroi de domaines à un bord, ceci en introduisant à la paroi de domaines un potentiel qui fait barrière.

Troisièmement et finalement, nous étudions le problème formulé sur un réseau cristallin, ce qui constitue la version entièrement quantique du problème (toujours dans l’approximation de champ moyen). Cette approche nous permet de dépasser les difficultés rencontrées à la limite quasi-classique : (i) l’anisotropie entre maintenant de façon naturelle à travers les deux termes aux liaisons fortes suivants : de saut et de pairage; (ii) ensuite, tous les termes d’ordre supérieurs (au delà de la limite quasi-classique) sont inclus automatiquement, ce qui entraîne une structure topologique des paroi de domaines en accord avec les prédictions du théorème d’index. À partir de la solution numérique auto-consistante des équations de Bogoliubov-de Gennes sur un réseau, nous sommes en mesure de donner la signature électronique (au travers de la fonction spectrale) des états liés chiraux de surface, ainsi que des états liés de la paroi de domaines, et ceci pour les deux cas suivants : (i) les surfaces sont alignées avec les axes cristallins, (ii) les surfaces sont tournées de 45°. Nous présentons une nouvelle propriété des états de surface à 45° qui n’a pas encore été signalée : les états chiraux de surface réalisent deux nouveaux points d’énergie zéro qui sont protégés par la symétrie particule-trou de l’échantillon homogène. Enfin, nous proposons une généralisation de l’argument de topologie faible proposé par Hatsugai en ce qui concerne l’existence de ces nouveaux états d’énergie zéro présents aux surfaces obliques.

Dans les perspectives, nous présentons la base de l’explication théorique d’une expérience récente, faite par Maeno et ses collaborateurs, où ils ont mesuré le courant critique de Josephson sur des jonctions Nb/Ru/Sr₂RuO₄. Ils rapportent des effets de bruit importants dans le courant critique mesuré lors
qu’on applique un courant piloté avec une valeur légèrement supérieure à la valeur critique, et tout cela pour des températures inférieures à $T_c$. Notre analyse est basée sur la structure correcte des parois de domaines stables et métastables, à partir des quelles nous simulons le courant critique en prenant en compte l’interaction de deux parois de domaines avec un vortex de Josephson à l’interface.
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Chapter 1

Introduction

1.1 Motivations

Shortly after the discovery of the superconductivity in Sr$_2$RuO$_4$ in 1994 by Maeno and coworkers [27] the proposal of an unconventional superconducting state has been made by Rice and Sigrist [29] (see also [30]). Since then the question of the symmetry of the superconducting state in Strontium Ruthenate has been debated and is not yet settled. Although there are many experimental evidences for the chiral $p$-wave state, the direct observation of domain walls—one of the most peculiar features of the time reversal breaking chiral $p$-wave state—has failed so far. Only Josephson interferometry experiments have been able to point explicitly to the presence of domain walls in Sr$_2$RuO$_4$. Such indirect approaches necessitate detailed theoretical interpretations. In this thesis we present a theoretical study of the domain walls in Sr$_2$RuO$_4$, assuming the chiral $p$-wave state, both at a macroscopic (the first part of the thesis) and microscopic level (the second part of the thesis). As a whole this thesis provides an exhaustive study of the structure of the domain walls in Sr$_2$RuO$_4$ at a mean-field single-band level. We successively study the Ginzburg-Landau theory, the quasi-classical (Eilenberger) theory and the lattice (Bogoliubov-de Gennes) theory, for all of which we give the numerical self-consistent solution. Our main results are:

(i) We give the phase diagram of the domain wall’s structure as a function of the electronic anisotropy of the material.

(ii) We give a detailed interpretation of Josephson experiments involving Sr$_2$RuO$_4$ where the domain walls are believed to play an important role [52, 60].

(iii) We explain the macroscopic structure of the domain walls from the structure of the topologically protected domain wall chiral bound states.

(iv) We reveal the violation of the topology by the quasi-classical theory for some domain wall configurations.

(v) From a lattice approach we give the electronic signature of the chiral edge states and the domain wall bound states in Sr$_2$RuO$_4$ assuming the chiral $p$-wave state. We also reveal peculiar band and geometry dependence of the edge and domain wall bound states.

Our aim is, on the one hand, to contribute to the identification and the characterization of the superconducting state of Sr$_2$RuO$_4$ and, on the other hand, to elucidate the microscopic structure of edges and domain walls within the chiral $p$-wave state. More detailed Motivations are given at the beginning of each part of the thesis.

1.2 Sr$_2$RuO$_4$ and the chiral $p$-wave state

Sr$_2$RuO$_4$ (Strontium Ruthenate) has a layered perovskite crystal structure corresponding to the body centered tetragonal lattice $I4/mmm$, see Fig. 1.1. The point group is then the tetragonal point group
$D_{4h}$. The low energy physics is principally determined by the $4d^4$ electrons of the ions Ru$^{4+}$ of the RuO$_2$ planes, see for instance Ref. [4, 5] for \textit{ab initio} results and Ref. [28] for a review of the experimental results. Due to the tetragonal crystal field surrounding each Ru atoms the $d$-orbitals are split into the \{A$_{1g}$, A$_{2g}$, B$_{2g}$, E$_{g}$\} irreducible representations of $D_{4h}$. At low energy only the $B_{2g}$ and $E_{g}$ states are occupied such that the electronic orbitals are described by the basis functions $d_{xy}$ and \{d$_{yz}$, d$_{zx}$\} (these are separated by the basal plane reflexion symmetry, $\sigma_h$). In the following we assume that there is no dispersion along the c-axis, i.e. the system is two-dimensional. A simplified three-band model\textsuperscript{1} gives the three $\alpha, \beta, \gamma$-Fermi surfaces shown on Fig. 1.2. These can be observed with extraordinary precision through de Haas-van Alphen measurements [43] and ARPES [1].

At low temperature Sr$_2$RuO$_4$ can be well described as a quasi-two dimensional Fermi liquid with strong mass enhancement (see Ref. [26]) subjected to a superconducting instability at $T_c = 1.5K$ [28]. Based on the anisotropic spin fluctuations observed in NMR and neutron scattering experiments [6, 7, 8, 42, 9], spin fluctuation mechanisms have been proposed for the pairing in Sr$_2$RuO$_4$. The spin-orbit coupling generically plays an important role in the determination of the pairing symmetry of the superconducting phase: The orbital anisotropy of the dynamical spin susceptibilities involved in the pairing interaction lifts the degeneracy of the pairing states among the irreducible representations of $D_{4h}$ favoring the chiral $p$-wave state [10, 12, 13, 15, 14, 17, 16].

Although the three bands are in principle important for the physics of Sr$_2$RuO$_4$, the detailed microscopic studies favor the scenario in which the $\gamma$-band is dominant for the superconductivity [11, 15, 18, 19, 101]\textsuperscript{2}. A recent study in the framework of functional renormalization group theory for Sr$_2$RuO$_4$ find a $p$-wave pairing tendency in the FRG flow and confirms the strongly dominant role played by the $\gamma$-band [21] with a strong $C_{4v}$-symmetric anisotropy of the gap. Furthermore, combining their renormalized paired interaction together with the spin-orbit coupling in an effective BCS-model they find the chiral $p$-wave state as the most stable superconducting state, which is in agreement with earlier analysis [11]. Based on those considerations we will restrict our study to the single $\gamma$-band assuming the chiral $p$-wave superconducting state. We will show that the anisotropy of the gap plays an essential role in the structure of the topological defects (here we focus on the domain walls) of the chiral $p$-wave state.

\textsuperscript{1}We derive in the appendix of Chapter 6 the most general tight-binding Hamiltonian for the $\{d_{yz}, d_{zx}, d_{xy}\}$-orbitals from the double point group taking the spin-orbit coupling into account.

\textsuperscript{2}An alternative approach based on incommensurate antiferromagnetic fluctuations and nesting in the $\{\alpha, \beta\}$-bands also leads to the chiral $p$-wave state [20, 13].

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![Figure 1.1: Layered perovskite crystal structure of Sr$_2$RuO$_4$ (identical to the high $T_c$ superconductor La$_2$CuO$_4$). The picture is taken from Ref. [28].](image-url)
1.2.1 Chiral $p$-wave state

Before to address the experimental evidences supporting the chiral $p$-wave state in Sr$_2$RuO$_4$ we first want to characterize the superconducting order parameter in terms of its symmetry. We have mentioned above that spin-orbit coupling is crucial for the electronic properties of Sr$_2$RuO$_4$ and most likely stabilizes the unconventional superconducting chiral $p$-wave state. We derive here the form of the superconducting order parameter (the gap function) allowed by symmetry when spin-orbit coupling is taken into account. It is done from general symmetry arguments such that it doesn’t depend on the details of the microscopic model (we note that this classification is standard, see for instance [54]).

The order parameter (the BCS gap function) can be decomposed as the product of a band, an orbital and a spin part, as

$$
\Delta_{mn,\alpha\beta}(k) \propto \langle c_{m,k,\alpha}c_{n,-k,\beta} \rangle ,
$$

where $m,n = yz,zx,xy$ are the band indices, $k$ is the Fourier coordinate conjugated to the relative coordinate of the Cooper pair $r_1 - r_2$, and $\{\alpha,\beta\}$ are the pseudo-spin indices. We note that $\{\alpha,\beta\}$ can be mapped onto the spin indices $\{\uparrow,\downarrow\}$ by switching off adiabatically the spin-orbit coupling [54]. From now on we will only consider the case $m = n = xy$ (i.e. the $\gamma$-band). Below we use the following parametrization of the gap function in terms of the $d$-vector [2, 3]

$$
\Delta_{\alpha\beta}(k) = i |d(k) \cdot \hat{\sigma}| \alpha\beta ,
$$

$$
d(k) = -\text{tr}\{\hat{\Delta}(k)i\hat{\sigma}_y\hat{\sigma}\}/2 .
$$

Let us start with the spin part. It is given by the combination of two spin-1/2 wave-functions. When the spin-orbit coupling is strong the spin degrees of freedom are attached to the momentum such that they transform together under spatial transformations. Hence the relevant irreducible representations correspond to the point group $D_{1h}$. The irreducible representation of a one-spin wave-function in $D_{1h}$ is given by $\Gamma_{\alpha\beta}^0 = \Gamma_{\alpha\beta}^+$. With the basis functions $\{\chi_\alpha,\chi_\beta\}^3$. The two-spin state can then be decomposed into one singlet and three triplet states as,

$$
\Gamma_0^+(1) \otimes \Gamma_0^+(2) = \Gamma_0^+ (1,2) + \Gamma_2^+ (1,2) + \Gamma_3^+ (1,2) ,
$$

\footnote{For $\lambda_{SO} = 0$ it is $\{\chi_\uparrow = \phi(s = 1/2, m_z = 1/2), \chi_\downarrow = \phi(s = 1/2, m_z = -1/2)\}$.}
with the corresponding basis functions given by,

\[ \Gamma_i^\pm = \Gamma^{S=0} \quad : \quad \frac{1}{\sqrt{2}} (\chi_\alpha(1)\chi_\beta(2) - \chi_\beta(1)\chi_\alpha(2)) \equiv \hat{l}, \]

\[ \Gamma_i^\pm = \Gamma^{S=1, M=0} \quad : \quad \frac{i}{\sqrt{2}} (\chi_\alpha(1)\chi_\beta(2) + \chi_\beta(1)\chi_\alpha(2)) \equiv \hat{\epsilon}, \]

\[ \Gamma_i^\pm = \Gamma^{S=1, M=\pm 1} \quad : \quad \left\{ \begin{array}{ll}
\frac{i}{\sqrt{2}} (\chi_\alpha(1)\chi_\beta(2) - \chi_\beta(1)\chi_\alpha(2)) \equiv \hat{x} \\
\frac{1}{\sqrt{2}} (\chi_\alpha(1)\chi_\beta(2) + \chi_\beta(1)\chi_\alpha(2)) \equiv \hat{y},
\end{array} \right. \]

where we have given the corresponding structure of the \( d \)-vector for each basis function. Since the wave function of the Cooper pair has to be totally anti-symmetric under the permutation of the electrons, the orbital part is even under inversion for the spin-singlet state (with the angular momentum quantum number \( l = 0, 2, 4, \ldots \)) and odd for the spin-triplet states (with \( l = 1, 3, \ldots \)). Restricting itself to the spin-triplet state (which is relevant for the chiral \( p \)-wave state), the orbital part is given by the irreducible representation \( \Gamma^{l=1} = \Gamma_5 \), with the lowest-order basis functions of a two-dimensional system \( \phi(k) \in \{k_x, k_y\} \). Coupling the spin and the orbital parts together (assuming strong spin-orbit coupling) we get the following decomposition,

\[ \Gamma^{l=1} \otimes (\Gamma^{S=1, M=0} + \Gamma^{S=1, M=\pm 1}) = \Gamma_5^\pm \otimes (\Gamma_5^+ + \Gamma_5^-) \]

\[ = \Gamma_5^+ + \Gamma_5^- + \Gamma_3^+ + \Gamma_4^- + \Gamma_5^- \], \hspace{1cm} \text{(1.7)}

with the corresponding basis functions \( \psi_{\Gamma, i}^\pm(k) \) listed in Tab. 1.1. It is easy to show that within the parametrization (1.3) the \( d \)-vector is simply given by

\[ d(k) = \left\{ \begin{array}{ll}
\frac{\Delta_0}{k_F} \psi_{\Gamma, i}^\pm(k), & \text{for 1D irred. rep.} \\
\frac{\eta_i}{k_F} \psi_{\Gamma, i}^\pm(k) + \eta_2 \psi_{\Gamma, j}^\pm(k), & \text{for 2D irred. rep.}
\end{array} \right. \]

\hspace{1cm} \text{(1.8)}

where \( |\eta|^2 = 1 \). Without any further specification the states listed in Tab. 1.1 are degenerated, i.e. they lead to the same condensation energy \( \Delta \) (such that \( \Delta = \Delta(\epsilon_\text{cond} = -\langle |\Delta(k)|^2 \rangle_{k_{\in F, \delta}} \)). However this degeneracy is lifted when we introduce an effective pairing interaction in which the spin-orbit coupling has been taken into account since then it leads to some asymmetry between the different spin configurations. As mentioned above, the effective mean-field pairing interaction (written in terms of the spin susceptibility) assuming a dominant \( \gamma \)-band \([11]\) and functional renormalization group results \([21]\) both show that the \( \Gamma_5^- \)-state is stabilized with \( (\eta_x, \eta_y) = (1, \pm i) \) such that time reversal symmetry is broken. This state is the so called chiral \( p \)-wave state.

**Table 1.1: Symmetry allowed order parameters for the tetragonal point group \( D_{4h} \).**

<table>
<thead>
<tr>
<th>( \Gamma_j )</th>
<th>( \psi_{\Gamma, i}^\pm(k) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Gamma_1^\pm )</td>
<td>( k_x \hat{x} + k_y \hat{y} )</td>
</tr>
<tr>
<td>( \Gamma_2^\pm )</td>
<td>( k_x \hat{y} - k_y \hat{x} )</td>
</tr>
<tr>
<td>( \Gamma_3^\pm )</td>
<td>( k_x \hat{x} - k_y \hat{y} )</td>
</tr>
<tr>
<td>( \Gamma_4^\pm )</td>
<td>( k_x \hat{y} + k_y \hat{x} )</td>
</tr>
<tr>
<td>( \Gamma_5^\pm )</td>
<td>( {k_x \hat{z}, k_y \hat{z}} )</td>
</tr>
</tbody>
</table>

\hspace{1cm} \text{(1.9)}

The chiral \( p \)-wave state belongs to the odd two-dimensional irreducible representation \( \Gamma_5^- \) (or \( E_u \)) of \( D_{4h} \). It has been obtained from the spin triplet state \( M \equiv S_z = 0 \) \( (\Gamma_5^+) \), i.e. it is an equal spin pairing state whose spins lie in the basal plane. In terms of the \( d \)-vector we get

\[ d(k) = \frac{\Delta_0}{k_F} (k_x \pm i k_y) \hat{z}, \]

\hspace{1cm} \text{(1.10)}

such that \( \Delta_{\uparrow \downarrow} = \Delta_{\downarrow \uparrow} = \Delta_0 \) and \( \Delta_{\uparrow \uparrow} = \Delta_{\downarrow \downarrow} = 0 \).
It is a $p$-orbital spin-triplet state and is called chiral because of its finite orbital angular momentum along of the $c$-axis, $L_z = \pm 1$. Since time reversal involves complex conjugation, it breaks time reversal symmetry. An other important property is its twofold degeneracy: this allows for the formation of domains with opposite chiralities that are separated by domain walls (this is analogous to a ferromagnet with an easy axis, see Ref. [22]).

1.2.2 Index theorem and bound states at topological defects

Volovik has shown [23, 24, 95] that time reversal symmetry breaking superconductors can be characterized by the topology of their ground state. As we will show in Chapter 4, the Bogolyubov-de Gennes model of the bulk chiral $p$-wave superconductor can be written as $H(k) = m(k) \cdot \hat{\sigma}$ with $m(k) = (\text{Re} \; d_z(k), \text{Im} \; d_z(k), \epsilon(k) - \mu)$ (assuming $\epsilon_k = \epsilon_k$). The unit vector $\hat{m}(k_x, k_y) = m/|m|$ can be seen as a mapping from the stereographic projection of the unit sphere $(k_x, k_y) \in \mathbb{R}^2 \cup \{\infty\} \simeq S^2$ to the unit sphere covered by the vectors $\hat{m}$, i.e. $\bigcup_k \hat{m}(k) \simeq S^2$ [25]. The number of wrapping of the unit sphere encompassed by this mapping is given by the winding number,

$$C = \frac{1}{4\pi} \int d^2 k \; \hat{m} \cdot \left( \frac{\partial \hat{m}}{\partial k_x} \times \frac{\partial \hat{m}}{\partial k_y} \right). \; \; \; (1.11)$$

It is a topological invariant with the value $C = \pm 1$ for $\mu > 0$, corresponding to the chirality of the superconducting state in (1.10), and with $C = 0$ for $\mu < 0$ (this case is not relevant for us). Formally we can build superconducting phases with higher winding numbers such that $C$ corresponds to the $Z$ topological invariant of the two-dimensional class D of Table I in Schnyder et al [83]. There is an index theorem [111, 112, 113] according to which between two bulk phases characterized by the topological invariants $C_1$ and $C_2$, the edge index $\nu$—which we define as the number of signed crossings of the Fermi energy $\mu$ by sub-gap modes (bound states) for a given spin—is given by $|C_1 - C_2|$. The direct consequence is the prediction of the existence in the chiral $p$-wave state of one zero-energy bound state (per spin) at the edges $(C_{\text{bulk}} - C_{\text{vacuum}} = 1 - 0 = 1)$ and two zero-energy bound states (per spin) at a domain wall that separates two domains of opposite chiralities $(C_+ - C_- = 1 - (-1) = 2)$.

1.2.3 Experimental evidences for the chiral $p$-wave state

Numerous experiments show evidences for the unconventional nature of superconductivity in Sr$_2$RuO$_4$. They especially point to the chiral $p$-wave state. We list the most important below. The thermodynamic properties of Sr$_2$RuO$_4$ first revealed discrepancies with the conventional properties. The heat capacity measurements reveal a linear dependence of $C_T/T$ over a wide range of temperatures $T$ which would suggest the presence of a line node in the gap structure, see Ref. [31]. Even if the picture is not completely consistent with that scenario, see Ref. [28] for a discussion, there is a clear discrepancy with the exponentially decreasing heat capacity expected for a fully gapped system\(^4\). It is also observed that superconductivity is strongly sensitive to nonmagnetic impurities [32]. While in a $s$-wave state the critical temperature remains unaffected under the introduction of nonmagnetic impurities (as it is expected from the Anderson theorem that is based on the conservation of time reversal symmetry [33], however see Ref. [34] for a counter example), it is well known that if there are gapless points or lines in the gap function they lead to a suppression of the critical temperature, see Ref. [35, 36].

SQUID interferometer experiments showed that the tunneling current at zero-field is maximum for devices with the contacts on the same side of the sample and minimum for devices with the contacts on the opposite sides. This can be understood if the order parameter undergoes a $\pi$-phase shift under inversion hence corresponding to an odd-parity ($p$-wave) pairing state [37].

NMR Knight shift measurements for magnetic fields parallel to the basal plane of the tetragonal crystal lattice—the RuO$_2$-plane—show no change in the spin susceptibility as the temperature is lowered through the superconducting phase transition [38]. This is compatible with an equal-spin spin-triplet pairing with the spin axis lying in the basal plane, i.e. $d \parallel \hat{z}$. We note however that NMR Knight shift measurements in magnetic fields parallel to the $c$-axis find a $d$-vector lying in the basal plane [39], which tends to show that very small magnetic field can flip the spin plane of the Cooper pairs.

\(^4\)Three-band models with a superconducting chiral $p$-wave state on the dominant $\gamma$-band seem to reproduce well the heat capacity measurements.
Muon spin relaxation measurements evince the existence of a spontaneous internal magnetic field below $T_c$ which suggests a state with broken time reversal symmetry [40]. Also the Kerr effect studies reveal the breaking of time reversal symmetry below $T_c$ [41]. Furthermore spin-polarized neutron scattering measurements also imply a spin-triplet state with spins lying in the basal plane [42].

**In the search of edge and domain wall currents**

Despite the numerous evidences pointing in the direction of the chiral $p$-wave state for Sr$_2$RuO$_4$, the direct observation of chiral edge states and domain walls remains controversial. On the one hand, the observation of edge states in Sr$_2$RuO$_4$ from tunneling experiments has been reported, see for instance Ref. [84], but the question of the chirality of those edge states is still under debate [70]. On the other hand, the attempt to observe by highly sensitive scanning probes the spontaneous magnetization expected at the edges or at domain walls of a chiral $p$-wave state has only given negative results so far [56, 57]. On the contrary, Josephson interferometry experiments have revealed to be quite successful as an alternative approach in the question of the existence of chiral bound states at the edges and domain walls in Sr$_2$RuO$_4$. This is an indirect approach and a detailed theoretical interpretation of the measurements is needed. We provide in this thesis such an interpretation for the Josephson experiments reported in Ref. [52] and Ref. [60]. We describe in more details the experiments in the **Motivations of Part I**.

**1.3 Outline**

This thesis is divided into two parts. The purpose of Part I is to study the macroscopic structure of the domain walls in Sr$_2$RuO$_4$ assuming the chiral $p$-wave state and to derive the consequences for the physics of Josephson junctions. This allows us to give a detailed interpretation of the experiments reported in Ref. [52] and Ref. [60]. The purpose of Part II is to study of the microscopic structure of topological defects in the chiral $p$-wave state from which we derive the electronic signature of the topological bound states present on the edges and within the domain walls.

A detailed outline is given in the introductory notes **Motivations of Part I** and **Motivations of Part II** at the beginning of each part. The outline of each chapter is given in a form of a short abstract at the beginning of each chapter.
Part I

Macroscopic properties of domain walls in $\text{Sr}_2\text{RuO}_4$
Motivations for Part I

In Ref. [52] Kidwingira \textit{et al} reported the results of a phase-sensitive Josephson interferometry experiment realized on several Josephson junctions made out of the conventional superconductor Pb and the unconventional superconductor \(\text{Sr}_2\text{RuO}_4\). The aim was to probe the internal symmetry of the superconducting state in a setup designed to reveal the discrepancy with the behavior of a conventional superconducting \(s\)-wave state. They measured the Josephson critical current through the junction as a function of the external magnetic field and showed several peculiar effects that are not observed in conventional \(s\)-wave superconductors. First of all, the diffraction pattern of the critical current versus the magnetic flux penetrating the junction showed remarkable differences from the conventional Fraunhofer pattern, the latter being characterized by the maximum of the Josephson critical current at zero field and the zeros of the critical current at integer values of the flux quantum. The measurements showed that the maximum of the Josephson critical current sometimes shifted from the zero field, as well as an asymmetry of the interference pattern between the positive and negative flux ranges. Furthermore they observed a high sensitivity of the measured signal on the junctions’ history. Peculiarly they clearly observed a stable hysteresis effect as the magnetic field was swept forth (say positive field) and back (then negative field) : the maximum of the critical current is realized at a positive field value after the system experiences a higher positive magnetic field, then it is realized at a negative field value after the system experiences a higher negative magnetic field. Last but not least, they reported a specific noise in the measurement of the voltage over time when driven currents just above the critical value were applied to the junction : the voltage switches between two (mostly) constant values. In their article Kidwingira \textit{et al} claim that those effects constitute a clear signature of the presence of chiral domains in \(\text{Sr}_2\text{RuO}_4\) as it is expected in the case of a chiral \(p\)-wave superconducting state.

More recently Bahr [60] reported a study on nano-scale Pb/\(\text{Sr}_2\text{RuO}_4\) Josephson junctions showing a clear transition as the junction’s size (interface length) was reduced from 4\(\mu\)m to 2\(\mu\)m. Above and down to 4\(\mu\)m the Josephson junctions shared most of the properties listed above, which is interpreted by Bahr as the evidence of the presence of a few domain walls inside small samples of \(\text{Sr}_2\text{RuO}_4\). Whereas at 2\(\mu\)m and lower only Fraunhofer-like interference patterns were observed, which is interpreted by Bahr as an evidence of the absence of domain walls. From these observations we can estimate the domain wall’s size to be of the order of a few micrometers, i.e. 4\(\mu\)m > \(\xi_{\text{DW}}\) ∼ 2\(\mu\)m.

Those experiments add to the list of the experimental evidences suggesting the chiral \(p\)-wave state as a good candidate for the superconducting state of \(\text{Sr}_2\text{RuO}_4\). However, as we have exposed in the introduction, there is not yet a general consensus among the physics community. The experiments we have described here are peculiar in the sense that they (indirectly) probe the internal structure of the superconducting state in a setup that is known to be highly sensitive to the symmetry of the pairing state. Therefore it is of great importance to provide a careful theoretical interpretation of those experiments with the aim to provide eventually a clear-cut characterization of the superconducting state in \(\text{Sr}_2\text{RuO}_4\).

In this part, we first derive the macroscopic structure of domain walls in \(\text{Sr}_2\text{RuO}_4\) assuming the chiral \(p\)-wave state. For this we derived a Ginzburg-Landau theory from the microscopic theory obtained for weak coupling and in the quasi-classical limit—in order to relate the Ginzburg-Landau parameters to the (averaged) orbital structure of the electronic band and the gap function (at the Fermi level) of the material. We give the solution of the numerical minimization of the full Ginzburg-Landau free energy, from which we derive a phase diagram of the domain wall’s structure versus the material parameters. We show that the anisotropy of the orbital electronic structure triggers a structural phase transition of the domain walls through which they acquire preferred spacial orientations and an additional global phase modulation. Those play an essential role in our explanation of the experimental findings exposed above. In Chapter 3 we derive a model of the Josephson junction—with a mechanism based on the internal structure of the domain walls—that accounts for most of the effects reported in Ref. [52] and Ref. [60].
Chapter 2

Ginzburg-Landau approach

Assuming the chiral p-wave superconducting state for Sr$_2$RuO$_4$, we derive a Ginzburg-Landau theory in order to study the structure of domain walls that separates domains of opposite chirality. The coefficients of the Ginzburg-Landau functional are derived from the quasi-classical theory and within the weak coupling limit. We find that the orbital anisotropy of the Fermi surface and of the gap function, as well as the orientation of the domain wall with respect to the main crystal axes are essential parameters for the structure of the stable and metastable domain walls. We give the results of the numerical minimization of the full Ginzburg-Landau functional for a representative set of parameters and characterize them in terms of the following two features : the domain wall type and the global gauge-independent phase shift across the domain wall. We eventually discuss the effect of the geometry on the domain wall (for a finite system).

This chapter shows that for realistic parameters (in regard to Sr$_2$RuO$_4$) the domain wall acquires a non trivial global phase shift across it. This result plays an essential role in the next chapter where we discuss the Josephson experiments reported in Ref. [52] and Ref. [60].

The results of an early study of the domain wall’s structure based on a variational ansatz of the gap order parameter are presented in the appendix of this chapter.

2.1 Introduction

In this chapter we study the stable and metastable domain wall configurations in Sr$_2$RuO$_4$ assuming the chiral p-wave state from the Ginzburg-Landau theory. The problem of the domain wall structure in unconventional superconductors is not new [48, 46, 47, 54, 61]. However a full self-consistent solution of the problem in view of Sr$_2$RuO$_4$ was still missing. The specificity of our work is that we specify our study to Sr$_2$RuO$_4$ and we go beyond the approximations assumed in previous works. First, following the approach of Ref. [61], we derive the expression of the Ginzburg-Landau coefficients as a function of (i) the anisotropy of the electronic structure (Fermi surface and gap function) of the material, and (ii) the domain wall angle with respect to the crystal axes. Second, following the early work of Sigrist (see for instance Ref. [46]) we give the solution of the numerical minimization of the full Ginzburg-Landau free energy. In particular, while the early studies [48, 46, 47, 54] were not dedicated to Sr$_2$RuO$_4$, the more recent work [61], that uses a variational ansatz of the order parameter, wrongly predicted the most stable domain wall to lie along one main crystal axis with a zero global phase shift across it. We will show that the anisotropy of the material triggers a structural phase transition into a state where the most stable domain wall is deflected from the main crystal directions and bears a non-zero global phase shift across it.

1 We present in the appendix of this chapter the numerical solution to this variational approach and give the correct expression of the approximated analytical expression of the free energy.
2.2 Ginzburg-Landau free energy

We introduce the basic order parameter of a chiral $p$-wave superconductor and its corresponding Ginzburg-Landau theory which will be used to study the structure of a spatial phase transition between the two degenerate chiral $p$-wave states in Sr$_2$RuO$_4$.

The chiral $p$-wave phase can be described with a two-component order parameter $\eta = (\eta_x, \eta_y)$ belonging to the irreducible odd representation $E_u$ of the tetragonal point group $D_{4h}$, i.e. in terms of the $d$-vector $[2, 3]$:

$$\mathbf{d}(k) = \hat{z}(\eta_x k_x + \eta_y k_y)/k_F. \quad (2.1)$$

We can derive the Ginzburg-Landau free energy functional through an expansion in powers of the order parameter and its gradients under the constraint that the functional remains invariant under all the transformations of the symmetry group of the system$^2 \mathcal{G} = D_{4h} \times K \times U(1)$ ($K$ stands for the time reversal operator) [54]. The free energy functional has then the following general form

$$\mathcal{F}_p[\eta_x, \eta_y, \mathbf{A}] = \int d^3r \left[ a_p(T)|\eta|^2 + b_1|\eta|^4 + \frac{b_2}{2}(\eta_x^* \eta_y^* + \eta_x^2 \eta_y^2) + b_3|\eta_x|^2|\eta_y|^2 \right. \left. \right.$$ 

$$+ K_1(|D_x \eta_x|^2 + |D_y \eta_y|^2) + K_2(|D_x \eta_y|^2 + |D_y \eta_x|^2) + \left\{ K_3(D_x \eta_x)^*(D_y \eta_y) \right. \left. \right.$$ 

$$+ K_4(D_x \eta_y)^*(D_y \eta_x) + c.c. \} + \frac{K_5(|D_x \eta_x|^2 + |D_y \eta_y|^2)^2 + \frac{B^2}{8\pi} \right), \quad (2.2)$$

where $v_p$ is the volume of the system and $\mathbf{D} = \nabla + i\gamma \mathbf{A}$ is the covariant derivative with $\gamma = 2e/\hbar c = 2\pi/\Phi_0$ ($\mathbf{A}$ is the vector potential with the magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$), $\Phi_0$ is the magnetic flux quantum. The material-dependent coefficients, $a_p = a'_p(T - T_{c,p})$ (with $a'_p > 0$), $b_i$, and $K_i$, are given in the next section for the weak coupling limit. In order to stabilize the chiral $p$-wave state in the bulk the coefficients have to satisfy the relations: $b_2 > 0$, $b_3 > b_1$ and $4b_1 > b_2 - b_3$ [55]. Minimizing the free energy functional with respect to the modulus $|\eta|$ in the homogeneous case, we obtain the uniform phase$^3$

$$\eta_{\pm} = \eta(1, \pm i), \quad \eta_t^2 = \frac{-a_p(t)}{4b_1 - b_2 + b_3}, \quad \eta_t \in \mathbb{R}, \quad t \equiv \frac{T}{T_c}, \quad (2.3)$$

such that the corresponding gap function ($d$-vector) is

$$d_{\pm}(k) = \hat{z} \eta_t(k_x \pm i k_y)/k_F. \quad (2.4)$$

This state is doubly degenerate and violates time reversal symmetry, as the operation of time reversal $\hat{K}$ yields $\hat{K}d_{\pm} = d_{\mp}^* = d_{\mp}$. We are interested in the situation of a system with several domains separated by domain walls.

2.2.1 Weak coupling coefficients

An alternative approach to the phenomenological Ginzburg-Landau theory sketched above is to derive the free energy from the quasi-classical theory, that is in the weak coupling limit and long wavelength limit (i.e. when the spatial variations of the fields are negligible over the distance of the lattice spacing). This is done in details in the appendix 5.B. Here, we merely summarize the results that are useful for the Ginzburg-Landau approach. We find that the coefficients of the functional (2.2) are determined by (i) the orbital structure of the Fermi surface and the gap function, both defined at a microscopic level, and (ii) the orientation of the domain wall with respect to the main crystal axes. We write the gap function in terms of the generic basis functions $\{\phi_x(k), \phi_y(k)\}$ of the irrep. $E_u$ as

$$d_z(k, x) = \phi_x(k)\eta_x(x) + \phi_y(k)\eta_y(x). \quad (2.5)$$

At the quasi-classical level (that is within the continuum limit) it is convenient to use for $\{\phi_x, \phi_y\}$ the Fermi surface harmonics which, in this case, are simply given by the Fermi velocity components at the

---

$^2$Note that because of the strong spin-orbit coupling, the spin degrees of freedom are frozen to the orbital degrees of freedom and the associated direct product SU(2) $\otimes D_{4h}$ reduces to $D_{4h}$.

$^3$We note that the corresponding bulk energy density is given by $\mathcal{F}_{\text{homog}}[\eta] = (-4b_1 + b_2 - b_3)\eta_t^4 + a_p\eta_t^2 = -\hbar^2/8\pi$, from which we define the critical magnetic field $H_c$. 

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Fermi level, i.e. $\phi_x = v_x(k_F) / \sqrt{\langle v_x^2 \rangle_{FS}}$ and $\phi_y = v_y(k_F) / \sqrt{\langle v_y^2 \rangle_{FS}}$, where $\langle \cdot \rangle_{FS}$ is the average over the Fermi surface of the system [73]. In this way the anisotropy of the gap function is identified with the anisotropy of the Fermi surface\(^4\).

It is convenient to work within the domain wall coordinates which we define as the following: $x_\perp$ is the coordinate along the direction perpendicular to the domain wall, and $x_||$ is the coordinate for the direction parallel to it, see Fig. 2.1. Rotating the domain wall by an angle $\bar{\theta}$ around the $\hat{z}$-axis, the order parameter transforms as\(^5\),

\[
d_{z} = \phi_{x} (\cos \bar{\theta} \eta_{\perp} - \sin \bar{\theta} \eta_{||}) + \phi_{y} (\sin \bar{\theta} \eta_{\perp} + \cos \bar{\theta} \eta_{||}) , \nonumber
d_{\perp} = \phi_{\perp} \eta_{\perp} + \phi_{\|} \eta_{||} , \tag{2.6}
\]

with

\[
\begin{cases}
\phi_{\perp} = \cos \bar{\theta} \phi_{x} + \sin \bar{\theta} \phi_{y} , \\
\phi_{\|} = - \sin \bar{\theta} \phi_{x} + \cos \bar{\theta} \phi_{y} .
\end{cases} \tag{2.7}
\]

Rewriting the free energy functional in the domain wall axes and setting $p = \sin^2(2\bar{\theta})$, we find the following Ginzburg-Landau coefficients,

\[
b_1 = \frac{b}{8} [3 + \nu - 2\nu p] , \quad b_2 = \frac{b}{4} [1 - \nu + 2\nu p] , \quad b_3 = - \frac{b}{4} [1 + 3\nu - 6\nu p] , \\
K_1 = \frac{K}{4} [3 + \nu - 2\nu p] , \quad K_2 = \frac{K}{4} [1 - \nu + 2\nu p] , \quad K_3 = K_4 , \tag{2.8}
\]

where we have used the Fermi surface Harmonics $\phi_i = \hat{\nu}_{FS, i}$. Following Ref. [45], the anisotropy parameter has been defined as

\[
\nu = \frac{\langle \phi^4_x \rangle_{FS} - 3 \langle \phi^2_x \phi^2_y \rangle_{FS}}{\langle \phi^4_y \rangle_{FS} + \langle \phi^2_x \phi^2_y \rangle_{FS}} , \tag{2.9}
\]

see also section 5.3 for more details. We have $\nu \in [-1, 1]$. For an isotropic system, e.g. a Fermi surface with a circular section, we have $\nu = 0$. If we deform the Fermi surface section into a square, we get $\nu = 1$ or $\nu = -1$ depending on the orientation of the square, see Fig. 2.2. Anticipating on the chapter 5 and 6, we note that the typical value of the anisotropy parameter for the material Sr$_2$RuO$_4$ is $\nu = -0.6$ (it depends on the choice for the values of the microscopic parameters).

\(^4\)This assumption is obviously violated on a lattice, see chapter 6.
\(^5\)The change of coordinates of a vector $(x, y)$ under the rotation of the coordinate axes by an angle $\theta$ (anti-clockwise) is given by

\[
\begin{pmatrix}
x' \\
y'
\end{pmatrix} = R_{\theta} \begin{pmatrix}
x \\
y
\end{pmatrix} = \begin{pmatrix}
\cos \theta & \sin \theta \\
-\sin \theta & \cos \theta
\end{pmatrix} \begin{pmatrix}
x \\
y
\end{pmatrix} = \begin{pmatrix}
\cos \theta x + \sin \theta y \\
-\sin \theta x + \cos \theta y
\end{pmatrix} ,
\]

and inversely

\[
\begin{pmatrix}
x \\
y
\end{pmatrix} = R_{\theta}^{-1} \begin{pmatrix}
x' \\
y'
\end{pmatrix} = \begin{pmatrix}
\cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{pmatrix} \begin{pmatrix}
x' \\
y'
\end{pmatrix} = \begin{pmatrix}
\cos \theta x' - \sin \theta y' \\
\sin \theta x' + \cos \theta y'
\end{pmatrix} ,
\]

where $R_{\theta}$ is the $\theta$-rotation matrix.
where the new coefficients are

From now on we will work mainly within the domain wall axes and we set (x, \parallel, \perp).

As we will see in the next section, the domain wall is characterized by a -phase shift in one of the two components of the order parameter. The parameters \( a, b, K > 0 \) are given in terms of the microscopic parameters as,

\[
\begin{align*}
    a_\nu(t) &= (t - 1) N_0 (\phi_2^2) \\
    b &= 2B_{\text{WC}} [\langle \phi_2^2 \rangle + \langle \phi_4^2 \rangle] \\
    K &= B_{\text{WC}} v_\parallel^2 [\langle \phi_2^2 \rangle + \langle \phi_4^2 \rangle], \\
    B_{\text{WC}} &= \frac{7}{16\pi^2 T^2 \Omega},
\end{align*}
\]

(2.10)

with the reduced temperature \( t = T/T_c \). Note that the GL coefficients satisfy the symmetry \( \{b_i, K_i\}_{\nu, \vartheta} = \{b, K\}_{-\nu, \vartheta \pm \pi/4} \).

The Ginzburg-Landau free energy is invariant under a \( C_4 \)-rotation of the coordinate axes. However, performing a rotation with an arbitrary angle \( \vartheta \in C_\infty \), the free energy is in general not invariant and it acquires the following extra terms,

\[
\begin{align*}
    F_\vartheta &= \int d^4r \left[ b_\nu (|\eta_\parallel|^2 - |\eta_\perp|^2) \left( \eta^\ast \eta_\parallel + \eta_\perp \eta^\ast_\parallel \right) \\
    &+ K_\vartheta \{ (D_\perp \eta_\perp) (D_\parallel \eta_\parallel)^* + (D_\perp \eta_\parallel) (D_\parallel \eta_\parallel)^* + (D_\parallel \eta_\parallel) (D_\parallel \eta_\parallel)^* + \text{c.c.} \} \right],
\end{align*}
\]

(2.11)

where the new coefficients are

\[
\begin{align*}
    b_\vartheta &= \frac{b}{4} \nu \sin 4\vartheta, \\
    K_\vartheta &= \frac{K}{4} \nu \sin 4\vartheta.
\end{align*}
\]

(2.12)

### 2.3 Domain wall structure

In this section we give a few definitions that are useful in order to characterize the domain wall’s structure. A domain wall is characterized by a \( \pi \)-phase shift in one of the two components of the order parameter \((\eta_x , \eta_y)\). Working in the domain wall axes, i.e. \( \eta \equiv (\eta_\perp , \eta_\parallel) \) (see Fig. 2.1), we can define two types of domain wall according to the following asymptotic configurations (L : left hand side, R : right hand side),

\[
\begin{align*}
    "\pi_\parallel - domain wall" : & \quad \eta_L = \eta_\perp \propto (1, -i) \iff \eta_R = \eta_\parallel \propto (1, i), \\
    "\pi_\perp - domain wall" : & \quad \eta_L = \eta_\perp \propto (-1, i) \iff \eta_R = \eta_\parallel \propto (1, i).
\end{align*}
\]

(2.13)

As we will see in the next section, the \( \pi_\parallel \)-domain wall is always more stable than the \( \pi_\perp \)-domain wall. From now on we will work mainly within the domain wall axes and we set \((x_\perp , x_\parallel) \equiv (x, y)\) (when used the main crystal axes are written with a hat, i.e. \(\hat{x}, \hat{y}\), and since we only consider rotations within the basal plane, we set \(\hat{z} \equiv z\)). The system is transitionally invariant along the \(y\)- and \(z\)-direction and the quantities only depend on \(x\) (i.e. the direction perpendicular to the domain wall). Therefor we can choose the following gauge for the vector potential, \( A = (0, A_y(x)) \).
We have to complete our picture of the domain wall structure with an additional element. In general, the order parameter acquires a gauge phase shift across the domain wall as

\[ \eta = \eta_+ \equiv s \, \eta \, e^{-i\alpha/2} (1, -i) \leftrightarrow \eta = \eta_- \equiv \eta \, e^{i\alpha/2} (1, i), \]

\[ s = \begin{cases} +1 & : \pi \\ -1 & : \pi \end{cases}, \quad \alpha = \alpha (\nu, \bar{\theta}). \]  

The phase \( \alpha \) is defined as the global gauge-invariant phase shift across the domain wall, i.e. in the case of a \( \pi \parallel \)-domain wall,

\[ \alpha \equiv \int_{-\infty}^{+\infty} dx \{ \partial_x \varphi_x (x) - \gamma A_x (x) \} = \varphi_x (+\infty) - \varphi_x (-\infty), \]

since in our gauge \( A_x \equiv 0 \) \((\gamma = 2\pi/\Phi_0 = 2e/\hbar c)\), where we used the parametrization \( \eta_x = |\eta_x| e^{i\varphi_x}. \) For the \( y \)-component we have \( \varphi_y (+\infty) - \varphi_y (-\infty) = \pi + \alpha \).

We define the domain wall energy per unit area as,

\[ f_{DW} \equiv \frac{F_{DW}}{L_y L_z} = \frac{F[\eta(x)] - F_{\text{homog}}}{L_y L_z}, \]

which we scale by \( f_0 \equiv K\eta^2_t/\xi_t \), see appendix 2.A.

### 2.4 Numerical results

In this section we present and discuss the results of the numerical minimization of the full Ginzburg-Landau functional for all the stable and metastable domain wall configurations. All the quantities are scaled according to the standard Ginzburg-Landau scaling factors listed in the appendix 2.A.

#### 2.4.1 Domain wall solution

We show on Fig. 2.3 the numerical solution for an isotropic system, i.e. the anisotropy parameter is \( \nu = 0 \) and the results are independent of the domain wall’s angle \( \bar{\theta} \). Fig. 2.3.A and Fig. 2.3.B show the \( \pi \parallel \)- and the \( \pi \perp \)-domain wall respectively. In the two cases, there is no extra phase shift, i.e. \( \alpha = 0 \). We note the sign change of the spontaneous current density that flows along the domain wall comparing the two domain wall solutions. We find for the domain wall energies,

\[ f_{DW}^{(\pi \parallel)} / f_0 = 0.5 \quad < \quad f_{DW}^{(\pi \perp)} / f_0 = 0.9, \]

i.e. the \( \pi \parallel \)-domain wall is the most stable. Nevertheless, the \( \pi \perp \)-domain wall is metastable and we can find it as a solution of the numerical minimization of the Ginzburg-Landau functional\(^6\). We remark the different domain wall widths, \( \xi_{DW}^{(\pi \parallel)} \approx 4\xi_t \) and \( \xi_{DW}^{(\pi \perp)} \approx 6\xi_t \) (with the Ginzburg-Landau coherence length defined as \( \xi_t = K/2\eta^2_t \)). In general we find that the sharpest domain wall is the most stable.

As was early reported in Ref. [46, 47, 54], we find a spontaneous supercurrent flowing along the domain wall associated with a spontaneous magnetization. This is a generic feature of time reversal symmetry breaking states in the vicinity of angular momentum jumps (see Ref. [48] for an early discussion in the context of heavy Fermion materials). We will show in the second part of this thesis that the domain wall currents are the signature of the presence of chiral bound states localized at the domain wall. We will also give an explanation of the inversion of the flow of the current comparing the stable and metastable domain walls, as it is a direct consequence of the different structure of the domain wall bound states.

---

\(^6\)This is done by setting the initial configuration and letting the solution relax through successive iterations. Since we do not use a global minimization algorithm, if the initial configuration corresponds to a metastable state the program remains locked in this state. We can then compare the energies of the different domain walls and tell which one corresponds to the global minimum.
We now consider the case of an anisotropic system, i.e. with $\nu \neq 0$. We are interested in the anisotropy range $\nu < 0$ (which corresponds to the $\gamma$-band of Sr$_2$RuO$_4$ as we will see in Part II of this thesis). The domain wall structure now depends on the domain wall orientation. While $\nu$ is determined by the intrinsic parameters of the material, the domain wall can have different orientations (due to geometric effect, atomic defects, etc.). Below we show the results for the anisotropy $\nu = -0.6$ (obtained from the fitting of the $\gamma$-band of Sr$_2$RuO$_4$) and the domain wall angles $\bar{\theta} = 0, \pi/4$.

We show on Fig. 2.4 the solution of a domain wall aligned along one main crystal axis, i.e. $\bar{\theta} = 0$, and
Figure 2.4: Numerical solution of the Ginzburg-Landau free energy minimization for $\nu = -0.6$ and $\bar{\theta} = 0$. We plot order parameter $\{\text{Re} \, \eta_x, \text{Im} \, \eta_x, \text{Re} \, \eta_y, \text{Im} \, \eta_y\}$, the current density $J_y$, the magnetic induction $B_z$, and the vector potential $A_y$. Fig.A shows the stable domain wall. Fig.B shows the metastable domain wall. The domain wall energy is given, according to Eq. (2.16). All the quantities are scaled according to the scaling factors defined in the appendix 2.A. The remaining external parameter is chosen as $\kappa_t = 3.5$.

for $\nu = -0.6$. Fig. 2.4.A and Fig. 2.4.B show the $\pi_{\parallel}$- and the $\pi_{\perp}$-domain wall solutions, respectively. We again note the sign change of the current density. Like in the isotropic case, the $\pi_{\parallel}$-domain wall is stable and the $\pi_{\perp}$-domain wall is metastable. Accordingly the widths of the domain wall are $\xi_{\parallel_{\text{DW}}} \approx 6\xi_t < \xi_{\perp_{\text{DW}}} \approx 8\xi_t$. Still as in the isotropic case, there is no extra phase shift across the domain wall, $\alpha = 0$. 

\[ f_{\text{DW}}^{(\pi_{\parallel})} / f_0 = 0.4 \]

\[ f_{\text{DW}}^{(\pi_{\perp})} / f_0 = 0.51 \]
Fig. 2.5 shows the results for a domain wall rotated by 45° with respect to one main crystal axis, i.e. \( \bar{\theta} = \pi/4 \), again for \( \nu = -0.6 \). In this case the \( \pi_\perp \)-domain wall is unstable\(^7\) and we only find a solution for the \( \pi_\parallel \)-domain wall. Contrary to the previous cases, the domain wall now acquires an extra global phase shift, \( \alpha = 0.25 \) rad (see the left column of Fig. 2.5). At the angles \( \bar{\theta} \mod \pi/4 = 0 \), the phase shifts \( \pm \alpha \) are degenerate (we show the other solution with \( \alpha < 0 \) on the right column of Fig. 2.5). This non-trivial phase shift will play a major role in the next chapter where we present a mechanism accounting for the influence of the domain walls on the Josephson effect in a Pb/Sr\(_2\)RuO\(_4\) junction. The domain wall in this case has a rather sharp profile with \( \xi_{DW}^{(\pi_\parallel)} \approx 3\xi_t \). Accordingly its energy, \( f_{DW}^{(\pi_\parallel)} = 0.32 \), lies below the other domain walls. We then have that the most stable domain wall lies spontaneously off the crystal axes due to the anisotropy of the system. We will see in the next section that the most stable configuration is realized at the angles \( \bar{\theta} \mod \pi/2 \approx \pm 0.21 \pi \) with the respective phase shifts \( \alpha \approx \pm 0.4 \) rad. We stress on the fact that the configurations \( (+|\bar{\theta}|, +|\alpha|) \) and \( (-|\bar{\theta}|, -|\alpha|) \) are degenerate and jumps from one to the other are allowed, while the configurations \( (+|\bar{\theta}|, -|\alpha|) \) and \( (-|\bar{\theta}|, +|\alpha|) \) do not correspond to minimum solutions (except for the special case \( \bar{\theta} = \pi/4 \), as we have seen above).

We finally show on Fig. 2.6 the global gauge-invariant phase shift across a domain wall, \( \alpha \), as a function of the anisotropy parameter, \( \nu \), for the domain wall angles \( \bar{\theta} = \pi/4 \) (full line) and \( \bar{\theta} = 0 \) (dashed line). There is a transition at a threshold value of the anisotropy, \( |\nu^*| \), above which the domain wall acquires a non-zero global phase shift, \( \alpha \neq 0 \). We note that \( \alpha \) is symmetric under the transformation \( (\nu, \bar{\theta}) \leftrightarrow (-\nu, \bar{\theta} \pm \pi/4) \) which is a consequence of the symmetry of the GL coefficients (2.8) mentioned above.

Domain wall structure for Sr\(_2\)RuO\(_4\)

Fig. 2.7 shows the domain wall energy, defined in Eq. (2.16), as a function of the domain wall angle, \( \bar{\theta} \), for the anisotropy \( \nu = -0.6 \). On Fig. 2.8 we plot the corresponding global phase shift across the domain wall, \( \alpha \), as a function of the angle \( \bar{\theta} \). We find two degenerated most stable domain wall configurations: one at \( \bar{\theta}_{min} = 0.21\pi \) with the phase shift \( \alpha = 0.32 \) rad, and an other at \( \bar{\theta}_{min} = -0.21\pi \) with the phase shift \( \alpha = -0.32 \) rad. An external perturbation might then provoke a jump of the domain wall from one of these two configurations to the other, hence changing abruptly the sign of its global phase shift. This key feature of the domain walls will be exploited in the next chapter. We remark that due to the \( \pi/2 \)-periodicity, one domain wall at a fixed angle \( \bar{\theta} \mod \pi/4 = 0 \) can be realized with the two phase shifts \( \alpha = \pm |\alpha(\pi/4)| \) (this is the special degeneracy at \( \bar{\theta} = \pi/4 \) mentioned above).

\(^7\)Starting with an initial \( \pi_\perp \)-domain wall configuration, it relaxes spontaneously to a \( \pi_\parallel \)-domain wall configuration.
Figure 2.5: Numerical solution of the Ginzburg-Landau free energy minimization for $\nu = -0.6 \, \text{and} \, \bar{\theta} = \pi/4$. We plot the order parameter $\{\text{Re} \, \eta_x, \text{Im} \, \eta_x, \text{Re} \, \eta_y, \text{Im} \, \eta_y\}$, the current density $J_y$, the magnetic induction $B_z$, and the vector potential $A_y$. The domain wall energy is given, according to Eq. (2.16). The $\pi_{\parallel}$-domain wall in this case is unstable and only the $\pi_{\perp}$-domain wall can be stabilized. There is a global phase shift $\alpha = \pm 0.25 \, \text{rad.}$ Fig.A shows the solution with $\alpha = 0.25 \, \text{rad}$ and Fig.B the solution with $\alpha = -0.25 \, \text{rad.}$ All the quantities are scaled according to the scaling factors defined in the appendix 2.A. The remaining external parameter is chosen as $\kappa_t = 3.5$. 

$\pi_{\parallel}$-domain wall for $(\nu, \bar{\theta}) = (-0.6, \pi/4), \quad f_{\text{DW}}^{(\pi_{\parallel})}/f_0 = 0.32$
Figure 2.6: Global gauge-invariant phase shift across a domain wall, $\alpha$, as function of the anisotropy of the Fermi surface, $\nu$, for different domain wall’s orientations: at $\bar{\theta} = \pi/4$ (full line) and at $\bar{\theta} = 0$ (dashed line).

Figure 2.7: Domain wall energy per unit area as a function of the domain wall angle, $\bar{\theta}$, for $\nu = -0.6$. The scaling factor is $f_0 \equiv K\eta^2/\xi_t$ (see Eq. (2.16)). This pattern is repeated with a $\pi/2$-periodicity.

Figure 2.8: Global gauge-invariant phase shift across the domain wall, $\alpha$, as a function of the domain wall angle, $\bar{\theta}$, for $\nu = -0.6$. This pattern is repeated with a $\pi/2$-periodicity.
2.4.2 Domain wall at the surface

We consider in this section the situation of a domain wall ending at the surface of the superconductor and being pinned at a defect somewhere in the bulk (by introducing a columnar pinning center along the \( \hat{z} \)-axis). We are interested in such a situation in view of our discussion, in the next chapter, of a Josephson junction intersected by domain walls.

There is now a compromise between the length of the domain wall and its orientation with respect to the crystal axes. Indeed the domain wall wants to be as short as possible and as close as possible to the orientation that minimizes its wall energy (we found in the previous section \( \bar{\theta}_{\text{min}} = \pm 0.21\pi \)).

Let us start with the situation where the surface normal vector \( \mathbf{n} \) is along one of the principal directions of the basal plane, say the \( \hat{x} \)-axis, i.e. \( \mathbf{n} = (1, 0, 0) \). We assume that a columnar defect pins the domain wall at a distance \( x_l \) from the surface (Fig. 2.9). Then the domain wall energy per unit length in the \( \hat{z} \)-direction, at an angle \( \bar{\theta} \) relative to the \( \hat{x} \)-axis, is given by

\[
E_d(\bar{\theta}) = x_l f_{\text{DW}} \cos \bar{\theta},
\]

(2.17)

with \( f_{\text{DW}} \) being defined in Eq. (2.16).

From the plot of \( E_d(\bar{\theta}) \) on Fig. 2.10 we find that the two most stable domain walls are realized at \( \bar{\theta}_{\text{min}} = \pm 0.17\pi \) with \( \alpha = \pm 0.375 \) rad, and the metastable state domain wall is realized at \( \bar{\theta} = 0 \) with \( \alpha = 0 \). We note that since \( f_{\text{DW}} \) is symmetric under \( (\bar{\theta}, \alpha) \rightarrow (-\bar{\theta}, -\alpha) \), so is \( E_d \).

If the surface normal vector does not lie along a main crystal axis but is tilted by an angle \( \theta_s \) anti-clock wise, i.e. \( \mathbf{n} = (\cos \theta_s, \sin \theta_s, 0) \) (written in the main crystal axes), the domain wall energy per unit surface is then given by,

\[
E_d(\bar{\theta}, \theta_s) = \frac{x_l f_{\text{DW}}}{\cos(\bar{\theta} - \theta_s)}.
\]

(2.18)

When \( \theta_s \neq 0 \) the degeneracy of the most stable states is lifted leaving only one stable and one metastable minimum, and the metastable state that we had at \( \bar{\theta} = 0 \) becomes unstable. We show on Fig. 2.11 the domain wall energy for the increasing surface angles \( \theta_s = 0 \rightarrow 0.05\pi \). We see that for \( \theta_s \rightarrow 0.05\pi \) there appears a metastable state at \( \bar{\theta} > \pi/4 \), while the stable state at \( -\bar{\theta}_{\text{min}} \) becomes unstable. These configurations are neither degenerate nor symmetric, unlike when \( \mathbf{n} = (1, 0, 0) \). The new metastable states correspond to domain wall configurations which are in principle accessible depending on the history of the system.

We summarize the allowed domain wall angles as a function of the surface angle in the following table,

<table>
<thead>
<tr>
<th>( \theta_s )</th>
<th>stable</th>
<th>metastable</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>( \bar{\theta} = \pm</td>
<td>\bar{\theta}_{\text{min}}</td>
</tr>
<tr>
<td>( 0 &lt; \theta_s &lt; \pi/4 )</td>
<td>( \bar{\theta} \approx</td>
<td>\bar{\theta}_{\text{min}}</td>
</tr>
<tr>
<td>( -\pi/4 &lt; \theta_s &lt; 0 )</td>
<td>( \bar{\theta} \approx -</td>
<td>\bar{\theta}_{\text{min}}</td>
</tr>
</tbody>
</table>
Figure 2.9: There are two degenerate configurations of the domain wall. The domain wall may jump between the two positions under an external excitation (in the next chapter, we study the effect of a magnetic field applied in the $z$-direction at the surface).

Figure 2.10: Domain wall energy per unit area, $E_d/x_l$, at the surface $n = (100)$, for $\nu = -0.6$.

Figure 2.11: Domain wall energy per unit area, $E_d/x_l$, as a function of the domain wall angle, for different surface angles (following the arrow): $\theta_s = 0, 0.05\pi, 0.1\pi, 0.15\pi, 0.2\pi, 0.25\pi$, for $\nu = -0.6$. 

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Appendix

2.A Scaling factors

The results from the Ginzburg-Landau theory are presented in the standard Ginzburg-Landau scaling factors:

\[
\eta_t^2 := \frac{-a_p(t)}{b},
\]

\[
\xi_t^2 := \frac{K}{2 b \eta_t^2},
\]

\[
\lambda_t^2 := \frac{1}{8 \pi \gamma^2 K \eta_t^2},
\]

\[
\kappa_t := \frac{\lambda_t}{\xi_t},
\]

\[
B_t^2 := 8 \pi b \eta_t^2,
\]

\[
J_t := \frac{c}{4 \pi \gamma \xi_t^2},
\]

\[
A_t := \frac{1}{\gamma \xi_t},
\]

with the reduced temperature \( t \equiv T/T_c \). We can rewrite the magnetic induction in the standard form as \( B_t = 1/(\sqrt{2} \gamma \xi_t \lambda_t) \). For the numerical results, we take \( \kappa_t = 3.5 \).

The free energy per unit area is scaled by,

\[
f_0 \equiv \frac{K \eta_0^2}{\xi_0} = \frac{v_F T_c N_0}{\Omega} \left( \frac{8 \langle \phi_x^2 \rangle^3 (1 - t)^3}{7 \zeta(3) [\langle \phi_x^2 \rangle + \langle \phi_y^2 \phi_x^2 \rangle]} \right)^{1/2}.
\]  

(2.20)

Note that \( \xi_t \propto \xi_0 (1 - t)^{-1/2} \) such that if we take instead, \( f = \frac{K \eta_t^2}{\xi_0} \), we would have \( f \propto (1 - t)^2 \).

2.B Domain wall structure from a variational ansatz

We give here the numerical solution (minimization of the Ginzburg-Landau free energy) for a variational ansatz of the order parameter. It can be seen as a first approximation; the most general results are presented in the main part of this chapter.

2.B.1 Free energy functional formulation

We first express the free energy functional in a new form which simplifies the rotation of the coordinate frame. We then always define the domain wall as the \( z-x \)-plane and the spatial variation of the order parameter occurs only along the corresponding \( y \)-axis perpendicular to this plane. For simplicity we keep the \( z \)-axis as fixed along the crystaline \( z \)-axis.

We introduce the parametrization [61],

\[
\eta_\pm = \frac{1}{2}(\pm \eta_x - i \eta_y), \quad D_\pm = D_x \pm i D_y,
\]

(2.21)
which inserted into the free energy leads to
\[
\mathcal{F}[\eta_+, \eta_-, A] = \int d^3r \left[ 2a_\rho (|\eta_+|^2 + |\eta_-|^2) + b \left\{ |\eta_+|^4 + |\eta_-|^4 + 4|\eta_+|^2|\eta_-|^2 \right\} + \nu (\eta_{+}^2 \eta_{-}^2 + \eta_{+}^2 \eta_{-}^2) + K \left\{ |D\eta_+|^2 + |D\eta_-|^2 - \frac{1}{2} (\nu(D_+ \eta_+)^{(D_+ \eta_-)} + (D_+ \eta_+)^*(D_+ \eta_-) + c.c.) \right\} + \frac{1}{8\pi} (\nabla \times A)^2 \right].
\]
(2.22)

In a weak-coupling approach the parameter \( \nu = \langle (v_x^2) - 3(v_x^2 v_y^2)/(v_x^2 + v_y^2) \rangle \) is a measure for the anisotropy of the Fermi surface (\( \nu = 0 \) for a cylindrical Fermi surface and \( \nu = 1 \) for a square-shaped Fermi surface) where \( v_{x,y,z} \) are the components of the Fermi velocity and \( \langle \cdot \rangle \) defines the average over the Fermi surface. The coefficients in Eq.(2.2) satisfy the following relations
\[
\begin{align*}
b_1 &= b \frac{3+\nu}{8}, \\
b_2 &= b \frac{1-\nu}{8}, \quad K_1 = K = K \frac{3+\nu}{8}, \\
b_3 &= -b \frac{1-\nu}{8}, \quad K_2 = K_3 = K_4 = K \frac{3-\nu}{8}.
\end{align*}
\]
(2.23)

where \( b \) and \( K \) are material dependent parameters.

This form of the free energy functional allows us now to deal easily with the rotation of the reference frame around the z-axis: \((x', y') = (x \cos \theta + y \sin \theta, y \cos \theta - x \sin \theta)\) with the angle \( \theta \) relative to the original x-axis in the tetragonal crystal. For the new coordinate frame, the order parameter and the gradients are transformed as \( \eta_{\pm} = e^{i\phi} \eta_{\pm} \) and \( D_{\pm} = e^{i\phi} D_{\pm} \). When we express (2.22) in the new coordinates, we have only to modify the two terms containing the parameter \( \nu \) by phase factors,
\[
\begin{align*}
&b \nu e^{i\phi} \frac{3+\nu}{8} \eta_{+}^2 \eta_{-}^2 + c.c., \\
&- \frac{K}{2} \left( \nu e^{i\phi} (D_{+} \eta_{+})^*(D_{-} \eta_{-}) + (D_{+} \eta_{+})^*(D_{-} \eta_{-}) + c.c. \right).
\end{align*}
\]

In this way we can use the angle \( \theta \) to define the coordinate frame. In the following we will omit the primes and always assume that we describe the domain wall in the corresponding frame.

2.B.2 Variational ansatz

We now turn to the structure of the domain wall which will depend qualitatively on the choice of parameters in the free energy. We choose here a variational approach to discuss behavior of the order parameter around the domain wall with the following ansatz which is most useful to eventually obtain the key information relevant for the Josephson effect,
\[
\eta_+ = \eta_0 e^{i\phi_+} \cos \chi \quad \text{and} \quad \eta_- = \eta_0 e^{i\phi_-} \sin \chi, \quad (2.24)
\]
with the boundary conditions within a given reference frame,
\[
\chi = \begin{cases} 
0 & y \rightarrow +\infty \\
\pi & y \rightarrow -\infty 
\end{cases},
\]
(2.25)

where we restrict the spatial dependence of the order parameter to the function \( \chi(y) \) and use relative the phase \( \alpha = \phi_+ - \phi_- \) as a further (variational) parameter. In this way the domain wall appears as an interface between the two superconducting domains which is additionally characterized by a phase difference \( \alpha \), similar to a Josephson junction or weak link [61].

For the later discussion of the Josephson effect with an \( s \)-wave superconductor, it will be useful to return to the order parameter components \( (\eta_x, \eta_y) \) which are expressed as
\[
\begin{align*}
\eta_x &= \eta_0 (e^{i\phi_+} \cos \chi - e^{i\phi_-} \sin \chi), \\
\eta_y &= i\eta_0 (e^{i\phi_+} \cos \chi + e^{i\phi_-} \sin \chi).
\end{align*}
\]
(2.26)

The chosen boundary conditions in (2.25) correspond to the situation,
\[
\begin{align*}
\eta(y = -\infty) &= \eta_0 (-1, i) e^{i\phi_-} \equiv \eta_-, \\
\eta(y = +\infty) &= \eta_0 (+1, i) e^{i\phi_+} \equiv \eta_+.
\end{align*}
\]
(2.27)
for which, in the parametrization \((\eta_x, \eta_y) = (|\eta_x| e^{i\phi_x}, |\eta_y| e^{i\phi_y})\), the phase shifts of the order parameters are given by
\[
\Delta \phi_x = \phi_x(+\infty) - \phi_x(-\infty) = \alpha - \pi,
\Delta \phi_y = \phi_y(+\infty) - \phi_y(-\infty) = \alpha.
\tag{2.28}
\]

Here \(\alpha\) plays the role of the total phase difference of the order parameter and also determines the current flow through the domain wall analogous to a Josephson junction.

With this variational ansatz we rewrite the free energy,
\[
\mathcal{F} = \int d^4r \left[ -b_0^4 + \frac{b_0^4}{2} (1 + \nu \cos(2\alpha - 4\theta)) \sin^2(2\chi) + K_0^2 \left[ |D \cos \chi|^2 + |D \sin \chi|^2 \right].
\]
\[
= \frac{1}{2} \left( e^{-i\alpha}(D_+ \cos \chi)^* (D_- \sin \chi) + \nu e^{i(\alpha - 4\theta)}(D_+ \sin \chi)^*(D_- \cos \chi) + c.c. \right) \right] + \frac{1}{8\pi} (\nabla \times A)^2,
\tag{2.29}
\]
where we substitute \(a_y = -b_0|\eta_y|^2\) using (2.3) and (2.23). Assuming homogeneity along the z- and x-axis, we take \(\chi = \chi(y)\) and \(A = A(y)\) with \(A_z = 0\), the free energy can be written as
\[
\mathcal{F} = \int d^4r \left[ -b_0^4 + K_0^2 \left[ \frac{Q}{4\xi_0^2} \sin^2(2\chi) + (\partial_y \chi)^2 + \gamma^2(A_x^2 + A_y^2)
\right.
\]
\[
+ C_+ \sin 2\chi \left( \gamma^2(A_y^2 - A_x^2) - (\partial_y \chi)^2 \right) + 2S_+ \gamma^2 A_x A_y \sin 2\chi
\]
\[
+ 2\gamma \partial_y \chi \left( S_+ A_y - C_- A_x \right) \right] + \frac{1}{8\pi} (\partial_y A_x)^2 \right],
\tag{2.30}
\]
where \(\xi_0^2 = K/2b_0^2\) defines the coherence length. Additionally we introduced
\[
Q = 1 + \nu \cos(2\alpha - 4\theta),
\]
\[
C_\pm = (\cos \alpha \pm \nu \cos(\alpha - 4\theta))/2,
\]
\[
S_\pm = (\sin \alpha \pm \nu \sin(\alpha - 4\theta))/2.
\tag{2.31}
\]
which are the only coefficients depending on the anisotropy parameter \(\nu\), the phase \(\alpha\) and the angle \(\theta\) of the domain wall orientation relative to the crystalline main axis (crystal x-axis).

Certain symmetries become immediately obvious here. The free energy is invariant under the rotation \(\theta \to \theta \pm \pi/2\) and the operation \((\theta, \nu) \to (\theta \pm \pi/4, -\nu)\) leaves the coefficients unchanged. It is also clear that the phase \(\alpha\) is closely linked to the orientation of the domain wall. A further aspect of symmetry is connected with the operation \((\theta, \alpha) \to (-\theta, -\alpha)\), leading to \(Q \to -Q\), \(C_\pm \to +C_\pm\) and \(S_\pm \to -S_\pm\).

The variational minimization of the free energy functional with respect to \(\chi\), \(A_x\) and \(A_y\) leads to the corresponding three equations:
\[
\partial_y^2 \chi = \frac{Q}{4\xi_0^2} \sin 4\chi - \gamma(S_+ \partial_y A_y - C_- \partial_y A_x)
\]
\[
+ \cos 2\chi \left[ C_+ \left( \gamma^2(A_y^2 - A_x^2) - (\partial_y \chi)^2 \right) + 2S_+ \gamma^2 A_x A_y \right] \sin 2\chi \partial_y^2 \chi,
\]
\[
\kappa^2 \xi_0^2 \gamma \partial_y^2 A_x - \gamma (1 - C_+ \sin 2\chi) A_x = S_- \gamma A_y \sin 2\chi - C_- \partial_y \chi,
\]
\[
A_y = -S_+ \partial_y \chi + S_- \gamma A_x \sin 2\chi \frac{1}{\gamma (1 + C_+ \sin 2\chi)}.
\tag{2.32}
\]
For a concise notation we introduce the Ginzburg-Landau parameter \(\kappa^2 = (\lambda/\xi_0^2)^2 = 1/(8\pi^2 K_0^2 \gamma^2 \xi_0^2)\) with \(\lambda = 1/(8\pi^2 K_0^2 \gamma^2 \xi_0^2)^{1/2}\) as the London penetration length. The third equation leads to \(A_y \to -A_y\) under \((\theta, \alpha) \to (-\theta, -\alpha)\). As a consequence we observe that the free energy is invariant under the operation \((\theta, \alpha, A_y) \to (-\theta, -\alpha, -A_y)\), which will be important again later in the analysis of the Josephson effect.

These equations will now be solved numerically, although we will also present in 2.C an approximate analytical solution. For this purpose it is useful to turn to the dimensionless variables, measuring lengths
in units of $\xi_0$, $\tilde{g} = y/\xi_0$, and using for the vector potential $a_i = \gamma \xi_0 A_i$. The free energy per unit area of the domain wall can then be written as

$$f = \frac{K_0^2}{\xi_0^2} \int d\tilde{g} \left[ -\frac{1}{2} + \frac{Q}{4} \sin^2 2\chi + (\partial_\tilde{g}\chi)^2 + a_b^2 + a_y^2 + C_+ \sin 2\chi (a_b^2 - a_y^2 - (\partial_\tilde{g}\chi)^2) 
+ 2S_- a_x a_y \sin 2\chi + 2\partial_\tilde{g}\chi (S_+ a_y - C_- a_x) + \kappa^2 (\partial_\tilde{g}a_x)^2 \right].$$

(2.33)

Figure 2.12: Domain wall energy as a function of the phase difference $\alpha = \phi_+ - \phi_-$ for rotations of the domain wall by the angles $\theta = 0$ (solid line), $\pi/8$ (dashed line) and $\pi/4$ (dotted line). The anisotropy parameter is chosen $\nu = -0.5$.

In Fig. 2.12 we show the domain wall energy per unit area as a function of $\alpha$ and $\theta$. We do not use here $\alpha$ as a variational parameter but search for the variational local minimum for given $\alpha$. For this calculations we choose the anisotropy parameter to be negative, $\nu = -0.5$. Note that the result for $\nu = 0.5$ follows immediately from the symmetry relation, $f(\alpha, \theta, \nu) = f(\alpha, \theta \pm \pi/4, -\nu)$. For $\theta = \pi/4$ we observe two degenerate minima of $f(\alpha, \theta, \nu)$ at $\alpha_{\text{min}} \approx \pm 0.46\pi$ corresponding to the stable domain wall configuration for given $\theta$ and $\nu$. For any other angle $\theta$ this degeneracy is lifted leading to a stable and metastable minimum, which are located at $\alpha = 0$ and $\alpha = \pi$, respectively, if $\theta = 0$.

The energy of the stable and metastable domain wall configuration depends on the angle $\theta$, as can be seen in Fig. 2.13 where we plot $f_{\text{min}}(\theta) \equiv f(\alpha_{\text{min}}(\theta), \theta)$ for $\nu = -0.5$ (the solid line marks the stable and the dashed line the metastable states). We find that a minimum of this energy occurs at an angle $\theta \approx \pm 0.21\pi$ away from $\theta = 0$. Analogously by symmetry such a minimum is found at $\theta \approx \pm (\pi/4 - 0.21\pi) = \pm 0.04\pi$ for $\nu = 0.5$. From this we conclude that there are special orientations for the domain wall which are energetically favorable and depend on the anisotropy properties of the superconductor. These special orientations need not to lie along symmetry axes or symmetry planes. Note that also the angle with respect to the $z$-axis is important in this respect, since domain walls parallel to $x$-$y$-plane are probably most stable. However, here we consider only the case of domain walls parallel to the $z$-axis, as they are generally most important for the modification of the Josephson effect.

As a reference we consider also the case of an isotropic Fermi surface ($\nu = 0$) which naturally does not show any dependence on the angle $\theta$. We find that the most stable domain wall state corresponds to the phase $\alpha = 0$ which agrees with the result obtained from a corresponding microscopic model calculation based on a quasi-classical approach [62].

In Fig. 2.15 we show the behavior of $\alpha_{\text{min}}$ as a function of $\nu$ for the angle $\theta = 0$. There are two obvious regions; for $\nu < \nu_c = 0.057$ the minimum corresponds to $\alpha_{\text{min}} = 0$ and for $\nu > \nu_c$ we find two degenerate values. In addition metastable states (indicated as dashed lines) appear at $\alpha_{\text{metastable}} = \pm \pi$ for $\nu < -0.12$. 26
Figure 2.13: Energy of stable (solid line) and metastable states (dashed line) of the domain wall in the bulk where the energy $f(\alpha, \theta)$ is minimized with respect to $\alpha$: $f_{\text{min}}(\theta) = f(\alpha_{\text{min}}, \theta)$, as a function of the angle of the domain wall for $\nu = -0.5$.

Figure 2.14: Domain wall energy for an isotropic Fermi surface, i.e. $\nu = 0$. 
2.C Analytical approximation

We start from the free energy functional (2.30) where we neglect the terms in $A_x$. Varying with respect to $\chi$ and $A_y$ gives, respectively,

$$\partial_y^2 \chi = \frac{Q}{4\xi_0} \sin 4\chi - S_+ \gamma (\partial_y A_y) + C_+ [\cos 2\chi (\gamma^2 A_y^2 + (\partial_y \chi)^2) + \sin 2\chi (\partial_y^2 \chi)] ,$$  \hspace{1cm} (2.34)

$$A_y = -\frac{S_+ \partial_y \chi}{\gamma (1 + C_+ \sin 2\chi)} .$$  \hspace{1cm} (2.35)

Following the argument of Ref.[61] we neglect the contribution of the third term of (2.34) and the $\sin 2\chi$ term in the denominator of $A_y$ in (2.35). This leads to the simplified equation for $\chi(y),$

$$\partial_y^2 \chi = \frac{\tilde{Q}}{4} \sin 4\chi ,$$  \hspace{1cm} (2.36)

where $\tilde{Q} = Q/[[C_0^2(1 - S_+^2)]]$. This has the following kink solution

$$\chi(y) = \arctan \left( e^{-\sqrt{\tilde{Q}}y} \right) ,$$  \hspace{1cm} (2.37)

which we use to determine $A_y$. Inserting $\chi$ and $A_y$ into the free energy functional we derive an analytical form of the variational domain wall energy per unit area,

$$f(\alpha, \theta) = K\xi^2 \sqrt{\tilde{Q}} \left\{ 1 - \frac{S_+^2}{2} + \frac{C_+ \pi}{8} + \frac{S_+^2}{C_+} \left[ \frac{1}{\sqrt{1 - C_+^2}} \arctan \frac{\sqrt{1 - C_+^2}}{1 + C_+} - \frac{\pi}{4} \right] \right\} .$$  \hspace{1cm} (2.38)

In Fig. 2.16.A we show the domain wall energy as a function of $\alpha$ for the different angles $\theta = 0, \pi/8, \pi/4$, with the anisotropy parameter chosen $\nu = -0.5$. We see that those results are qualitatively and even quantitatively close to the numerical results plotted in Fig. 2.12. In Fig. 2.16.B we plot the free energy density at $\nu = 0$. Here some short-comings of the above approximation becomes obvious, since there a two minima of the energy in contrast to the single one of the numerical result shown in Fig. 2.14. This discrepancy originates from neglecting the vector potential $A_x$ and the corresponding terms in the free energy.
Figure 2.16: Domain wall energy as a function of the phase difference $\alpha = \phi_+ - \phi_-$, derived from the analytical approximation. A: Anisotropic case with $\nu = -0.5$. B: Isotropic case, $\nu = 0$. The angle of the domain wall with respect to the crystal $x$-axis are chosen $\theta = 0, \pi/8$ and $\pi/4$. 
Chapter 3

Influence of the domain walls on the Josephson effect in a Pb/Sr$_2$RuO$_4$ junction

Based on the results of the previous chapter concerning the domain walls’ structure in a chiral $p$-wave superconductor, we develop a generic mechanism that accounts for the Josephson interference experiment on Pb/Sr$_2$RuO$_4$ junctions reported by Kidwingira et al [52] and Bahr [60]. We derive a simple model for the Josephson current in the limit of a short junction assuming that several domain walls intersect the interface. Our model is written for an arbitrary orientation of the interface with respect to the main crystal axes.

With our model we can reproduce with a good qualitative agreement the characteristic deviations from the Fraunhofer interference pattern of the critical Josephson current as a function of the magnetic field revealed by the experimental findings: see Fig. 3.6 (our simulations) and Fig. 3.7 (measurements from Ref. [52]).

We also discuss the limit of a small junction where only a few domain walls are allowed in the system: see Fig. 3.8 (our simulations and measurements from Ref. [60]).

Furthermore our model is able to account for peculiar hysteretic patterns of the critical current observed in experiments: see Fig. 3.9 (our simulations) and Fig. 3.10 (measurements from Ref. [52]). We also consider the effect of a misalignment of the interface with respect to the crystal main directions and predict a strong asymmetry of the hysteretic pattern, see Fig. 3.11.

Finally we give an estimate of the domain walls’ width and we give an explanation of the switching noise of the voltage over time when a driven current slightly above the critical value is applied to the junction.

3.1 Introduction

We derive in this chapter a model of the Josephson critical current for the experimental setups of Ref. [52] and Ref. [60]. It is based on the results of the previous chapter where we have derived the structure of the stable domain walls in Sr$_2$RuO$_4$ assuming the chiral $p$-wave state. While this chapter follows the presentation of the second part of Ref. [72], we have renewed most of the materials and we have generalized the model by including the orientation of the interface as a tunable parameter.
Figure 3.1: Josephson junction between Pb and Sr$_2$RuO$_4$ in the chiral p-wave state. The dimensions of the junction are $\Delta x \times \Delta y \times \Delta z = 2L_x \times L \times L_z$. The normal vector to the Pb surface is $\mathbf{n}_s$, and the normal vector to the Sr$_2$RuO$_4$ surface is $\mathbf{n}_p$.

3.2 Josephson coupling between s- and p-wave superconductors

We derive here the general expression of the Josephson current density that flows through the Josephson junction with Pb on one side (left) and Sr$_2$RuO$_4$ on the other (right). The geometry we consider is characterized by the surface normal vectors $\mathbf{n}_s$ and $\mathbf{n}_p$ at the interface (s for Pb and p for SRO) each written in the main crystal axes of the corresponding material [54], see Fig. 3.1. In this chapter $(x, y)$ refers to the junction coordinates as drawn on Fig. 3.1.

3.2.1 Bulk terms

The conventional superconductor (Pb) is described by a scalar order parameter $\psi(r)$ corresponding to the spin-singlet pairing state of highest possible symmetry ("s-wave" pairing state). The Ginzburg-Landau free energy functional has the standard form,

$$F_s[\psi, A] = \int d^3r \left[ a_s(T)|\psi|^2 + b_s|\psi|^4 + K_s |D\psi|^2 + \frac{B^2}{8\pi} \right],$$

with $D = \nabla + i\gamma A$ the gauge-invariant derivative and $\gamma = 2e/\hbar c = 2\pi/\Phi_0$ ($A$ is the vector potential with the magnetic field $B = \nabla \times A$), $\Phi_0$ is the magnetic flux quantum, $a_s(T) = a'_s(T - T_{c,s})$, $b_s$ and $K_s$ are parameters that can be derived from a microscopic theory in the weak coupling limit [53].

The free energy for the chiral p-wave superconductor (Sr$_2$RuO$_4$) with the two-dimensional order parameter $\eta = (\eta_x, \eta_y)$ is given in the previous chapter by Eq. (2.2).

3.2.2 Surface term

It was first believed that a Josephson tunneling with frequency $2eV/h$ (lowest-order) between conventional s-wave and p-wave states is forbidden due to the parity mismatch of the two pairing states. This is true if we assume a non-magnetic barrier, i.e. represented by a time reversal and spin-rotation invariant tunneling Hamiltonian [49]. It was then shown that a Josephson coupling to the lowest-order is obtained if the interface is spin active: This is done by introducing a spin-flip term in the tunneling Hamiltonian that allows spin-orbit scattering of quasiparticles such that, since the total angular momentum of the Cooper pair has to be conserved, it leads to a finite coupling between pairing states of different parity [65]. The barrier is magnetic if the spin-orbit coupling on each side of the junction strongly differs, in which case spin independent tunneling Hamiltonian cannot be a valid model of the interface [50]. Let us consider the case of a junction with, on one side, low spin-orbit coupling and, on the other side, strong spin-orbit coupling. Then the eigenstates of the low spin-orbit coupling side are well represented
by pure spin states, whereas the eigenstates of the strong spin-orbit coupling side are represented in terms of pseudo-spin states (linear combination of pure spin states). As a consequence a spin-mixing transfer Hamiltonian is necessary to connect the two sides. In other words the spin mismatch between the respective quasiparticles is overcome through spin flips at the interface together with the mixing of the parity. This argument can be generalized when the spin-orbit coupling is strong on both sides as in the case of Pb and Sr$_2$RuO$_4$ [1]. The strong spin-orbit coupling possibly leads to a strong Josephson coupling but an estimate is not easy because of the complexity of the band structure$^1$.

Based on a group theory analysis, it can be shown that the lowest-order Josephson coupling between the $s$-wave order parameter $\psi$ and the $p$-wave order parameter $\eta$ for an interface with normal vector $n_p$ has the form [54, 65],

$$\mathcal{F}_J = t(n_p) \int d^2r \{ \psi^*(\eta \times n_p) \cdot \hat{z} + \psi(\eta^* \times n_p) \cdot \hat{z} \} ,$$  \hspace{1cm} (3.2)

if the $d$-vector is parallel to the $\hat{z}$-axis as for the chiral $p$-wave state. Here $t(n)$ denotes the coupling strength$^2$ and the integral is taken over the interface.

Using $\mathcal{F}_J$ as a boundary term in the Ginzburg-Landau equations and taking the variational differentiation of the total free energy of the system with respect to $\psi^*$, we find

$$\delta \mathcal{F}[\delta \psi^*] = \delta \mathcal{F}_s[\delta \psi^*] + \delta \mathcal{F}_J[\delta \psi^*] = 0 ,$$

$$\Rightarrow \int d^3r \left\{ -K_s D^2 \psi + a_s \psi + b_s |\psi|^2 \right\} \delta \psi^* + \int d^2r \left\{ -K_s n_s \cdot D \psi + t (\eta \times n_p) \cdot \hat{z} \right\} \delta \psi^* = 0 .$$

From the cancelation of the surface term we then have the relation at the interface

$$K_s n_s \cdot D \psi \big|_i = t (\eta \times n_p) \cdot \hat{z} .$$ \hspace{1cm} (3.3)

The current density on the left hand side (in the Pb bulk) is given through the variational minimization of the free energy $\mathcal{F}_s$ with respect to the vector potential, that is

$$\delta \mathcal{F}_s[\delta A] = 0 , \Rightarrow J \equiv \frac{c}{4 \pi} \text{rot} B = -\frac{\delta [\mathcal{F}_s - \mathcal{F}_{\text{magn}}]}{\delta A} = \frac{2 e K_s}{\hbar} \text{Im} \{ \psi^* D \psi \} ,$$ \hspace{1cm} (3.4)

where $\mathcal{F}_{\text{magn}} = \int d^3r B^2 / 8 \pi$ is the magnetic part of $\mathcal{F}_s$. The current density at the interface flowing along the normal vector $n_s$ (that is the $x$-direction of the junction) is then given by

$$J_x = \frac{2 e K_s}{\hbar} \{ \psi^* n_s \cdot D \psi - \text{c.c.} \} ,$$

$$= \frac{2 e t}{\hbar} [\psi^*(\eta \times n_p) \cdot \hat{z} - \text{c.c.}] ,$$ \hspace{1cm} (3.5)

where we have used the relation Eq. (3.3) that holds at the interface.

Assuming that the interface makes an angle $\theta_i$ with the main crystal axes, see Fig. 3.2, we find $n_p = (-\cos \theta_i, -\sin \theta_i)$. If a domain wall crosses the bulk of Sr$_2$RuO$_4$ with the angle $\theta = -\pi/2 + \theta_b$ (w.r.t. the crystal $\hat{x}$-axis), see Fig. 3.2, it then makes an angle $\theta_b - \theta_i$ with respect to the $x$-axis of the interface. The order parameter in the interface axes is then given by$^3$

$$\begin{cases} 
\eta_x & = \sin (\theta_b - \theta_i) \eta_\perp + \cos (\theta_b - \theta_i) \eta_\parallel , \\
\eta_y & = -\cos (\theta_b - \theta_i) \eta_\perp + \sin (\theta_b - \theta_i) \eta_\parallel .
\end{cases}$$ \hspace{1cm} (3.6)

$^1$The spin-orbit coupling is a microscopic quantity which has to be determined indirectly through a comparison of the computed electronic bands with experimental data (for instance, dHvA or ARPES).

$^2$Not to be confused with the reduced temperature defined in the previous chapter.

$^3$We have

$$\begin{bmatrix} \eta_x \\ \eta_y \end{bmatrix} = R_{\theta_b}^{-1} \begin{bmatrix} \eta_\parallel \\ -\eta_\perp \end{bmatrix} = R_{\theta_b}^{-1} R_{\theta_\perp = -\pi/2 + \theta_b} \begin{bmatrix} \eta_\perp \\ \eta_\parallel \end{bmatrix} ,$$

where $R_{\theta} = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$ is the $\theta$-rotation matrix.
As a consequence, we find for the general Josephson current-phase relation of the junction,

\[
J_x = \frac{2e\ell}{\hbar} \{ \psi^{*} (\cos \theta_i \eta_y - \sin \theta_i \eta_x) - \text{c.c.} \} = \frac{4e\ell}{\hbar} |\psi| (|\eta_y| \cos \theta_i \sin \varphi_y - |\eta_x| \sin \theta_i \sin \varphi_x) ,
\]

with \( \varphi_{x,y} = \phi_{x,y} - \phi_s \) as the phase difference between the order parameter of the chiral \( p \)-wave and the \( s \)-wave superconductor, using the parameterization \( \eta_i = |\eta_i| e^{i\phi_i} \) for \( i = x, y \). Setting \( \theta_i = 0 \) (i.e. the interface is aligned with one main crystal axis), the Josephson coupling reduces to

\[
J_x = J_0 \sin \varphi_y ,
\]

with \( J_0 = (4e\ell/\hbar)|\psi| |\eta_y| \). In this geometry only the \( \eta_y \)-component of the chiral \( p \)-wave state contributes to the Josephson coupling. This is the component parallel to the interface (the nodes point towards the interface). Only this component can combine with the spin to conserve the total angular momentum of the Cooper pair in the tunneling through the interface. In the following we will take \( J_0 \) to be constant for simplicity.

3.3 Interference pattern

We want to calculate the Josephson critical current assuming that several domain walls intersect the Josephson junction from the \( \text{Sr}_2\text{RuO}_4 \) side, as schematically represented on Fig. 3.3. In the following we model the domain wall as a step-like phase shift at the point of intersection\(^4\).

3.3.1 Junction in a uniform magnetic field

Analogously to ordinary Josephson junctions we find also in junctions between an \( s \)- and a chiral \( p \)-wave superconductor a relation between the derivative of the phase \( \varphi_{x,y} = \phi_{x,y} - \phi_s \) with respect to the coordinate along the contact and the magnetic field threading perpendicularly.

We assume that a uniform magnetic field \( H \) is applied in the \( z \)-direction. From the conditions that the current density along the \( y \)-direction \((i)\) vanishes deep inside the bulk of \( \text{Pb} \), and \((ii)\) is determined only

\(^4\)This approach is justified if we assume that the Josephson coupling is weak. Since then the Josephson currents are small and the Josephson penetration depth \( \Lambda_J \) defined below is longer than the extension of the junction, hence it is much longer than the width of a domain wall [66].
Figure 3.3: Josephson junction between Pb and Sr$_2$RuO$_4$ in the chiral p-wave state with several domain walls intersecting the interface. The dimensions of the junction are $\Delta x \times \Delta y \times \Delta z = 2L_x \times L \times L_z$.

by the domain walls’ structure deep inside the bulk of Sr$_2$RuO$_4$, we find the following gauge invariant relations for the derivative of the phases on each side of the junction ($0 \ll a < L_x$),

$$\partial_y \phi_x = \frac{2\pi}{\Phi_0} A_y(-a,y) = 0,$$  \hspace{1cm} (3.9)

$$\partial_y \phi_y = \frac{2\pi}{\Phi_0} A_y(a,y) = \partial_y \phi^{(y)},$$  \hspace{1cm} (3.10)

$$\partial_y \phi_x = \frac{2\pi}{\Phi_0} A_y(a,y) = \partial_y \phi^{(x)},$$  \hspace{1cm} (3.11)

where we have used Eq. (3.4) for the first relation and where the phases $\phi(x,y)$ are intrinsic quantities that account for the presence of domain walls in the bulk of the chiral p-wave superconductor.

Let us first consider the phase $\phi_y$ which is the only one relevant for the Josephson current when $\theta_i = 0$, see Eq. (3.8). Combining the second and the first equation above we obtain,

$$\partial_y \phi_y = \frac{2\pi}{\Phi_0} d_{\text{eff}} B_z(y) + \partial_y \phi^{(y)}(y),$$  \hspace{1cm} (3.12)

where $B_z(y)$ is the magnetic induction that penetrates through the interface and is screened over the effective width of the Josephson contact (parallel to $\eta_y$) $d_{\text{eff}} = d + \lambda_s + \lambda_p$, which includes the width $d$ and the London penetration depths on both sides, $\lambda_s, \lambda_p$ (for Pb $\lambda_s \approx 35\text{nm}$ and for Sr$_2$RuO$_4$ $\lambda_p \approx 160\text{nm}$). We note that the source term $\partial_y \phi^{(y)}$ can be interpreted as a local magnetic field due to the presence of a domain wall.

From Eq. (3.8) and Ampere’s law, $J = (e/4\pi)\partial B_z/\partial y$, we find that the spatial variation of the phase $\varphi_y(y)$ obeys the extended Sine-Gordon equation,

$$\partial_y^2 \varphi_y = \frac{1}{\Lambda_J^2} \sin \varphi_y + \partial_y^2 \phi^{(y)},$$  \hspace{1cm} (3.13)

with the Josephson penetration depth $\Lambda_J = (e\Phi_0/8\pi^2 J_0 d_{\text{eff}})^{1/2}$. Assuming now that $\Lambda_J$ is larger than the extension $L$ of the Josephson junction along the $y$-direction, we find that $\varphi_y$ is given approximately by

$$\partial_y \varphi_y = \frac{2\pi}{\Phi_0} d_{\text{eff}} H + \partial_y \phi^{(y)} \Rightarrow \varphi_y(y) = ky + \phi^{(y)}(y) + \beta_y,$$  \hspace{1cm} (3.14)

where $k = 2\pi H d_{\text{eff}}/\Phi_0$ and $\beta_y$ is an integration constant.

Repeating the same procedure for the phase $\varphi_x$ we find

$$\varphi_x(y) = ky + \phi^{(x)}(y) + \beta_x.$$  \hspace{1cm} (3.15)
The total current is then
\[ I = L_z J_0 \int_{-L/2}^{+L/2} dy \left[ \cos \theta_i \sin \left( k y + \phi^{(y)}(y) + \beta_y \right) - \sin \theta_i \left( \frac{\eta_x(y)}{\eta_y(y)} \right) \sin \left( k y + \phi^{(x)}(y) + \beta_x \right) \right], \] (3.16)
with \( L_z \) the extension of the junction along the \( z \)-direction. We will see below that the constant \( \beta_x \) is related to \( \beta_y \). This allows us now to discuss the effect of domain walls on the interference pattern in the maximal Josephson current obtained by maximizing \( I \) with respect to \( \beta_y \).

### 3.3.2 Phase \( \phi(y) \)

Before addressing the question of the interference pattern it is necessary to determine the change of the phase \( \phi^{(y)}(y) \) when there is a domain wall in \( \text{Sr}_2\text{RuO}_4 \). We consider here a single domain wall that reaches the Josephson junction’s interface with the angle \( \theta_b - \theta_i \) with respect to the junction \( z \)-axis, see Fig. 3.2. In the configuration of Fig. 3.2 the domain wall solution exposed in the previous chapter gives
\[
\begin{align*}
\phi_x(y = \pm \infty) &= \pm (\hat{\theta}_b - \theta_i - \alpha/2) \\
\phi_y(y = \pm \infty) &= \pm (\hat{\theta}_b + \theta_i + \alpha/2 + \pi/2) 
\end{align*}
\]

The total phase shift of the order parameter is then by,
\[
\begin{align*}
\Delta \phi_x &= \alpha (\hat{\theta}_b) - 2 (\hat{\theta}_b - \theta_i) + \pi, \\
\Delta \phi_y &= \alpha (\hat{\theta}_b) - 2 (\hat{\theta}_b - \theta_i) ,
\end{align*}
\] (3.17, 3.18)
with \( \Delta \phi_x = \phi_x(\pm \infty) - \phi_x(\pm \infty) \). Note that due to the \( C_{4z} \)-symmetry of \( \text{Sr}_2\text{RuO}_4 \) we have \( \alpha(\hat{\theta}) = \alpha(\hat{\theta}_b) \) (see Fig. 2.8).

The phase shift \( \Delta \phi^{(y)} \) through the domain wall is then given through the integration of Eq. (3.10) along the \( y \)-axis, which together with Eq. (3.18), readily gives
\[
\begin{align*}
\Delta \phi^{(y)}(\hat{\theta}_b - \theta_i) &= \Delta \phi_y - \frac{2\pi}{\Phi_0} \int_{-\infty}^{+\infty} dy A_y , \\
&= \alpha (\hat{\theta}_b) - 2 (\hat{\theta}_b - \theta_i) + \tan (\hat{\theta}_b - \theta_i) \frac{2\pi}{\Phi_0} \int_{-\infty}^{+\infty} dx_{\perp} A_{||}(x_{\perp}) ,
\end{align*}
\] (3.19)
after transforming $dyA_y$ into the domain wall coordinates according to Fig. 3.2.

We listed in the previous chapter the stable and metastable configurations of a domain wall for different ranges of the interface’s angle, see Tab. 2.19. We found that at $\theta_i = 0$ there are two degenerate stable domain wall configurations at the angles $\theta_{b,min} = 0.17\pi$ for which the global phase shift in the domain wall axes are $\alpha(\pm \theta_{b,min}) = \pm 0.375 \text{ rad}$ (see Fig. 2.10). We find for those states $\Delta\phi_{\eta}(y=0(\pm \theta_{b,min})) = \mp 1 \text{ rad}$. When $\theta_i \neq 0$ we have shown that one of the states becomes metastable (see Fig. 2.11). Strictly speaking the stable and metastable angles depend on the interface angle, i.e. $\theta_{b,min} = \theta_{b,min}(\theta_i)$. We show on Fig. 3.4 the plot of the phase shift across a domain wall that separates the state $\eta_+$ at $y < 0$ and the state $\eta_-$ at $y > 0$. $\Delta\phi_{\eta_+ \rightarrow \eta_-}$, as a function of the interface angle $\theta_i$ and for the different stable and metastable domain wall angles. The phase shift of the reversed configuration, i.e. we permute the states $\eta_+$ all the rest remaining the same, is simply given by $\Delta\phi_{\eta_- \rightarrow \eta_+} = - \Delta\phi_{\eta_+ \rightarrow \eta_-}$ (see Fig. 3.5). Finally there is also a metastable state at $\theta_i$ for $\theta_b = 0$ with $\alpha(0) = 0$, for which we find $\Delta\phi(0) = 0$. This state becomes unstable when $|\theta_i| > 0$.

From Eq. (3.17) we find for the phase shift $\Delta\phi^{(x)}$ the simple relation

$$\Delta\phi^{(x)} = \Delta\phi^{(y)} + \pi \ . \ (3.20)$$

In order to determine the constant $\beta_x$ we fix the boundary condition at $y = 0$ assuming that Sr$_2$RuO$_4$ is in the state $\eta_+ = (1, i) e^{\alpha/2}$ (written in the domain wall axes). Transforming to the junction axes, that is $\eta(y=0) = (i, 1) e^{\alpha/2}$, we find the relation $\phi_y(0) - \phi_y(0)$ mod $2\pi = \pi/2$. In general we have

$$[\beta_y - \beta_x]_{\eta(0) = \eta_+} = \frac{\pi}{2}, \quad [\beta_y - \beta_x]_{\eta(0) = \eta_-} = -\frac{\pi}{2} \ . \ (3.21)$$

### 3.3.3 Model for intersecting domain walls

We extend now our model to a Josephson junction intersected by several domain walls. When only one domain wall reaches the interface at the position $y = y_1$, the Josephson phase is simply given by

$$\varphi_y(y) = k y + \phi_y^{(y)}(y) + \beta_y = k y + \Delta\phi_{\eta_+}^{(y)}(y-y_1) + \beta_y \ . \ (3.22)$$

Here $\Delta\phi_{\eta_+}^{(y)}$ denotes the phase shift at the domain wall as calculated in the previous section. The index $\mu_i$ labels the allowed configurations of the domain walls, $\pm|\theta_{b,min}|$ (which can be both stable minima or, one stable and one metastable domain walls, depending on the interface’s angle $\theta_i$). We illustrate them (for $\theta_i = 0$) on Fig. 3.5 which gives the possible phase shifts of two successive domain walls, $\Delta\phi_{\mu_i}^{(y)}$ for $i = 1, 2$ and $\mu_i = -, +$. It is admissible to use a step function $\Theta(y)$ to describe the spatial change of the phase, since the extension of the domain wall is small compared to the length of the Josephson junction and the Josephson penetration depth $\Lambda_J$. This leads to a piecewise constant phase shift.

The generalization to an array of domain walls is straightforward. For $N$ successive domain walls, the Josephson phase difference across the junction is given by

$$\varphi_y(y) = \beta_y + \sum_{i=1}^{N} \Delta\phi_{\mu_i}^{(y)}(y-y_1) + k y \ , \ (3.23)$$

where $\varphi_y(y)$ depends on the configuration $\{\mu_1, \mu_2, \ldots, \mu_N\}$ of all domain walls. We will now show that the distortion of the Josephson interference pattern through $\varphi_y(y)$ depends on these configurations. The Josephson phase difference $\varphi_x$ is given analogously with the domain wall phase shift given by Eq. (3.20) and the constant $\beta_x$ fixed through the boundary condition at $y = 0$, Eq. (3.21).

### 3.3.4 Modified interference pattern

The total Josephson current which traverses the junction is given by Eq. (3.16). Using our piece-wise constant approximation for $\phi^{(y,x)}(y)$ and imposing the boundary condition $\eta(y=0) = \eta_+$, we obtain readily the following expression,

$$\frac{I(\Phi)}{I_0} = \frac{\Phi_0}{\pi \Phi_0} \sum_{n=0}^{N} \sin \left( \beta_y + (-1)^n\theta_i + \sum_{j=0}^{n} \Delta\phi_{\mu_j}^{(y)} + \frac{\pi \Phi (y_{n+1} + y_n)}{\Phi_0 \Phi_0} \left( \frac{y_{n+1} - y_n}{L} \right) \right) \sin \left( \frac{\pi \Phi (y_{n+1} - y_n)}{\Phi_0} \right) \ . \ (3.24)$$

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Figure 3.5: The two stable configurations of two successive domain walls (here $\theta_i = 0$) and their respective phase shift, $\Delta\phi^{(y)}_{\mu_j}$.

where we have made the approximation $|\eta_x(y)|/|\eta_y(y)| \approx 1$, and with $\Delta\phi_{\eta_0} = 0$, $y_{N+1} = L/2$, $y_0 = -L/2$ and $I_0 = SJ_0$ ($S = L_2L$ being the interface area), and $kL\Phi_0 = 2\pi\Phi$. Note that if we chose the boundary condition $\eta(y = 0) = \eta_+$ instead, the factor in front of $\theta_i$ becomes $(-1)^{n+1}$.

The Josephson critical current, i.e. the maximal supercurrent allowed for this configuration, is obtained by the maximization of $I$ with respect to $\beta_y$. This condition reads

$$\frac{\partial I}{\partial \beta_y}(\beta_{\text{max}}) = 0,$$

leading to

$$\beta_{\text{max}} = \arctan \left( \frac{A_1}{A_2} \right),$$

with

$$A_1 = \sum_{n=0}^{N} \cos \left( (-1)^n \theta_i + \frac{\pi\Phi (y_{n+1} + y_n)}{\Phi_0 L} \right) \sin \left( \frac{\pi\Phi (y_{n+1} - y_n)}{\Phi_0 L} \right),$$

$$A_2 = \sum_{n=0}^{N} \sin \left( (-1)^n \theta_i + \frac{\pi\Phi (y_{n+1} + y_n)}{\Phi_0 L} \right) \sin \left( \frac{\pi\Phi (y_{n+1} - y_n)}{\Phi_0 L} \right).$$

The Josephson current can be written as

$$I I_0 = \frac{\Phi_0}{\pi \Phi} \{ A_1 \sin \beta + A_2 \cos \beta \},$$

from which we find eventually

$$\frac{I_{\text{max}}}{I_0} = \frac{\Phi_0}{\pi \Phi} \{ A_1 \sin \beta_{\text{max}} + A_2 \cos \beta_{\text{max}} \} = \frac{\Phi_0}{\pi \Phi} \sqrt{A_1^2 + A_2^2}.$$

On Fig. 3.6 we show two simulations for interference pattern of the Josephson critical current in a magnetic field, using two random domain wall configurations (indicated in the inserted panels) where we assumed $N = 10$ for the number of intersecting domain walls. The randomness occurs in the positions of domain walls as well as in the sequence of $\{\mu_1, \ldots, \mu_N\}$. The deviation from the standard Fraunhofer
Figure 3.6: Simulation of the Josephson critical current as a function of the external magnetic flux for ten intersecting domain walls randomly configured with (a) a zero total phase shift, and (b) a total phase shift $-4|\Delta \phi|$. The anisotropy parameter is chosen $\nu = -0.6$. In the both cases we assume an interface aligned with the main crystal axes, i.e. $\theta_i = 0$.

Figure 3.7: Experiments: Critical current measured by Kidwingira et al [52]. (a) Fraunhofer-like pattern. (b) Unconventional pattern. Pictures from Ref. [52].

pattern is obvious. We show on Fig. 3.7 two examples of measured critical current taken from Kidwingira et al [52]. We see a quite good qualitative agreement.

The effect of the size of the junction on the interference pattern of the critical current has been investigated experimentally by Bahr [60]. We show on Fig. 3.8 (a) and (b) the simulations assuming a small junction with two and three domain walls intersecting the interface. We have assumed that due to the small size of the junction the domain walls are lying close to the center of the junction, this is what is responsible for the characteristic patterns obtained. We compare our findings with the measurements for a junction of size $L = 4 \mu m$ shown on Fig. 3.8 (c) and (d), taken from [60]. We find a surprisingly good qualitative agreement. Bahr [60] shows that for shorter junctions, i.e. with the size $L = 2 \mu m$ and below, the interference pattern is always mainly Fraunhofer-like which he interprets as the sign of the absence of domain wall in the junction due to the spatial restriction. This leads to the following estimate of the upper bound for the domain wall width $\xi_{DW} \leq 1 \mu m$.

In all those examples, the maximum of the Josephson current lies rather close to $H = 0$. This feature has to do with the fact that, in the case of generic random configurations, the phase shift does not vary much overall, i.e. $|\phi(y = L/2) - \phi(y = -L/2)| \ll 2\pi$. Stronger deviations can be observed, if we bias the domain wall configuration in a way as to have a larger net shift, e.g. by assuming for all domain walls the same sign of $\Delta \phi$. As we will see in the next section, this can happen as a consequence of the
interaction of the external magnetic field and the domain walls at the interface.

### 3.3.5 Hysteresis effect

An important feature supporting the idea that domain walls are involved in producing the irregular interference pattern is the observation of hysteresis effects by Kidwingira et al., when the external magnetic field was cycled between positive and negative maximal fields [52] (see also [60]). They argued that the applied magnetic field induces a rearrangement of the domain walls in the sample, and they substantiated their claim by simulations looking at the effect of shifted domain wall positions. Since the domain walls are pinned at defects of the sample large shifts in positions are rather unlikely.

Hysteresis effects are rather easily discussed within our simplified model in Eq. (3.23, 3.24, 3.29). The free energy of the junction in a magnetic field can be approximated by

$$ F(\beta_y, \Phi, \{\mu_1,\ldots,\mu_N\}) - F_0 = - \frac{I_0 \Phi_0}{2 \pi c L} \sum_{n=0}^{N} \int_{y_n}^{y_{n+1}} dy \cos \left( \beta_y + \sum_{j=0}^{n} \Delta \phi_{j,\mu_j} + \frac{2 g \pi \Phi}{L \Phi_0} \right), $$

(3.30)

for $\theta_i = 0$. We neglect the change of the intersection points $y_n$ for different configurations $\mu_n$ and examine the condition to minimize the free energy. Moreover we assume that the interface is smooth and that we
has the same two essentially degenerate configurations for all domain walls, see Fig. 3.5:

\[
\begin{align*}
\Delta \phi_- &= \Delta \phi_{y|-\bar{\theta}_{b,m}|} (|\bar{\theta}_{b,m}|) = \Delta \phi_{y|\bar{\eta}-\bar{\eta}_+|} (-|\bar{\theta}_{b,m}|) < 0, \\
\Delta \phi_+ &= \Delta \phi_{y|\bar{\eta}_+\bar{\eta}_-|} (|\bar{\theta}_{b,m}|) = \Delta \phi_{y|\bar{\eta}_+\bar{\eta}_-|} (|\bar{\theta}_{b,m}|) > 0.
\end{align*}
\]

Thus, \( n_p \) is assumed to lie very close to a high-symmetry axis of SrRuO\(_4\), say \( n_p = (-100) \) and \( \theta_i = 0 \). For values \( \Phi > 0 \) the free energy in Eq. (3.30) can be lowered by choosing \( \Delta \phi_{y\mu_i} = \Delta \phi_- \), because under this condition

\[
\sum_{j=0}^n \Delta \phi_{y\mu_i} \approx \Delta \phi_- \frac{N(y + L/2)}{L} < 0.
\]

Note that there are special values of \( \Phi \) where the full “polarization” of \( \Delta \phi \) may not be the best choice. However, considering a sweep of the field to maximal value \( \Phi_{\text{max}} \) and back would favor Eq. (3.32). The same argument can be used for negative fluxes, driving the domain walls to adopt \( \Delta \phi_{y\mu_i} = \Delta \phi_+ \).

Starting at zero field, the domain walls shall be essentially randomly configured. Such a situation would lead to a critical current pattern as shown on Fig. 3.6. If the magnetic field is increased up to a sufficiently high value, then the domain walls would likely polarize after a certain waiting time. When we decrease now the field to measure the interference pattern, we observe the interference pattern modified

\[
\text{Figure 3.9: Hysteresis effect: shift of the maximum of the critical Josephson current for positive field (solid line) and negative field (dashed line). (a) Symmetric shift for positive and negative field. (b) Asymmetric shift due to an incomplete polarization of the domain walls (here one domain wall has not jumped as we reached negative field). In the both cases the interface is aligned with the crystal axes, i.e., } \theta_i = 0.
\]

\[
\text{Figure 3.10: Experiment: Hysteretic pattern of the critical Josephson current, from Kidwingira et al [52].}
\]
by the polarized domain walls. After reaching a sufficiently large negative field value, the domain walls polarize in the opposite way. Therefore, tuning the field back towards positive values we find an altered interference pattern of the critical current. Simulation results taking the two (polarized) domain wall configurations into account are shown on Fig. 3.9. The most striking feature is the shift of the maximum of the critical current. On Fig. (a) all the domain walls are polarized and the phase shift is symmetric for positive and negative fields. On Fig. (b) we assume that when reaching the maximum negative field one domain wall didn’t jump into its other stable configuration which results in an asymmetric phase shift (also the maximum critical current has different values for positive and negative fields). These curves are obtained assuming that changes of domain wall configurations during the field sweep, when the critical currents is measured, can be neglected. We show on Fig. 3.10 (a) the experimental counterpart.

Reorganizations of the domain wall configurations during the field sweep would most likely lead to discontinuities in the critical current. This kind of behavior is also observed in a set of measurements by Kidwingira et al [52], see Fig. 3.10 (b), where the field sweeping range is restricted to rather small fields only. Also in this case a hysteretic behavior of critical current (dependence on the field sweep direction) is observed, though less pronounced. It is not unlikely that some part of the noise on these data can be interpreted as an effect due to the domain walls.

Note that for metastable domain wall states a polarization would only be possible if the energy expense of the metastable configurations is sufficiently small. We consider now geometries for which this is true. We show on Fig. 3.11 the effect of changing the interface’s orientation with respect to the main crystal axes. In this case the force of the magnetic field on the domain wall has to be strong enough to stabilize some domain walls, each over two, in their metastable state (remember Fig. 3.4). We see that a change in the geometry of the junction would lead to strong effects on the critical current. Peculiarly we find that it leads to an accentuation of the asymmetry of the hysteretic effect, i.e. $I_{c,max}(−|Φ|) ≠ I_{c,max}(|Φ|)$.

We finish this part by noting that taking the possible creeping of the pinning points of the domain walls would also lead to remarkable effects on the interference patterns.

### 3.3.6 Estimate of the domain wall width

Turning back to the hysteresis effect with polarized domain wall configurations, we might use the shift of the position of the maximal critical current in order to estimate the density of domain walls. We denote the flux of the maximal current as $Φ_{mc}$, which can be determined approximately by the condition

$$\frac{2πΦ_{mc}}{Φ_0} ≈ − N \sum_{i=1}^{N} \Delta φ_{i,μ} = − [φ(y)(L/2) − φ(y)(−L/2)] = − N \Delta φ_± , \quad (3.33)$$

assuming for the last equality a completely polarized domain wall configuration where all domain walls contribute the same phase shift $Δφ_±$. First, we conclude that for a sweep down from the positive field side, for which all the domain walls contribute by $Δ_−$, the maximum lies at $Φ_{mc} > 0$ (opposite for the opposite sweep direction) in accordance with experimental findings. The number of domain walls
intersecting the Josephson junction is then given by

\[ N \approx \frac{2\pi \Phi_{mc}}{\Delta \phi \pm \Phi_0} = \frac{2\pi |\Phi_{mc}|}{|\Delta \phi| \Phi_0}. \]  

(3.34)

Kidwingira et al find in a measurement of hysteresis effect the magnetic field \( B_{mc} \approx 0.8G \) (Fig. 3.10) which yields a flux \( \Phi_{mc} = d_{eff}LB_{max} \approx 16 \times G \mu m^2 \approx 0.8\Phi_0 \). For this estimate of \( \Phi_{mc} \) we took \( L \approx 100\mu m \) and \( \lambda_z = 35\mu m \), \( d = 10\mu m \) and \( \lambda_p = 160nm \).

Using Eq. (3.19) with \( \nu = -0.6 \) we find \( |\Delta \phi^{(v)}| = 1 \) rad. From this we obtain \( N \approx 10 \) which leads to a mean distance between two domain walls of \( d_{DW} \approx 9.3\mu m \). We then have an upper bound for the domain wall width \( \xi_{DW} < d_{DW} \).

### 3.3.7 Noise effect

Kidwingira et al [52] also reported the presence of peculiar noise in the time dependence of the voltage of the junction in a constant current slightly above the critical current. We show their experimental data on Fig. 3.12.

![Figure 3.12: Switching noise in the voltage of a junction biased at a constant current greater than the critical current, from Kidwingira et al [52].](image)

This feature can be well understood in terms of the dynamics of domain walls. As we have seen above, the modification of the domain wall configuration \( \{\mu_1, \ldots, \mu_N\} \) changes the critical current. The current-voltage characteristics of a Josephson junction for currents \( I \) immediately above the critical current \( I_c \) is very non-linear such that a slight change in the critical current induces a jump in the voltage, see Fig. 3.13. The noise feature of Fig. 3.12 suggests that the critical current fluctuates between two values, which could correspond to two domain wall configurations.

The issue of the faceting of the interface has also been addressed in Ref. [72], where it is argued that it would only slightly shift the maximal critical current in the interference pattern with no hysteresis effect such that alone it cannot be responsible for the effects observed here.

### 3.4 Long Josephson junction solution

For completeness we address here a further interesting feature connected with a domain wall intersecting the interface. We have seen that the phase profile of the Josephson junction, \( \varphi_y \), is governed by the Sine-Gordon equation,

\[ \partial_y^2 \varphi_y = \frac{1}{\Lambda_y^2} \sin \varphi_y + \partial_y^2 \varphi^{(y)}. \]  

(3.35)

In the limit of \( \Lambda_y \) being much shorter than the extension of the junction the solution has a kink shape which is slightly modified by the last term of the right-hand side. It is clear that within the length scale...
of \( \Lambda_J \) from the domain wall, localized say at \( y_0 \), \( \varphi_y(y) \) approaches a constant value (sharp kink profile), such that we have the following boundary conditions: \( \varphi_y( y \ll y_0 - \Lambda_J ) = 0 \) and \( \varphi_y( y \gg y_0 + \Lambda_J ) = n2\pi \) (where \( n \) is a positive integer). As mentioned above the derivative \( \partial_y \varphi \) corresponds to a magnetic field localized at the line of intersection between the domain wall and the interface, i.e. the domain wall generates a well localized magnetic flux-line at the interface [61, 46]. The magnetic flux enclosed by the junction is simply given by,

\[
\Phi = \int_{-L/2}^{L/2} [A_y(+a, y) - A_y(-a, y)] dy \\
= \int_{-L/2}^{L/2} \frac{\Phi_0}{2\pi} \left[ \partial_y \varphi(y) - \partial_y \phi(\theta)(y) \right] dy \\
\approx \frac{\Phi_0}{2\pi n2\pi - \frac{\Phi_0}{2\pi} \Delta \phi_{\pm}},
\]

(3.36)

and the minimal possible fluxes are then given by,

\[
\Phi \approx -\frac{\Delta \phi_{\pm}}{2\pi} \Phi_0, \left( 1 - \frac{\Delta \phi_{\pm}}{2\pi} \right) \Phi_0.
\]

(3.37)

Since \( |\Delta \phi_{\pm}| \leq 2\pi \), those are fractional vortices which are generally a sign of broken time reversal symmetry [61, 67]. The detection of such well-localized fluxes could be used to detect the position of domain walls.

### 3.5 Conclusions

Motivated by the Josephson interferometry experiments on Josephson junctions between Sr\(_2\)RuO\(_4\) and the conventional superconductor Pb reported by of Kidwingira et al. [52], we studied the effect of domain walls on the Josephson interference effect in a magnetic field assuming that Sr\(_2\)RuO\(_4\) is a chiral \( p \)-wave superconductor. We also discussed the more recent experimental investigations on nano-scale Pb/Sr\(_2\)RuO\(_4\) Josephson junctions reported by Bahr in Ref. [60].

For this purpose we used the results of Chapter 2 that gives the stable and metastable domain wall structures obtained from the numerical minimization of the full Ginzburg-Landau free energy for Sr\(_2\)RuO\(_4\)—derived from the microscopic equations in the weak coupling and quasi-classical limits, see appendix 5.B. The anisotropy of the electronic band structure and the gap function—entered through the Fermi velocity harmonics—plays an important role, as it influences the global phase shift of the superconducting order parameter across a domain wall that separates domains of opposite chiralities. Furthermore, we found that the anisotropy also determines the energetically most favorable orientation of the domain wall. For realistic material parameters we found that the domain wall can be in two degenerated stable states with opposite phase shifts. We showed in the present chapter that if the
interface of a Josephson junction is intersected by domain walls, the domain wall phase shift and their respective locations are crucial for the Josephson effect in an external magnetic field. Furthermore, we argued that the interaction between the magnetic field and the domain walls at the interface lifts the degeneracy of the domain walls’ orientation, i.e. the domain wall orientation is polarized by strong enough external magnetic fields.

We summarize in the following the most important experimental features reported by Kidwingira et al [52] and Bahr [60] for which our theory gives a good qualitative explanation. (1) The interference pattern in a single junction deviates from the standard Fraunhofer pattern not only through irregularities, but also shows an asymmetry between positive and negative magnetic fields. In general the maximum critical current is shifted off the zero-field point. This can be attributed to the localized phase shifts of the superconducting order parameter introduced by domain walls intersecting the interface between Sr$_2$RuO$_4$ and Pb. (2) Kidwingira et al report a strong variability of the interference pattern between different samples. This may be explained by the fact that the samples were prepared in different ways, with possibly different normal vector directions and different degrees of faceting. Indeed, we have shown that a variation in the interface’s orientation can have a strong effect on the interference pattern. (3) Bahr has studied the effect of the size of the junction on the Josephson effect for Pb/Sr$_2$RuO$_4$ junctions. He shows a clear transition for the size $L = 2\mu m$ below which the junctions mainly appear Fraunhofer-like. We have compared our simulations for two and three domain walls with the measurements done by Bahr on a junction with the size $L = 4\mu m$ and found very good qualitative agreement. (4) Cycling the field continuously covering a positive and negative field range, a hysteretic behavior in the interference pattern appears. This can be understood in terms of the field-driven polarization of the domain walls. Indeed, we have shown that the anisotropy of the material induces the existence of two stable configurations corresponding to two inequivalent orientations of the domain wall. While the two domain wall orientations are degenerated in energy at zero field, the application of an external magnetic field lifts the degeneracy and the domain wall moves towards the most stable state leading to a change in the interference pattern. (5) A careful observation of the experimental data for the hysteresis effect shows that the maxima of the critical current at positive and negative fields are not symmetric. Taking the interface’s orientation into account we show that as its misalignment with the crystal axes increases so increases the asymmetry of the hysteretic pattern. (6) Finally, Kidwingira et al reports a specific noise effect observed in the voltage measurements as a function of time at driven currents slightly above the critical value (with jumps between mainly two constant values of the voltage). This can be well understood in terms of the jump of a domain wall between a stable and a metastable configuration.
Part II

Microscopic properties of domain walls in Sr$_2$RuO$_4$
Motivations for Part II

Up to now our analysis has been concerned with the study of the macroscopic structure of the domain walls as obtained from the Ginzburg-Landau theory. We found the following features: the existence of a spontaneous current flowing along the domain wall, the sign dependance of this current on the domain wall type ($\pi_{||}$- or $\pi_{\perp}$-domain wall), and the role of the electronic band structure of $\text{Sr}_2\text{RuO}_4$ as well as the gap function anisotropy in the determination of the most stable domain wall structure—i.e. the domain wall orientation and the global phase shift across it.

We want now to address the question of the microscopic origin of those features of the domain walls. This is the purpose of the second part of this thesis.

We start in Chapter 4 with the study of the Bogoliubov-de Gennes and Andreev equations from the point of view of symmetry and topology. There we discuss the implications of the charge-conjugation symmetry and the index theorem for the bound states present at topological defects (edge and domain wall). We then derive the domain wall spectrum from the analytical solution of the Andreev equation derived for two approximated (non-self-consistent) domain wall configurations: first assuming a sharp domain wall (with a step-like shape); then assuming a simple smooth ansatz of the gap function. On the one hand, we show that the quasi-classical limit can sometimes break the topology (depending on the domain wall configuration), leading to the necessity to treat the full quantum model. On the other hand, the domain wall energy obtained from the non-self-consistent solutions is not accurate and it is necessary to solve the full self-consistent problem in order to find the most stable domain wall configuration. This is the purpose of Chapter 5.

In Chapter 5 we overcome the limitation of the non-self-consistent approach in order to determine the most stable domain wall structure. Therein we give the numerical self-consistent solution of the quasi-classical Green’s function equations (Eilenberger-Riccati) for the problem of a domain wall in $\text{Sr}_2\text{RuO}_4$. We find a strikingly good qualitative agreement with the Ginzburg-Landau results. From this approach we can relate the features of the domain wall listed above to the chiral bound states localized at the domain wall. Furthermore we study the effect of a potential barrier at a domain wall and consider the transition from a domain wall to an edge (by increasing the potential barrier). This allows us to describe a smooth transition from the domain wall bound states to the well known chiral edge states. However, despite the good agreement of the self-consistent macroscopic structure of the domain wall with the Ginzburg-Landau findings, the topological pathology of the quasi-classical limit (mentioned above) leads to the missing of a fraction of the spectral weight of the domain wall bound states around the zero-energy level (i.e. at the Fermi level). This constitutes an explicit breaking of the topology since the bound states, that are predicted by the index theorem, are topologically protected. We note that this limitation of the quasi-classical limit had not been acknowledged in earlier works.

Chapter 6 is dedicated to the study the lattice Bogoliubov-de Gennes equations which overcome all the limitations of the quasi-classical approach: the anisotropy of the system enters naturally (the band structure is distinguished from the pairing anisotropy) and the topological structure of the domain wall problem is now always well defined. The lattice approach constitutes the full quantum version of the domain wall problem for $\text{Sr}_2\text{RuO}_4$ (at the mean-field and single-band level). We give the numerical self-consistent solution and show that it agrees strikingly well with the Ginzburg-Landau and the quasi-classical solutions regarding the macroscopic structure of the domain walls. We note that the chiral edge states and the domain wall bound states are treated on the same footing (the edge states are imposed by the finiteness of the system). This approach provides a full picture of the domain wall bound states. Moreover we report a new feature of the chiral edge states at $45^\circ$-rotated edges: we observe two extra zero-energy points within each chiral edge state branch at $k_y = \pm k_0 \neq 0$. Peculiarly, we give the electronic signature of the chiral edge states and domain wall bound states for the aligned-edge and rotated-edge geometries in $\text{Sr}_2\text{RuO}_4$ assuming the chiral $p$-wave state, hence providing a clear-cut frame for future STM experiments.
Chapter 4

Bogoliubov-de Gennes and Andreev equations

We derive the effective Andreev equation for an anisotropic system in the continuum limit. We also give the full Bogoliubov-de Gennes equation in the isotropic limit for the case of a domain wall configuration. We then introduce the quasi-classical Green’s function and the Eilenberger equation following the approach of Zaitsev.

We derive some general results concerning the solutions of the Andreev equation. We then review the topological properties of the full Bogoliubov-de Gennes equation following the approach of Volovik: Chern number, index theorem, Fermi points and zero-energy bound states.

We derive the explicit analytical solution (non-selfconsistent) of the Andreev equation assuming (i) a sharp domain wall (i.e. step-like gap function), and (ii) a simplified smooth ansatz of the gap function. From those we compute the spectrum and the spectral function of the Andreev bound states at a domain wall. We show that in general the Andreev spectrum breaks the topology of the full quantum model (through discontinuities in the bound state branches) leading to the necessity to go beyond the quasi-classical limit. We also discuss the Zaitsev versus the Blonder Tinkham Kapliwijk boundary conditions.

4.1 Introduction

Motivated by the results of the first part where we studied the macroscopic structure of the domain walls within the Ginzburg-Landau theory for Sr$_2$RuO$_4$ assuming the chiral $p$-wave state, we want now to address the question of their electronic structure. We adopt here the approach of the quasiparticle wave function obtained from the Andreev equation as opposed to the Green’s function approach which is the object of the next chapter.

In this chapter we concentrate ourself on the symmetry and the topological properties of the domain wall problem. This chapter can be seen as an introduction into the study of the microscopic structure of domain walls at the non-self-consistent level. It sets the conceptual framework that will be used in the following chapter where we present the numerical self-consistent solution of the quasi-classical Eilenberger equation. One of the main conclusions of this chapter is that the correct topology of the spectrum is in general broken in the quasi-classical limit such that we have to go beyond$^1$.

We mention the work by Samokhin [71] where the problem of a sharp domain wall from the Andreev equation is treated. However, neither the question of a good quantum number representation—i.e. the necessity to combine the two sectors, $k_x$ and $-k_x$, of the Andreev wave function—, nor the breaking of the topology in the quasi-classical limit were addressed.

$^1$This is done in the last chapter where we present the lattice approach of the domain wall problem.

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4.2 Effective Andreev equation

In this section we derive the effective Andreev equation in the continuous limit for an anisotropic system—that is taking the underlying lattice structure into account.

We have derived in the appendix 5.A the Gorkov equation for the chiral $p$-wave state in the Nambu representation,

$$[i \omega_m \mathbf{\hat{1}} - \mathbf{H}] G_{\uparrow \downarrow}(\mathbf{k}, \mathbf{r}, \omega_m) = \mathbf{\hat{1}} , \quad (4.1)$$

where $\mathbf{r}$ is the center of mass coordinate of a Cooper pair, and $\mathbf{k}$ is the Fourier coordinate conjugated to the relative coordinate $\mathbf{r}_1 - \mathbf{r}_2$. The Bogoliubov-de Gennes equation is given by the associated eigenvalue equation,

$$\begin{pmatrix} \hat{h}_c - \mu & \Delta [-i \nabla \mathbf{r}, \mathbf{r}] \\ \Delta^*[i \nabla \mathbf{r}, \mathbf{r}] & -\hat{h}_c^* + \mu \end{pmatrix} \psi_n(\mathbf{r}) = E_n \psi_n(\mathbf{r}) , \quad (4.2)$$

with the gap function (up to the first order in the gradient),

$$\Delta [-i \nabla \mathbf{r}, \mathbf{r}] = \frac{1}{2k_F} \left( [-i \nabla_x, \Delta_x(\mathbf{r})] + [-i \nabla_y, \Delta_y(\mathbf{r})] \right) , \quad (4.3)$$

and with the normal crystal Hamiltonian given by,

$$\hat{h}_c = \hat{h}_0 + U_c(\mathbf{\hat{r}}) , \quad (4.4)$$

$$\hat{h}_0 = \frac{1}{2m} \left( \nabla_{\mathbf{r}}(\mathbf{\hat{r}}) + \gamma \mathbf{A}(\mathbf{\hat{r}}) \right)^2 ,$$

with $U_c(\mathbf{r})$ the periodic lattice potential (we have set $\hbar \equiv 1$ and $\gamma = \hbar c/e$). Note that $\nabla_{\mathbf{r}} = -i \nabla$. This equation constitutes the full quantum model of the system in the continuous limit. Below we derive the effective Andreev equation taking the lattice anisotropy into account.

Let us write the eigenfunctions as the product,

$$\psi_n(\mathbf{r}) \to \psi^\uparrow_\mathbf{k}(\mathbf{r}) \psi^\downarrow_\mathbf{k}(\mathbf{r}) = \psi^\uparrow_\mathbf{k}(\mathbf{r}) \left( \begin{array}{c} u^\uparrow_\mathbf{k}(\mathbf{r}) \\ u^\downarrow_\mathbf{k}(\mathbf{r}) \end{array} \right) , \quad (4.5)$$

where $\psi^\uparrow_\mathbf{k}(\mathbf{r})$ is an eigenfunction of the normal Schrödinger equation, i.e.

$$\hat{h}_c[A = 0] \psi^\uparrow_\mathbf{k}(\mathbf{r}) = \left[ -\nabla_{\mathbf{r}}^2 + U_c(\mathbf{\hat{r}}) \right] \psi^\uparrow_\mathbf{k}(\mathbf{r}) = \epsilon(\mathbf{k}) \psi^\uparrow_\mathbf{k}(\mathbf{r}) , \quad (4.6)$$

where $\epsilon(\mathbf{k})$ is the electronic band energy. We have assumed that the vector potential corresponds to a spontaneous local magnetization generated by the inhomogeneity of the gap function, i.e. it is intrinsic to the superconducting phase and it doesn’t appear in this equation. From the Bloch’s theorem we can decompose the normal eigenfunction as $\psi^\uparrow_\mathbf{k}(\mathbf{r}) = e^{i \mathbf{k} \cdot \mathbf{r}} u^\uparrow_\mathbf{k}(\mathbf{r})$ and the band energy can be rewritten as,

$$\epsilon(\mathbf{k}) = \frac{1}{2m} \left( \mathbf{k}^2 - 2 i \mathbf{k} \cdot \frac{\nabla_{\mathbf{r}} u^\uparrow_\mathbf{k}(\mathbf{r})}{u^\uparrow_\mathbf{k}(\mathbf{r})} - \frac{\nabla_{\mathbf{r}}^2 u^\uparrow_\mathbf{k}(\mathbf{r})}{u^\uparrow_\mathbf{k}(\mathbf{r})} \right) . \quad (4.7)$$

Inserting the ansatz (4.5) in the BdG equation (4.2), we get the following effective BdG equation,

$$\begin{pmatrix} \xi_\mathbf{k} + \mathbf{v}(\mathbf{k}) \cdot (-i \nabla \mathbf{r} + \gamma \mathbf{A}) + \hat{h}_0 & \Delta[\mathbf{k}, \mathbf{r}, -i \nabla \mathbf{r}] \\ \Delta^*[\mathbf{k}, \mathbf{r}, -i \nabla \mathbf{r}] & -\xi_\mathbf{k} + \mathbf{v}(\mathbf{k}) \cdot (i \nabla \mathbf{r} + \gamma \mathbf{A}) - \hat{h}_0^* \end{pmatrix} \psi_\mathbf{k}(\mathbf{r}) = E_n(\mathbf{k}) \psi_\mathbf{k}(\mathbf{r}) , \quad (4.8)$$

where $\xi_\mathbf{k} = \epsilon(\mathbf{k}) - \mu$, $\hat{h}_0 = \hat{h}_c[U_c = 0]$, and the velocity is given by,

$$\mathbf{v}(\mathbf{k}) = \frac{1}{m} \frac{i \nabla_{\mathbf{r}} u^\uparrow_\mathbf{k}(\mathbf{r})}{u^\uparrow_\mathbf{k}(\mathbf{r})} = \frac{\mathbf{k}}{m} - \frac{i}{m} \frac{\nabla_{\mathbf{r}} u^\uparrow_\mathbf{k}(\mathbf{r})}{u^\uparrow_\mathbf{k}(\mathbf{r})} = \frac{\partial \epsilon(\mathbf{k})}{\partial \mathbf{k}} . \quad (4.9)$$
The gap function is now given by\(^2\),

\[
\Delta[k, r, -i\nabla r] = \frac{1}{k_F} \left[ m v(k) \cdot \Delta(r) - i \left( \frac{1}{2} \nabla r \cdot \Delta(r) + \Delta(r) \cdot \nabla r \right) \right]. \tag{4.10}
\]

Restricting to the states at the Fermi level, i.e. \(|k| = k_F\), and assuming that the typical length scale of the spatial variations, \(\xi\), is very large compared to the lattice spacing \(1/k_F\), i.e.

\[
\left| \frac{\nabla^2 \psi^n_k(r)}{k_F \cdot \nabla r \psi^n_k(r)} \right| \sim \frac{1}{(k_F \cdot \hat{n}) \xi} \sim \frac{1}{k_F \xi} \ll 1, \tag{4.11}
\]

we neglect all the terms of the order of \((k_F \xi)^{-n}\) for \(n \geq 1\) (Andreev approximation) and we get the Andreev equation,

\[
\begin{pmatrix}
-iv(k_F) \cdot \nabla r + \gamma v(k_F) \cdot A \\ \Delta^\prime(k_F, r)
\end{pmatrix}
\begin{pmatrix}
\Delta(k_F, r) \\
iv(k_F) \cdot \nabla r + \gamma v(k_F) \cdot A
\end{pmatrix}
\psi^n_k(r) = E_n(k_F) \psi^n_k(r). \tag{4.12}
\]

We can interpret it as the linear expansion of the Bogoliubov-de Gennes equation around the bulk Fermi point \(k_F\). We note that the condition (4.11) for the Andreev approximation is violated for the trajectories with \(k_F \cdot \hat{n} \rightarrow 0\). As we will see this leads to an important limitation of the quasi-classical limit since the Andreev equation is pathological as the coefficient \(|v(k_F) \cdot \hat{n}|^{-1}\) becomes singular.

### 4.3 Good quantum number

Let us assume that the system is inhomogeneous along the \(x\)-direction and translationally invariant along the \(y\)-direction. In the following we will choose for the vector potential the following gauge \(A = (0, A_y(x))\). In this geometry only \(k_0\) is a good quantum number for the full quantum BdG model Eq. (4.2). We then see that the effective BdG equation Eq. (4.8), which is defined for the full wave vector \(k\), doesn’t have the same structure. In the following we derive the relationship between the spectrum of the two models.

Since in this chapter we will be mainly interested in the topological properties of the domain wall problem it is sufficient to consider the isotropic limit. Indeed, we can think of the anisotropic system as being obtained from the isotropic model after switching on the crystal potential \(U_c\) adiabatically such that we do not close the bulk gap of the system, hence preserving the topological structure of the problem.

Taking the limit of a vanishing crystal potential, i.e. \(U_c(x) = 0\), the Bloch wave-functions are simply given by plane-waves. Since the problem is translationally invariant in the \(y\)-direction we can expand the wave function as \(\Psi_n(r) = \sum_{k_y} e^{ik_y x} \psi^n_{k_y}(x)\), which leads to the equation,

\[
\mathcal{H}_{BdG}^{BdG} \Psi^n_{k_y}(x) = E_n(k_y) \Psi^n_{k_y}(x), \tag{4.13}
\]

with the full Bogoliubov-de Gennes Hamiltonian now given by,

\[
\mathcal{H}_{BdG}^{BdG} = \left( \frac{k_y^2 + \gamma^2 A_y^2(x)}{2m} - \mu - \frac{\partial_x^2}{2m} \right) \hat{\sigma}_3 + \frac{k_y}{m} \gamma A_y(x) \hat{\sigma}_1
\]

\[
+ \left( -i \frac{1}{2k_F} (\partial_x \Re \Delta_x) - i \frac{1}{k_F} \Im \Delta_x \partial_x + \frac{k_y}{k_F} \Im \Delta_y \right) \hat{\sigma}_1
\]

\[
- \left( -i \frac{1}{2k_F} (\partial_x \Im \Delta_x) - i \frac{1}{k_F} \Im \Delta_x \partial_x + \frac{k_y}{k_F} \Re \Delta_y \right) \hat{\sigma}_2. \tag{4.14}
\]

Introducing the expansion \(\psi^n_{k_y}(x) = \sum_{k_x} c_{k_x} e^{i k_x x} \psi^n_{k_x}(x)\), we find,

\[
\mathcal{H}_{BdG}^{BdG} \Psi^n_{k_y}(x) = \sum_{k_x} c_{k_x} e^{i k_x x} \mathcal{H}_{BdG}^{BdG} \psi^n_{k_x}(x), \tag{4.15}
\]

\(^2\)Note that

\[
\Delta^\dagger[k, r, -i\nabla r] = \frac{1}{k_F} \left[ m v(k) \cdot \Delta^\ast(r) - i \left( \frac{1}{2} \nabla r \cdot \Delta^\ast(r) + \Delta^\ast(r) \cdot \nabla r \right) \right],
\]

where we have used \(\nabla_F^2 = -\nabla r\).
with the effective Bogoliubov-de Gennes Hamiltonian,

\[ \hat{\mathcal{H}}_{\text{BdG}}^{\theta} = \left( \frac{k_x^2 + k_y^2 + \gamma^2 \Delta_y^2}{2m} - \mu - \frac{i k_x}{m} \partial_x - \frac{\partial_y^2}{2m} \right) \sigma_3 + \frac{k_y}{m} \gamma \Delta_y(x) \hat{1} \]

\[ + \frac{1}{k_F} \Re \Delta_x + \frac{k_y}{k_F} \Im \Delta_y - \frac{i}{2k_F} (\partial_x \Re \Delta_x) - \frac{i}{k_F} \Im \Delta_x \partial_x \right) \sigma_1 \]

\[ - \frac{1}{k_F} \Im \Delta_x \partial_x + \frac{k_y}{k_F} \Im \Delta_y - \frac{i}{2k_F} (\partial_x \Im \Delta_x) - \frac{i}{k_F} \Im \Delta_x \partial_x \right) \sigma_2 . \] (4.16)

Let us fix now \( k_y = k_{F,y} \). We introduce the polar coordinates \( k_F = k_F(\cos \theta_k, \sin \theta_k) \) and define \( \theta_y = \arcsin(k_y/k_F) \). We now approximate the BdG equation as the following,

\[ \mathcal{H}_{\theta_k}^{\text{BdG}} \psi_{\theta_k}^n(x) \approx c_{\theta_k} e^{ik_F \cos \theta_k x} \mathcal{H}_{\theta_k}^{\text{BdG}} \psi_{\theta_k}^n(x) + c_{\pi-\theta_k} e^{-ik_F \cos \theta_k x} \mathcal{H}_{\pi-\theta_k}^{\text{BdG}} \psi_{\pi-\theta_k}^n(x) , \]

\[ \approx c_{\theta_k} e^{ik_F \cos \theta_k x} \mathcal{H}_{\theta_k}^{A} \tilde{\psi}_{\theta_k}^n(x) + c_{\pi-\theta_k} e^{-ik_F \cos \theta_k x} \mathcal{H}_{\pi-\theta_k}^{A} \tilde{\psi}_{\pi-\theta_k}^n(x) , \] (4.17)

where the Andreev Hamiltonian is now given by,

\[ \mathcal{H}_{\theta_k}^{A} = -iv_F \cos \theta_k \partial_x \sigma_3 + v_F \sin \theta_k \gamma \Delta_y(x) \hat{1} + [\cos \theta_k \Re \Delta_x(x) + \sin \theta_k \Im \Delta_y(x)] \sigma_1 \]

\[ - [\cos \theta_k \Im \Delta_x(x) + \sin \theta_k \Re \Delta_y(x)] \sigma_2 , \] (4.18)

which was obtained after taking the quasi-classical limit, i.e. assuming \( a \equiv k_F \xi \gg 1 \). We note that since \( \max \Delta_y \sim H_{c2} \xi, \) and \( H_{c2} \sim (\gamma \xi^2)^{-1} \), we have \( \gamma^2 \Delta_y^2 \sim k_F \gamma \Delta_y \left( \gamma H_{c2} \xi/k_F \right) \sim k_F \gamma \Delta_y a^{-1} \ll a \). We also see that for this geometry the Andreev equation has singular coefficients for the directions \( \theta_k = \pm \pi/2 \).

The Andreev equation for the bound states reads,

\[ \mathcal{H}_{\theta_k}^{A} \tilde{\psi}_{\theta_k}^n(x) = \tilde{E}_b(\theta_k) \tilde{\psi}_{\theta_k}^n(x) , \] (4.19)

from which we eventually find,

\[ E_b(\theta_y) \approx \sum_{\theta_1, \theta_2} \tilde{E}_b(\theta_1) c_{\theta_2}^* c_{\theta_1} f_{\theta_1, \theta_2}^b , \]

(4.20)

where \( \theta_1, \theta_2 \in \{ \theta_k, \pi - \theta_k \} \), and with

\[ f_{\theta_1, \theta_2}^b = \int_{-\infty}^{\infty} dx \ e^{ik_F(\cos \theta_1 - \cos \theta_2)x} \left( \tilde{\psi}_{\theta_2}^b(x) \right) \dagger \tilde{\psi}_{\theta_1}^b(x) . \] (4.21)

While the expression of the spectrum Eq. (4.20) conserves the symmetry structure of the original full quantum model, i.e. the BdG equation (4.15), it is only valid as long as the quasi-classical limit doesn’t break down. We will see that the singularity points of the Andreev equation lead to discontinuities in the Andreev spectrum which in turn can lead to the breaking of the topology of the full quantum problem.

### 4.3.1 Quasi-classical Green’s function and Eilenberger equation

We derive here the quasi-classical Green’s function and the Gorkov equations in the quasi-classical limit (Eilenberger equations) following Zaitsev [85]. We start from the general equation,

\[ \left[ i \omega_n \hat{1} - \mathcal{H}_{\theta_k}^{\text{BdG}}(x) \right] G(x, x', k_y, \omega_m) = \delta(x - x') \hat{1} . \] (4.22)

obtained after Fourier transforming the Green’s function \( G(x, x', \omega_m) \) in \( y - y' \rightarrow k_y \). Let us decompose the full Green’s function in terms of the sum,

\[ G(x, x', k_y, \omega_m) \approx e^{i k_y (x-x')} G_a(x, x', k(\theta_k), \omega_m) + e^{-i k_y (x-x')} G_b(x, x', k(\pi - \theta_k), \omega_m) , \]

\[ + e^{i k_y (x+x')} G_a(x, x', k(\theta_k), \omega_m) + e^{-i k_y (x+x')} G_b(x, x', k(\pi - \theta_k), \omega_m) , \] (4.23)
where \( k(\theta_k) = (k_x, k_y) \) and \( k(\pi - \theta_k) = (-k_x, k_y) \). In the following we will neglect the terms \( G_b(x, x', k, \omega_m) \) that account for the interference between right and left moving quasiparticles. For \( x \neq x' \), the general Green’s function equation reduces to,

\[
[i \omega_m \bar{1} - \mathcal{H}_{BG}^k(x)] G_a(x, x', k, \omega_m) = 0 ,
\]

and from the connection conditions of the full Green’s function for \( x' \rightarrow x \pm 0 \), see [85], we find,

\[
(1 + \partial_x) [G_a(x + 0, x, k, \omega_m) - G_a(x - 0, x, k, \omega_m)] = -\frac{m}{ik_x} .
\]

In the following we make the approximation, \( G_a(x, x', k, \omega_m) \rightarrow \bar{G}(x, x', k_F, \omega_m) \), where the new function satisfies the Green’s function equation,

\[
[i \omega_m \bar{1} - \mathcal{H}_{BG}^k(x)] \bar{G}(x, x', k_F, \omega_m) = 0 ,
\]

where we have taken the quasi-classical limit (i.e. assuming \( k_F \xi \gg 1 \)). The connection relation is now,

\[
\bar{G}(x + 0, x, k_F, \omega_m) - \bar{G}(x - 0, x, k_F, \omega_m) = -\frac{1}{2iv_F} ,
\]

where we have neglected the terms \( \partial_x \bar{G} \), since in the quasi-classical limit we have \( |\xi^{-1} \partial_\xi \bar{G}| \ll |k_x \bar{G}| \).

Obviously when \( k_x \rightarrow 0 \) this condition is violated, and so is the validity of the relation (4.27).

Still following Ref. [85], we construct a function that is continuous at the point \( x = x' \),

\[
g(x, x', \theta_k, \omega_m) = \text{sign}[v_x(\theta_k)] (2iv_x(\theta_k)\bar{G}(x, x', k_F, \omega_m) - \text{sign}[x - x']) ,
\]

i.e. \( \lim_{x' \rightarrow x} g(x, x', \theta_k, \omega_m) = g(x, \theta_k, \omega_m) \). We can show that this function satisfies the following equation,

\[
v_x(\theta_k) \partial_x g(x, \theta_k, \omega_m) = \left[(i \omega_m + \gamma v_y A_y)\bar{1} + \Delta_1 \sigma_1 - \Delta_2 \sigma_2, g(x, \theta_k, \omega_m)\right] ,
\]

where we have decomposed the gap function into its real and imaginary parts, \( \Delta = \Delta_1 + i \Delta_2 \). This is the Eilenberger equation for the quasi-classical Green’s function \( g(x, \theta_k, \omega_m) \).

We finally have that in the quasi-classical limit the full Green’s function is approximated by,

\[
\lim_{x' \rightarrow x} G(x, x', k_F, \omega_m) \approx \frac{1}{2iv_F} [g(x, \theta_k, \omega_m) + g(x, \pi - \theta_k, \omega_m)] .
\]

In the following we use the fact that the spectrum of the bound states is given by the poles of this expression.

**Zaitsev and BTK boundary conditions**

In Ref. [85] Zaitsev derives the boundary conditions in the quasi-classical limit for the Green’s function \( \bar{G} \) defined above. This is a valid approximation only if the Andreev approximation \( (k_F \xi \gg 1) \) is valid in the relevant region of the spectrum. Hence whenever \( k_x \rightarrow 0 \) we should not expect those boundary conditions to be reliable. In Ref. [97] Blonder Tinkham and Klapwijk (BTK) introduce the boundary conditions for the BdG wave function (which is nothing but the continuity condition for the total wave function of the problem). While it is not restricted to the quasi-classical limit and is then more general than the Zaitsev boundary conditions, it necessitates the analytical expression of the solution to the full BdG equation. Unfortunately this is not known in general.

In the sections 4.6 and 4.7 we solve two simplified versions (non-self-consistent) of the domain wall problem from the Andreev equation and we discuss the limitation of the quasi-classical limit and the use of the Zaitsev and BTK boundary conditions when we only know the analytical expression of the Andreev solutions.

### 4.4 Symmetries of the Andreev equation

We present in this section some general results concerning the structure of the solutions to the Andreev equation. We show that the charge-conjugation symmetry of the Andreev spectrum is sufficient (together with specular boundary condition) to find the position of the zero-energy chiral edge states, whereas the knowledge of the topological structure of the full BdG equation is necessary in order to prove the existence of zero-energy bound states on a domain wall (this is the topic of the next section).
Domain wall Hamiltonian

The Andreev equation with an edge or a domain wall at \( x = 0 \) can be written as (see section 4.2 for a derivation),

\[
\mathcal{H}^A[-i\partial_x, \theta_k, x] \psi^n_{\theta_k}(x) = E_n(\theta_k) \psi^n_{\theta_k}(x),
\]

with

\[
\mathcal{H}^A[-i\partial_x, \theta_k, x] = \left[ -iv_x(\theta_k)\partial_x \sigma_3 + \gamma v_y(\theta_k)A_y(x)\hat{1} + \Delta_1(\theta_k, x)\sigma_1 - \Delta_2(\theta_k, x)\sigma_2 \right],
\]

and

\[
\psi^n_{\theta_k}(x) = \left( \begin{array}{c} u^n_{\theta_k}(x) \\ v^n_{\theta_k}(x) \end{array} \right),
\]

where \( \theta_k \) refers to one point of the Fermi surface \( (\theta_k = \arctan k_{F_y}/k_{F_x}) \), and the real and imaginary parts of the gap function, \( \Delta(\theta_k, x) = \phi(\theta_k) \cdot \Delta(x) \), are in general given by

\[
\begin{cases}
\Delta_1(\theta_k, x) = \phi_x(\theta_k)\Re \Delta_x(x) + \phi_y(\theta_k)\Re \Delta_y(x), \\
\Delta_2(\theta_k, x) = \phi_x(\theta_k)\Im \Delta_x(x) + \phi_y(\theta_k)\Im \Delta_y(x).
\end{cases}
\]

The domain wall is characterized by the following gap function’s structure, where \( s = 1 \) corresponds to the \( \pi_\parallel \)-domain wall and \( s = -1 \) to the \( \pi_\perp \)-domain wall (see chapter 2 for a definition),

\[
\begin{cases}
\Delta_1(\theta_k, -\infty) = s\Delta_1(\theta_k, +\infty), \\
\Delta_2(\theta_k, -\infty) = -s\Delta_2(\theta_k, +\infty),
\end{cases}
\]

such that if \( s = 1 : \Delta_2(\theta_k, 0) = 0 \); else if \( s = -1 : \Delta_1(\theta_k, 0) = 0 \).

Furthermore we introduce the following parametrization of the gap function far from the domain wall,

\[
\begin{cases}
\Delta_1(\theta_k, x \to \pm \infty) = s_1 \left( \phi_x(\theta_k)\cos \frac{\alpha}{2} - \phi_y(\theta_k)\sin \frac{\alpha}{2} \right), \\
\Delta_2(\theta_k, x \to \infty) = s_2 \left( \phi_x(\theta_k)\sin \frac{\alpha}{2} + \phi_y(\theta_k)\cos \frac{\alpha}{2} \right),
\end{cases}
\]

where \( s_1 = (\pm 1)^j \) and \( s_2 = (\pm 1)^{j+1} \) with \( j = (3 + s)/2 \), such that

\[
\alpha = 0 \Rightarrow \begin{cases}
\Delta_1 = \Delta_x \\
\Delta_2 = \Delta_y.
\end{cases}
\]

Symmetries

We start by noting that for each given energy \( E_n(\theta_k) \), the Andreev equation has at most two orthogonal eigenfunctions, \( \{ \psi^n_{\theta_k}(x), \psi^n_{\theta_k}(x) \} \). It is then easy to show that

\[
\partial_x \left[ u^n_{\theta_k}(x)\psi^n_{\theta_k}(x) - v^n_{\theta_k}(x)u^n_{\theta_k}(x) \right] = 0.
\]

An important property of the Andreev equation for the chiral \( p \)-wave state is the charge-conjugation symmetry\(^3\). If \( \psi^n_{\theta_k}(x) \) is an eigenstate with the energy \( E_n(\theta_k) \), then the state \( \psi^n_{\theta_k, \pi}(x) = \psi^{\pi n}_{\theta_k, \pi}(x) \) is also an eigenstate with the energy \( E_{\pi n}(\theta_k) = -E_n(\theta_k \pm \pi) \). This symmetry of the spectrum is illustrated in Fig. 4.1.

---

\(^3\)We note the following other generic feature of the Andreev equation. If \( \psi^n_{\theta_k} = (u^n_{\theta_k}, v^n_{\theta_k}) \) is an eigenstate with the energy \( E_n(\theta_k) \), then the state \( \psi^n_{\theta_{k, \pi}} = (u^n_{\theta_k}, v^n_{\theta_k})^{\ast} \) is also an eigenstate with the same energy, \( E_{\pi n}(\theta_k) = E_n(\theta_k) \). We will show below that the bound states are not degenerated, from which it follows that the two wave functions represent the same state, i.e. \( \psi^n_{\theta_k} \sim \psi^n_{\theta_{k, \pi}} \). On the other hand, the scattering states can be degenerated such that the state \( \tilde{n}_1 \) can be different than \( n_1 \).
Bound states

In inhomogeneous systems the Andreev equation can have bound state solutions. Their energy is smaller than the bulk gap and they are localized at the spatial defects (edge, domain wall, vortex), i.e.

$$|E_b(\theta_k)| < |\Delta(\theta_k, \text{bulk})|, \quad b = 1, \ldots, N_b,$$

(4.39)

where $N_b$ is the number of bound states at a given $\theta_k$. The localization of the bound states means that they vanish as we move away from the defect, i.e. $\psi^{b_i}_{\theta_k}(x \to \pm \infty) = 0$.

Using the relation (4.38) we can show that the bound states are never degenerate, i.e.

$$E_b(\theta_k) = E_b(\theta_k) \Rightarrow \psi^{b_i'}_{\theta_k}(x) \propto \psi^{b_j}_{\theta_k}(x),$$

(4.42)

and there is only one eigenstate $\psi^{b_i}_{\theta_k}(x)$ for a given bound state energy $E_b(\theta_k)$.

The spectrum of the bound state $b$ crosses the Fermi level if it is continuous and

$$E_b(\theta_k)E_b(\theta_k \pm \pi) < 0.$$  

(4.43)

The charge-conjugation symmetry tells us that if there is one bound state $\psi^{b_i}_{\theta_k}$ with the energy $E_b(\theta_k)$, then there must be one bound state $\psi^{b_j}_{\theta_k}$ with the energy $E_b(\theta_k) = -E_b(\theta_k \pm \pi)$. We stress the fact that up to this point, even if we can assume the existence of bound states (due to the inhomogeneity of the gap function), we cannot predict the existence of zero-energy bound states—see for instance the spectrum plotted on Fig. 4.1.

---

4The following demonstration for the Andreev equation is taken from [89]. Let us assume that there are two orthogonal eigenstates $\{\psi^{b_1}_{\theta_k}(x), \psi^{b_2}_{\theta_k}(x)\}$ for the bound state energy $E_b(\theta_k)$. From equation (4.38) and using the fact that the bound states decay to zero far from the defect, we can write $\psi^{b_2}_{\theta_k}(x) = f(x)\psi^{b_1}_{\theta_k}(x)$, with $f(x) \in \mathbb{C}$. Taking the difference $\mathcal{H}^{\theta_k}\psi^{b_2}_{\theta_k}(x) - \mathcal{H}^{\theta_k}f(x)\psi^{b_1}_{\theta_k}(x) = 0$ we find, $\partial_x f(x) = 0$, thus $\psi^{b_1} = \psi^{b_2}$ and they represent the same state. We note that this argument is specific to the Andreev model!

Let us consider now the effective BdG equation (4.16). With the second order derivative $\partial_x^2$ we find the following equation for the function $f$,

$$\partial_x^2 f(x)u_1(x)v_1(x) + (1 + 2imv_\pi)\partial_x f(x)\partial_x [u_1(x)\partial_x v_1(x)] = 0,$$

(4.40)

which gives

$$f(x) = C_2 + C_1 \int_{-\infty}^{x} e^{-(1 + 2imv_\pi)y}u_1(y)\partial_x v_1(y) dy.$$

(4.41)

Now since $\psi^{b_1} \sim \exp(-|x|^\beta) \to 0$ for $x \to \pm \infty$, we have $C_1 = 0$, such that the bound state solutions of the BdG equation at a given $\theta_k$ are also non-degenerate.
Let us assume that we have the extra symmetry $E_b(\theta_k \pm \pi) = -E_b(\theta_k)$, which means that $E_{b'}(\theta_k) = E_b(\theta_k)$. Then, because of the non-degeneracy of the bound states, the states $\{b, b'\}$ have to be the same. If the spectrum of the bound state $-E_b(\theta_k)$ for $\theta_k \in (-\pi, \pi)$ is a continuous function of $\theta_k$, it has to cross the Fermi level and we have a zero energy state. However we will see that at the singularity points of the Andreev equation (for the coefficient $1/v_y$), there are discontinuities in the spectrum of the bound states such that in general we cannot conclude to the existence of zero-energy bound states.

An other way to go is to make use of the index theorem which relates the number of zero-energy bound states to the Chern number of the system in the different bulk regions. This is the topic of the section 4.5.

### 4.4.1 Chiral edge states

We discuss here the special case of the bound states present at the edges and for which the quasi-classical limit works well since—as we will show in the section 4.6—the relevant part of the spectrum lies outside the singularity points, i.e. $\sigma_{\text{edge}}(\mathcal{H}_b) \approx \{E_b(\theta_k)| -\pi/2 < \theta_k < \pi/2\}$. We show that their eigenvalue branches cross the Fermi level at $\theta_k \mod \pi = 0$.

The edge is characterized by the following structure of the gap function,

\[
\begin{cases}
\Delta(\theta_k, x < 0) & \neq 0, \\
\Delta(\theta_k, x > 0) & = 0.
\end{cases}
\]  

(4.44)

In the case of an edge between the bulk and the vacuum—anticipating the results of the next section—the index theorem tells us that there is only one bound state branch crossing the Fermi level and connecting continuously the lower eigenvalue continuum to the upper continuum. We call it the chiral edge state. From the charge-conjugation symmetry discussed above we know that for each bound state with the energy $E_b(\theta_k)$ there is another one with the energy $E_{b'}(\theta_k) = -E_b(\theta_k + \pi)$. The index theorem tells us that they have to be the same, such that $E_{b'}(\theta_k) = E_b(\theta_k)$. Therefore we find,

\[E_b(\theta_k \pm \pi) = -E_b(\theta_k).\]

(4.45)

We stress the fact that this result comes from the combination of the charge-conjugation symmetry of the system and the index theorem telling us the number of edge states crossing the Fermi level and connecting the negative part of the spectrum to the positive part.

Let us now consider the location $(\theta_k)$ of the zero energy edge state. For this we assume specular reflection at the surface, i.e. the states $\psi^b_{\theta_k}$ and $\psi^b_{\theta_k-\pi}$ are connected by reflection, such that

\[E_b(\pi - \theta_k) = E_b(\theta_k),\]

(4.46)

where $\theta_k$ is the angle with respect to the surface normal vector $n = (1, 0, 0)$. We then find that for quasiparticles moving perpendicularly to the surface, i.e. $\theta_k = 0$, together with equation (4.45), we have

\[E_b(0) = E_b(\pi) = -E_b(0) \Rightarrow E_b(0) = 0!\]

(4.47)

i.e. there is a single chiral edge branch crossing the zero energy line at $\theta_k = 0$, that is far from the singularity points $\pm \pi/2$. This result is general and holds for the full quantum model of the system Eq. (4.15).

### 4.5 Topology

As it has been mentioned in the introduction, the chiral $p$-wave state is a topological superconductor for which we can define a $\mathbb{Z}$ topological invariant associated to the bulk of the material. Then we can use an index theorem in order to predict the existence of bound states at the topological defects, i.e. in the regions where there is a jump between different values of the bulk topological invariant (for instance, edges and domain walls). In this section we briefly review the main concepts and results from this topological point of view. As pointed above, it is enough to consider the isotropic model since we can think of the anisotropic system as obtained through the adiabatic switching on of the periodic crystal field in such a way that we do not change the topology of the problem (that is without closing the bulk gap). Here we only consider the full quantum Bogoliubov-de Gennes model, $\mathcal{H}_{k_y}$, given in Eq. (4.15).
We will show in the next sections that the quasi-classical Andreev model, $H_{dG}$, given in Eq. (4.18), in general doesn’t conserve the topology of the problem and it is not a good starting point for studying the topology.

**Bulk Chern number**

Taking the limit $x \to \pm \infty$ we find the bulk Hamiltonian through the transformation,

$$e^{-i k_x x} H_{dG}^{BdG} (x \to \pm \infty) e^{i k_x x} = \left( \frac{k_x^2 + k_y^2}{2m} - \mu - i \frac{k_x}{m} \sigma_x - \frac{\partial \varphi_x}{2m} \right) \hat{\sigma}_3 + \left( \frac{k_x}{k_F} \hat{n} \Delta_x + \frac{k_y}{k_F} \hat{n} \Delta_y - i \frac{1}{k_F} \hat{n} \Delta_x \sigma_x \right) \hat{\sigma}_1 - \left( \frac{k_x}{k_F} \hat{n} \Delta_x + \frac{k_y}{k_F} \Delta_y - i \hat{n} \Delta_x \sigma_x \right) \hat{\sigma}_2 . \quad (4.48)$$

Neglecting all the gradient terms and using the parameterization of Eq. (4.36), the bulk Hamiltonian can be rewritten as,

$$
\begin{aligned}
H_{\text{bulk}}^{BdG} (k) &= m(k) \cdot \hat{\sigma}, \\
m(k) &= \left( s_1 \frac{k}{k_F} \cos(\theta_k + \alpha/2) \Delta_0 , - s_2 \frac{k}{k_F} \sin(\theta_k + \alpha/2) \Delta_0 , \left( \frac{k^2}{2m} - \mu \right) \right),
\end{aligned} \quad (4.49)
$$

where we have used the polar coordinates $(\theta_k, \alpha)$, defined through $k = \hat{k} k$ and $\hat{k} = (\cos \theta_k, \sin \theta_k)$.

The unit vector $\hat{m} = m/m$ can be seen as a mapping from the stereographic projection of the unit sphere in the reciprocal space, $(k_x, k_y) \in \mathbb{R}^2 \cup \{\infty\} \simeq S^2$, to the unit sphere in the Hilbert space, i.e.

$$\bigcup_{k \in \mathbb{R}^2 \cup \{\infty\}} \hat{m}(k) \simeq S^2 . \quad (4.50)$$

In general the topology of the ground state can be characterized by the winding number of this mapping,

$$C = \frac{1}{4\pi} \int_0^{+\infty} dk \int_0^{2\pi} d\theta_k \hat{m} \cdot \left( \frac{\partial \hat{m}}{\partial k} \times \frac{\partial \hat{m}}{\partial \theta_k} \right) . \quad (4.51)$$

We are only interested in the case $\mu > 0$ for which we find,

$$C = s_1 s_2 1 . \quad (4.52)$$

Note that it doesn’t depend on $\alpha$. For a $\pi_f$-domain wall ($s = 1 \Rightarrow s_1 = 1$) we get $C = s_2 1$, where $s_2$ gives the chirality of the bulk (i.e. $s_2 = L_z/L = \pm 1$).

The number $|C|$ computes the degree of covering of the origin $O = (0, 0, 0)$ (in the $m$-space) by the surface $\bigcup_{k \in \mathbb{R}^2 \cup \{\infty\}} \hat{m}(k)$, see for instance [109]. We plot on Fig. 4.2 the surface defined by the vectors $\hat{m}$ for the parameters’ range $(\theta_k, k) \in (0, 1.5\pi] \cup [0, 4k_F]$. The origin is represented by the black point. When the parameters run over the whole range $(k, \theta_k) \in (0, 2\pi]\cup[0, \infty]$, the surface $\bigcup_{k \in \mathbb{R}^2 \cup \{\infty\}} \hat{m}(k)$ covers the origin with the degree one.\(^5\)

**Bulk-edge correspondence**

We briefly review in this section different approaches for the proof of the bulk-edge correspondence in the continuous limit and discuss their limitation with regard to our problem.

We start with the approach of Volovik [95] and Gurarie [96]. We argue that their result is limited to the validity of the quasi-classical limit and hence is not general enough for the case of domain walls in the chiral $p$-wave state.

\(^5\)We note that, strictly speaking, the Hamiltonian discussed by Volovik in Ref. [24] doesn’t satisfies the topological results presented in the paper. Volovik discuss the case of a $d + id$ superconductor, with the gap $\Delta_1/\Delta_0 = \cos \theta_k^2 - \sin \theta_k^2$ and $\Delta_2/\Delta_0 = 2 \cos \theta_k \sin \theta_k$, and the dispersion relation $\epsilon(k) = k^2/2m - \mu$, i.e. the components of the gap function are normalized: instead of $k/k_F$, Volovik takes $\kappa/|k|$. It is then obvious that the mapping $m(k)$ doesn’t cover the origin since at $k = 0$ we find that $\bigcup_{\theta_k \in (0,2\pi]} m(\theta_k, k = 0)$ is the unit circle contained in the plane $m_x = -\mu$ (i.e. it is open instead of closing to a point). Nevertheless, the Hamiltonians discussed by Volovik in Ref. [95] are defined in the correct way.
Figure 4.2: Covering of the origin by the surface $\bigcup_{k \in A} \mathbf{m}(k)$ for $(\theta_k, k) \in A = (0, 1.5\pi] \cup [0, 4k_F]$. The covering is complete and of degree one for $(\theta_k, k) \in (0, 2\pi] \cup [0, +\infty]$.

Due to the translational invariance along the $y$-direction, $k_y$ is a good quantum number and we have seen in the section 4.3.1 that the Green’s function of the system $G(x, x', k_y, \omega_m)$ satisfies Eq. (4.22) with the Hamiltonian $H_{BdG}^{k_y}$ given on Eq. (4.15). In the following we write $G^{-1}(x, x', k_y, \omega_m)$ for the inverse of the Green’s function. Volovik showed that the spectral flow of the system can be expressed through the following topological invariant,

$$N_1(k_y) = \text{tr} \int dx \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi i} G^{-1}(x, k_y, \omega) \partial_\omega G(x, k_y, \omega),$$

(4.53)

where we have taken the limit $x' \to x$. Indeed, writing the eigenvalues of the Green’s function as $\lambda_b(\omega, k_y) = [i\omega - E_b(k_y)]^{-1}$, we find

$$N_1(k_y) = \int \frac{d\omega}{2\pi i} \partial_\omega \int dx \text{ tr } \log G(x, k_y, \omega) = \int \frac{d\omega}{2\pi i} \partial_\omega \log \det_{k_y} G(x, k_y, \omega),$$

$$= \sum_b \int \frac{d\omega}{2\pi i} \partial_\omega \log \lambda_b(\omega, k_y),$$

$$= \frac{1}{2} \sum_b \text{sign}[E_b(k_y)],$$

(4.54)

where $E_b(k_y)$ are the poles of the Green’s function at $\omega = 0$. Assuming that the bound state spectrum can be expanded as $E_b(k_y) \sim c_0(k_y - k_0)$ in the vicinity of a zero-energy point $k_0$, i.e. in the limit $k_y \to k_0$, we find that the spectral flow is given by the difference,

$$N_1(k_y \to +\infty) - N_1(k_y \to -\infty) = \sum_b \text{sign}[c_b] \equiv \nu_\sigma.$$

(4.55)

The spectral flow $\nu_\sigma$ is defined as the number of bound state branches that cross the gap and connects continuously the lower eigenvalue continuum to the upper continuum.

---

6The velocity $c_0$ can always be made non-zero by adiabatically tuning $\mu$. 

60
Introducing the Wigner transform of the Green’s function, we now have

\[ N_1(k_y) = \int \frac{dk_x}{2\pi} \int \frac{dxd\omega}{2\pi i} \text{tr} \ G^{-1}(x, k, \omega) \partial_x G(x, k, \omega), \quad (4.56) \]

\[ = \frac{e_{\alpha\beta\gamma}}{24\pi^2} \text{tr} \int dxd\omega G^{-1} \partial_{k_x} \partial_{k_y} G^{-1} \partial_{k_y} G, \quad (4.57) \]

where we have introduced the gradient expansion of the inverse Green’s function, see [96], and where the sum is taken over \( \alpha, \beta, \gamma \in \{ k_x, k_y, k_z \} \). This quantity can be related to the following local \( x \)-dependent Chern number,

\[ N_3(x) = \frac{e_{\alpha\beta\gamma}}{24\pi^2} \text{tr} \int d\omega dk_x dk_y G^{-1} \partial_{k_x} \partial_{k_y} G G^{-1} \partial_{k_y} G, \quad (4.58) \]

where the sum is taken over \( \alpha, \beta, \gamma \in \{ \omega, k_x, k_y \} \). It is easy to show that if we take the limit \( x \to \pm\infty \) and substitute the bulk Green’s function by \( G_{\text{bulk}}(\omega, k) = [i\omega - \mathcal{H}_{\text{bulk}}^G(k)]^{-1} \), we find \( N_3(\pm\infty) = C_{\text{right/left}} \), so it is nothing but the winding number (or degree of covering) of the bulk Hamiltonian defined previously.

From there we can derive the bulk-edge correspondence [95, 96] that relates the spectral flow of the edge Hamiltonian to the Chern number of the bulk through,

\[ C_{\text{right}} - C_{\text{left}} \equiv N_3(x = +\infty) - N_3(x = -\infty) = N_1(k_y = +\infty) - N_1(k_y = -\infty) \equiv \nu \sigma. \quad (4.59) \]

This formal proof of the index theorem has been derived under the assumptions that (i) \( G \) has no singularities within the integration region (which is satisfied since by construction of the edge Hamiltonian the poles of the Green’s function lie at \( x = 0 \) and \( k \approx k_F \)), and, more critically, (ii) the inverse of the Green’s function can be approximated through its gradient expansion. The second assumption is then restricted to validity of the quasi-classical limit. We will see in the two last sections of this chapter that this is in general not the case.

An other approach has been presented by Fukui et al in Ref. [92] where they give the explicit proof of the index theorem for a certain class of Hamiltonians (they look at Dirac Hamiltonians with higher order derivatives). However their proof is restricted to Hamiltonians for which the coefficients of the gradient terms are independent of \( x \). In our case, see Eq. (4.15), we have the term \( \Delta_x(x)(-i\partial_x/k_F) \) and the method of Ref. [92] doesn’t apply.

To our knowledge only the approaches by Graf and Porta [112] and by Avila et al [113] (see also Hatsugai [111]) give a proof of the index theorem that is general enough to apply to our problem. We note that there are written in terms of lattice models (the continuous limit is then only a special case). It is beyond the scope of this work to review them here.

**Quasi-classical Fermi points and zero-energy bound states**

Now comes the question of the position of the zero-energy bound states which existence is predicted by the index theorem. Following Volovik in [95], it appears that if the zero-energy bound states are in a region where the quasi-classical limit is valid (i.e. \( k_x \xi \gg 1 \)), then we can deduce their position from the...
"classical" Hamiltonian that is obtained through the substitution \(-i \partial_x \rightarrow k_x\) in the full Hamiltonian Eq. (4.15). We get,

\[
\mathcal{H}_{cl}(k, x) = \left( \frac{k_x^2 + k_y^2 + \gamma^2 A_F^2(x)}{2m} - \mu \right) \sigma_3 + \frac{k_y}{m} \gamma A_y(x) \mathbf{1}
\]

\[
+ \left( \frac{k_x}{k_F} \Re \Delta_x(x) + \frac{k_y}{k_F} \Im \Delta_y(x) \right) \sigma_1
\]

\[
- \left( \frac{k_x}{k_F} \Im \Delta_x(x) + \frac{k_y}{k_F} \Re \Delta_y(x) \right) \sigma_2 .
\]

(4.60)

If we look at a point \((k, x)\) which lies within the validity range of the quasi-classical limit, then the Andreev equation corresponds to the first order Taylor expansion of the "classical" Hamiltonian, \(\mathcal{H}_{cl}(k, x)\), around this point. As a consequence the positions of the zero-energy bound states are given by the zeros (or Fermi points) of \(\mathcal{H}_{cl}(k, x)\).

If we consider a domain wall configuration between the two chiral states, the index theorem predicts the existence of \(N_3(R) - N_3(L) = 1 - (-1) = 2\) bound states on the domain wall.

- Let us first consider the case of a \(\pi_\perp\)-domain wall with \(\alpha = 0\). At the domain wall the gap function is then given by \(\Delta_x(0) = 0\) and \(\Delta_y(0) = 3 \Delta_y(0) \neq 0\). The zeros are then readily given by,

\[
m_{cl}(k_0, x_0 = 0) = 0 ,
\]

\[
\Rightarrow \begin{cases} 
    k_{0,1(2)} = \sqrt{2m\mu - \gamma^2 A_F^2(0)} , \\
    \theta_{k_{0,1}} = 0 , \\
    \theta_{k_{0,2}} = \pi .
\end{cases}
\]

(4.61)

From those Fermi points, \((k_0, x_0)\), we can deduce the position of the zero-energy bound states of the full quantum model \(\mathcal{H}_{bdg}^{\text{full}}\) : we have \(E_b(k_{0,0}) = 0\) at \(k_{y,0} = 0\). The two zero-energy bound states predicted by the index theorem are then degenerated.

- We consider now the case of a \(\pi_\parallel\)-domain wall with \(\alpha \neq 0\); we neglect the vector potential for simplicity. The gap function at the domain wall (i.e. at \(x = 0\)) is now given by \(\Delta_x(0) = \Re \Delta_x(0) \neq 0\) and \(\Delta_y(0) = \Im \Delta_y(0) \neq 0\). The Fermi points \((m_{cl}(k_0, 0) = 0)\) are then given by

\[
\begin{cases} 
    k_0 = \sqrt{2m\mu} , \\
    \theta_{k_0} = -\arctan \left( \frac{\Im \Delta_y(0)}{\Re \Delta_x(0)} \right) \pm \pi .
\end{cases}
\]

(4.62)

We then deduce the presence of zero-energy bound states of the full quantum model at \(k_{y,0} = \pm k_0 \sin \theta_{k_0}\). The two zero-energy bound states are not degenerated anymore.

Unfortunately this approach doesn’t work for zero-energy bound states that lie in a region of the spectrum where the quasi-classical approach is not valid. Let us consider for instance a \(\pi_\parallel\)-domain wall with \(\alpha = 0\); we again neglect the vector potential for simplicity. In this case the gap function at the domain wall \((x = 0)\) is given by \(\Delta_x(0) = \Re \Delta_x(0) \neq 0\) and \(\Delta_y(0) = 0\). We then find the Fermi points at \(k_0 = \sqrt{2m\mu}\), and \(\theta_{k_0} = \pm \pi/2\). But since \(k_x \rightarrow 0\) as \(\theta_k \rightarrow \pm \pi/2\), the quasi-classical limit doesn’t hold and \(\mathcal{H}_{cl}(k, x)\) cannot be used to deduce the position of the zero-energy bound states of the full quantum model \(\mathcal{H}_{bdg}^{\text{full}}\). We will show explicitly in the two last sections the breaking of the topology in the quasi-classical limit for this case.

We finish this part by noting that when (1) the quasi-classical limit is valid in a neighborhood of the Fermi points, (2) one part of the gap function is constant in space (i.e. \(\partial_x \Delta_i = 0\), for \(i = 1\) or \(i = 2\)), and (3) we neglect the vector potential, then there exists an elegant proof of the existence of zero-energy states based on the super-symmetry of the Andreev equation, see Ref. [91] and the references therein.

We don’t review it here since, in general, it doesn’t apply to our problem.

### 4.6 Sharp domain wall

In this section we derive the spectrum of the bound states present at the domain wall assuming a step-like gap function. We have on each side of the domain wall,

\[
\Delta_L = \Delta_- \equiv s\Delta_0(1, -i)e^{-i\alpha/2} , \quad \Delta_R = \Delta_+ \equiv \Delta_0(1, i)e^{i\alpha/2} ,
\]

(4.63)
Consequently the BdG wave function is decomposed on each side of the domain wall as, \[ \Delta_{\pm}(\theta_k) = \phi(\theta_k) \cdot \Delta_{\pm}, \] where \( s = 1 \) corresponds to a \( \pi_{\uparrow} \)-domain wall, and \( s = -1 \) corresponds to a \( \pi_{\downarrow} \)-domain wall. In the following we will chose \((\phi_x, \phi_y) = (\tilde{v}_x, \tilde{v}_y) = v_F(\theta_k)(\cos \theta_c, \sin \theta_c)\) for simplicity, where \( \tilde{v}_i \equiv v_i(\theta_k)/v_F \) and \( \theta_i(\theta_k) = \arctan(v_y(\theta_k)/v_x(\theta_k)) \). The gap function can then be rewritten as the following,

\[ \Delta_{\pm}(\theta_k) = s\Delta_0 \cdot \tilde{v}_F(\theta_k) \exp \left\{ \pm i \left( s\theta_v + \frac{\alpha}{2} \right) \right\}. \] (4.64)

In the following we only consider the \( \pi_{\uparrow} \)-domain wall, i.e. we set \( s = +1 \).

The Andreev equation with a constant gap can be readily solved making the ansatz,

\[ \psi_{\theta_k}(x) = \left( \begin{array}{c} u \\ v \end{array} \right) e^{\frac{i}{\kappa} v_x(\theta_k)^x}, \] (4.65)

from which we find the two solutions,

\[ \kappa_{\pm} = \mp \sqrt{\Delta^2 - E^2}, \quad \eta_{\pm} = \left( \frac{v}{u} \right)_{\pm} = \frac{E + i\kappa_{\pm}}{\Delta}. \] (4.66)

In the following we will focus on the bound state solutions for which \( \kappa \in \mathbb{R} \) and \( \kappa/x_v(\theta_k) < 0 \), i.e.

\[ \kappa = -\text{sign}[v_x(\theta_k)]|\kappa|, \quad \text{for } x > 0, \]

\[ \kappa = \text{sign}[v_x(\theta_k)]|\kappa|, \quad \text{for } x < 0. \] (4.67)

Following the section 4.3, we expand the BdG wave functions at the Fermi level in terms of the Andreev wave functions as,

\[ \Psi_{k_F} (x) = \sum_{k_{F,x}, k_{F,y}} c_{k_{F,x}} e^{i k_{F,x}x} \psi_{\kappa}(x), \]

\[ = c_{\theta_k} e^{i k_{F,x}(\theta_k)x} \psi_{\theta_k}(x) + c_{\theta_{\pi - \theta_k}} e^{i k_{F,x}(\pi - \theta_k)x} \psi_{\pi - \theta_k}(x). \] (4.68)

Consequently the BdG wave function is decomposed on each side of the domain wall as,

\[ \Psi_L = A_L \Psi_1 + B_L \Psi_2, \quad \Psi_R = A_R \Psi_1 + B_R \Psi_2, \] (4.69)

where the different components are drawn on Fig. 4.3. We find

\[ \Psi_L = A_L \left( \begin{array}{c} 1 \\ \eta_L(\theta_k) \end{array} \right) e^{i k_x(\theta_k)x + i k_y y + \frac{\kappa(\theta_k)}{\hbar v_x(\theta_k)} x} + B_L \left( \begin{array}{c} 1 \\ \eta_L(\pi - \theta_k) \end{array} \right) e^{i k_x(\pi - \theta_k)x + i k_y y - \frac{\kappa(\pi - \theta_k)}{\hbar v_x(\pi - \theta_k)} x}, \]

\[ \Psi_R = A_R \left( \begin{array}{c} 1 \\ \eta_R(\theta_k) \end{array} \right) e^{i k_x(\theta_k)x + i k_y y - \frac{\kappa(\theta_k)}{\hbar v_x(\theta_k)} x} + B_R \left( \begin{array}{c} 1 \\ \eta_R(\pi - \theta_k) \end{array} \right) e^{i k_x(\pi - \theta_k)x + i k_y y + \frac{\kappa(\pi - \theta_k)}{\hbar v_x(\pi - \theta_k)} x}, \] (4.70)

![Wave function components at a domain wall.](image)
This spectrum has then the same structure as the full BdG spectrum $E$.

We directly see that the solution to the equation (4.79) satisfies the following symmetries,

$$
\begin{align*}
\eta_L(\theta_k) &= \frac{\tilde{E} + i\tilde{k}(\theta_k)}{\Delta^*(\theta_k)}, \\
\eta_R(\theta_k) &= \frac{\tilde{E} - i\tilde{k}(\theta_k)}{\Delta(\theta_k)},
\end{align*}
$$

(4.71)

with $\tilde{E} = E/(\Delta_0\tilde{\kappa}_F(\theta_e))$ and $\tilde{k}(\theta_k) = \text{sign}[\cos \theta_e(\theta_k)]\sqrt{1 - \tilde{E}^2}$.

Now we introduce the continuity conditions at the interface for the BdG wave functions,

$$
\begin{align*}
\Psi_L(0) &= \Psi_R(0), \\
\partial_x \Psi_L(0) + k_F Z \Psi(0) &= \partial_x \Psi_R(0),
\end{align*}
$$

(4.72)

where, following Blonder et al [97], we have included the effect of a potential barrier of the form $U(x) = U_0\delta(x)$, with $Z = 2mU_0/\hbar^2k_F$.

Inserting the BdG wave functions into the boundary conditions we get a homogeneous system of four linear equations that has non-trivial solutions under the following compatibility condition,

$$
\hbar^2 v_F^2 k_x^2 \left( m_1 - m_2 \right) + 4Z \hbar v_x k_x \text{sign}[v_x] |\alpha| + 4\kappa^2 = 0,
$$

(4.73)

with

$$
\begin{align*}
m_1 &= \eta_R^*(\pi - \theta_k) \eta_R^+(\theta_k) + \eta_R^+(\pi - \theta_k) \eta_R^-(\theta_k) = -2 \cos \alpha, \\
m_2 &= \eta_R^+(\theta_k) \eta_R^+(\pi - \theta_k) + \eta_R^+(\pi - \theta_k) \eta_R^-(\theta_k) \\
&= 2 \cos 2\theta_e \left( 1 - 2\tilde{E}^2 \right) + 4\tilde{E} \text{ sign}[\cos \theta_e] \sqrt{1 - \tilde{E}^2} \sin 2\theta_e, \\
m_3 &= \eta_R^+(\pi - \theta_k) \eta_R^+(\pi - \theta_k) + \eta_R^+(\theta_k) \eta_R^-(\theta_k) = 2
\end{align*}
$$

(4.74)

Let us now introduce the following dimensionless quantity,

$$
a = k_F \frac{\hbar v_F}{\Delta_0} = k_F \xi_0,
$$

(4.75)

that is a measure for the validity of the Andreev approximation (i.e. the limit $k_F\xi_0 \gg 1$) in the bulk of the system. In the case of Strontium Ruthenate we have $a \approx 1200$ (the $\gamma$-band parameters are : $k_F = 0.753 \, \text{Å}^{-1}$, $v_F = 5.5 \times 10^4 \, \text{ms}^{-1}$, $\Delta_0 = 0.23 \, \text{meV}$; the values taken from [28]).

**Symmetry**

We directly see that the solution to the equation (4.79) satisfies the following symmetries,

$$
\begin{align*}
E(\pi - \theta_k) &= E(\theta_k), \\
E(-\theta_k) &= -E(\theta_k).
\end{align*}
$$

(4.76)

(4.77)

This spectrum has then the same structure as the full BdG spectrum $E_{k_y}$ labeled by the good quantum number $k_y$, see section 4.3.

We also note that independently of the value of the phase shift through the domain wall, $\alpha$, there will be no bound state current flowing perpendicularly through the domain wall (i.e. along the $x$ direction) since we have, after substituting $\theta_k = \theta_k' + \pi/2$,

$$
E(\pi/2 - \theta_k') = E(\pi/2 + \theta_k'),
$$

(4.78)

i.e. the spectrum is symmetric around $\theta_k = \pi/2$ and the bound state current flowing along the negative $x$-direction compensates the current flowing along the positive $x$-direction.
4.6.1 Transparent domain wall

Considering a perfectly transparent domain wall ($Z = 0$) we get the following equation for the spectrum of the bound states,

\[ a^2 \cos^2 \theta_k \cos^2 \theta \left [ \left ( 1 - 2 \tilde{E}^2 \right ) \cos 2 \theta \psi_k + 2 \tilde{E} \text{sign}[\cos \theta \psi_k] \sqrt{1 - \tilde{E}^2} \sin 2 \theta \psi_k + \cos \alpha \right ] + \left ( 1 - \tilde{E}^2 \right ) \left [ \left ( 1 - 2 \tilde{E}^2 \right ) \cos 2 \theta \psi_k + 2 \tilde{E} \text{sign}[\cos \theta \psi_k] \sqrt{1 - \tilde{E}^2} \sin 2 \theta \psi_k - 1 \right ] = 0. \]  

(4.79)

Lowest order solution

Let us first only keep the zero-order terms in $a^{-1} = (k_F \xi_0)^{-1}$. This is the quasi-classical limit and it corresponds to neglecting the terms $|\partial_x \psi_{\theta_k}|$ as compared to the terms $|k_x \psi_{\theta_k}|$. The equation (4.79) then reduces to,

\[ (1 - 2 \tilde{E}^2) \cos 2 \theta \psi_k + 2 \tilde{E} \text{sign}[\cos \theta \psi_k] \sqrt{1 - \tilde{E}^2} \sin 2 \theta \psi_k + \cos \alpha = 0, \]  

(4.80)

from which we find the following solutions,

\[
\begin{align*}
E_{\psi}^{\pm} (\theta_y) &= -s_{\psi_k}^\pm \Delta_0 \psi_{\theta_k} (\theta_0) \cos (\theta_0 \pm \alpha/2), \\
\Delta_0 &= \text{sign}[\sin(\theta_0 \pm \alpha/2) \cos \theta_0],
\end{align*}
\]  

(4.81)

where we have chosen the good quantum number as $\theta_y = \arcsin(k_F \psi_0/k_F)$. For simplicity we will only consider the isotropic limit, i.e. $\theta_x = \theta_y$ (we will show the spectrum with non-zero anisotropy in the next section). We plot the bound state spectrum in Fig. 4.4: (a) for $\alpha = 0$ the spectrum is doubly degenerated, and (b) for $|\alpha| = 0.2 \pi$ the spectrum splits into two distinct branches. We note that the topology of the problem is not well defined since the bound state branches are cut at $\theta_y = \pm \pi/2$ before they reach the opposite continuum. In the case $\alpha = 0$, it is even not clear that bound state branches cross the Fermi level\footnote{We will see in the next chapter that when we take the vector potential into account, the bound state branches do not cross the Fermi level at all! This leads to the vanishing of a part of the bound state’s spectral weight and constitutes a striking breaking of the topology of the problem.}. This shows the limitation of the quasi-classical solution. Since this feature is of a topological nature—i.e. the breaking of the topology of the full quantum problem—, it will be conserved in all the quasi-classical solutions independently of the degree of precision of the solution: here, with...

Figure 4.4: Lowest order domain wall spectrum as a function of $\theta_y = \arcsin(k_F \psi_0/k_F)$: (a) for $\alpha = 0$, and (b) for $\alpha = \pm 0.2 \pi$. The both are for a fully transparent domain wall, i.e. $T = 1$. 

\[ (a) : \alpha = 0, \ T = 1 \]  

\[ (b) : \alpha = \pm 0.2 \pi, \ T = 1 \]
Higher order corrections

We now look at the effect of taking the higher order terms in $a^{-1}$ in Eq. (4.79), that is in some sense going beyond the quasi-classical approximation. We show the numerical solution of the spectrum on Fig. 4.5 for the same parameters as in the previous case ($\alpha = 0, \pm \pi$ and $T = 1$). The main effect of the higher order corrections is to reestablish the topology of the full quantum problem: the bound state branches are now connecting continuously the lower and the upper energy continuums. We then have that the substitution of the Andreev wave functions in the continuity condition for the BdG wave functions, equation (4.72), is sufficient here to recover the correct topology. Unfortunately, we will see in the next section (with a smooth ansatz for the gap function) that it is not always the case.

4.6.2 Effect of a potential barrier

We assume now that there is a potential barrier at the domain wall, i.e. $Z \neq 0$. The transparency of the barrier is defined as $T = 4/(Z^2 + 4)$. Keeping only the zero-order terms in $a^{-1}$, we find the equation,

$$
\left(1 - 2\tilde{E}^2\right) \cos 2\theta_v + 2\tilde{E} \text{sign}[\cos \theta_v] \sqrt{1 - \tilde{E}^2} \sin 2\theta_v + T \cos \alpha + T - 1 = 0.
$$

The solutions can be written as,

$$
\left\{
\begin{array}{l}
E(\theta_v) = s^{\pm}_{\theta_v} \Delta_0 \bar{v}_F(\theta_v) \left(\sin \theta_v \sqrt{1 - \tilde{E}^2} \cos^2 \left(\frac{\alpha}{2}\right) \pm \cos \theta_v \sqrt{T} \cos \left(\frac{\alpha}{2}\right)\right), \\
s^{\pm}_{\theta_v} = \text{sign} \left[\frac{1}{\pi} \arctan \left(\sqrt{T} \cos(\alpha/2)\right) \mp \theta_v\right].
\end{array}
\right.
$$

We show the solution on Fig. 4.6: the infinity barrier case, i.e. $T = 0$, is given by the blue line; the red lines show the spectrum when we decrease the barrier up to $T = 0.1$.

We see that the spectrum at $T = 0$, that is the well known signature of the chiral edge states, is doubly degenerated—we have one chiral edge state on each side of the interface—and, as we increase the transparency of the interface, it is split into two inequivalent branches (red lines).
Figure 4.6: Lowest order domain wall spectrum as a function of $\theta = \arcsin(k_{F,y}/k_F)$ : for $T = 0$ (blue line) and $T = 0.1$ (red line).

The effect of higher order corrections for small $T$ is small (most of the bound state spectrum lies in the range $-\pi/2 + 0^+ < \theta_k < \pi/2 - 0^+$ where the quasi-classical limit is valid), and we don’t include those plots.

4.7 Smooth domain wall ansatz

In this section we derive the analytical solution to the Andreev equation for the domain wall problem assuming a simplified smooth ansatz for the gap function (non-self-consistent). Our initial motivation for seeking the analytical solution with a smooth gap was to be able to derive the free energy of the system. Indeed it was shown that the discontinuities in the gap functions and its derivatives lead to spurious terms in the Ginzburg-Landau free energy when derived from the specific gap function, see Ref. [91] and references therein. It was found that those spurious terms disappear by removing the discontinuities of the gap function. This was shown explicitly by Eilenberger and Jacobs in Ref. [98] for a simple gap function’s shape from which they derived the analytical solution to the Andreev equation. We follow the same idea here.

We derive the spectrum of the Andreev bound states and then compute the spectral function of the system (which contains all the states : the bound states and the scattering states). We also give the Ginzburg-Landau free energy for this ansatz. We note that, while this analytical solution is not self-consistent and gives wrong domain wall energies, i.e. we cannot derive from it the correct domain configuration in its most stable state, we will see—anticipating on the results of the next chapter—that there is a surprisingly good qualitative agreement of the spectral function obtained from the numerical self-consistent solution (presented in the next chapter) when we fix the parameters, $\alpha, \tilde{\theta}$, to their values for a stable domain wall.

**Ansatz**

The Andreev equation can be rewritten as,

\[
-iv_x(\theta_k) \frac{\partial}{\partial x} \sigma_3 + \Delta_1(\theta_k, x)\sigma_1 - \Delta_2(\theta_k, x)\sigma_2 - E \hat{\sigma}_1 \begin{pmatrix} u(x, \theta_k, E) \\ v(x, \theta_k, E) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix},
\]

where we have neglected the vector potential for simplicity. From now on we assume the following ansatz for the gap function,

\[
\begin{align*}
\Delta_1(\theta_k) &= \Delta_0 \tilde{v}_F(\theta_v) \cos(\theta_v + \alpha/2), \\
\Delta_2(\theta_k, x) &= \Delta_0 \tilde{v}_F(\theta_v) \sin(\theta_v + \alpha/2) \tanh (x/\xi),
\end{align*}
\]
where we have used the same parameterization of the gap function as in equation (4.64). Since $\partial_z \Delta_1 = 0$, the Andreev equation can be diagonalized, and for the simple ansatz, $\Delta_2(x) \sim \tanh(x/\xi)$, we can derive an analytical solution to the Andreev equation. It is done in detail in the appendix.

Let us now introduce the functions,

$$a(x, \theta_k, E) = \frac{iu_-(x, \theta_k, E)}{v_-(x, \theta_k, E)} , \quad b(x, \theta_k, E) = \frac{iv_+(x, \theta_k, E)}{u_+(x, \theta_k, E)} \, ,$$

which are defined through the solution of the Andreev equation obtained for the following boundary conditions,

$$\begin{cases}
\lim_{x \rightarrow -\infty} v_-(x, \theta_k, E) & = \eta_L(\theta_k) , \\
\lim_{x \rightarrow +\infty} v_+(x, \theta_k, E) & = \eta_R(\theta_k) ,
\end{cases}$$

where the functions $\eta_{L,R}$ were defined in Eq. (4.71) of the previous section. The explicit expressions of the functions $a$ and $b$ are given in terms of associated Legendre polynomials of the first kind, see Eq. (4.115) in the appendix.

The quasi-classical Green’s function introduced in section 4.3.1—satisfying the Eilenberger equation—is simply given by (Riccati parametrization),

$$g(x, \theta_k, E) = \frac{1 - a(x, \theta_k, E)b(x, \theta_k, E)}{1 + a(x, \theta_k, E)b(x, \theta_k, E)} \, ,$$

from which we get the spectral function of the system through,

$$A(x, \theta_k, E) = \text{Re} \left\{ g(x, \theta_k, E + i0^+) \right\} \, .$$

The spectrum of the bound states is given by the poles of the spectral function at the sub-gap energies, i.e. $|E| < \Delta_0$. Using the analytical solution Eq. (4.115) we find the following equation for the spectrum of the bound states,

$$\sin(\theta_v + \alpha/2)\tilde{E} + \text{sign}[\cos(\theta_v)] \cos(\theta_v + \alpha/2) \sqrt{1 - E^2} = 0 \, ,$$

with the solution,

$$\begin{cases}
E_\nu(\theta_k) & = -s_{\theta_k} \frac{\Delta_0}{v_F} \cos(\theta_v + \alpha/2) , \\
s_{\theta_v} & = \text{sign}[\sin(\theta_v + \alpha/2) \cos(\theta_v)] \, .
\end{cases}$$

We note that this solution is identical to one of the two branches derived in the previous section for the case of a sharp domain wall.

In section 4.3 we have stressed the fact that $k_x$ is not a good quantum number for the full quantum problem. We have given in equation (4.30) the full Green’s function in the quasi-classical limit that is obtained through the addition of the two sectors, $\theta_k$ and $\pi - \theta_k$ (right moving and left moving quasiparticle, respectively). Therefore the full spectral function is given by,

$$A_\Sigma(x, \theta_y, E) = A(x, \theta_k, E) + A(x, \pi - \theta_k, E) \, ,$$

where we have defined the good quantum number as $\theta_y = \arcsin(k_{F,y}/k_F)$.

We plot the spectral function and the spectrum of a $\pi_0$-domain wall on Fig. 4.7 (we show the solution with the full angular resolution in the appendix). We see clearly the discontinuities at $\theta_k = \pm \pi/2$—by discontinuity we mean that the bound state branches are not connecting continuously the lower energy continuum to the upper continuum—due to the singularity of the Andreev equation at $v_x \rightarrow 0$. We will see that those non-self-consistent results are in a surprisingly good qualitative agreement with the numerical self-consistent solution that is presented in the next chapter.
Figure 4.7: Spectral function, $A(\theta_k, E, x = 0)$, and bound state spectrum, $E_b(\theta_k)$, of a $\pi\parallel$-domain wall ($s = 1$).

Ginzburg-Landau free energy

Inserting the ansatz in the Ginzburg-Landau free energy we get

$$F_{DW} - F_{\text{homog}} = \xi_t \frac{\xi_t}{\eta} \left( 3 + 8l^2 - 4l^2 \cos \alpha + \nu(-4l^2 \cos \alpha + \cos 2\alpha) \cos 4\bar{\theta} \right),$$

(4.93)

where $l = \xi_t / \xi_{DW}$. We plot the GL free energy on Fig. 4.8. While the general structure of the spectrum is in a good agreement with the numerical self-consistent solution (as we will see in the next chapter), the domain wall energy is less accurate such that we need to solve the full self-consistent problem in order to find the most stable domain wall configuration.

4.7.1 Higher order corrections

We have mentioned in section 4.3.1 that the boundary conditions derived by Zaitsev in [85] are only valid in the quasi-classical limit (there are derived for the quasi-classical Green’s functions $\bar{G}$ and not for the full Green’s function $G$). Hence it is not possible to recover the topology of the original quantum problem from them, since we need to go beyond the quasi-classical limit.

On the contrary, the BTK boundary condition—that is nothing but a continuity condition for the full BdG wave function—is more general. We have seen in the section on the sharp domain wall solution that inserting the Andreev wave functions into the BTK boundary condition Eq. (4.72) and keeping
higher order terms in $a^{-1} = (k_F \xi)^{-1}$, we could recover the correct topology of the full quantum problem. However, if we do the same here, by making use of the analytical Andreev wave functions $(u_{\pm}(x), v_{\pm}(x))$ derived in this section for a smooth gap function, the corrections from the higher order terms are spurious and we cannot recover the correct topology. Therefore it seems that this naive attempt to go beyond the quasi-classical limit by inserting the Andreev wave function into the BTK continuity condition doesn’t work in general. This is one of the main motivations for looking at the lattice formulation of the problem in chapter 6.

4.8 Conclusions

Motivated by the question of the microscopic origin to the macroscopic domain wall structure as obtained from the Ginzburg-Landau theory for Sr$_2$RuO$_2$ (assuming the chiral $p$-wave state), we have derived the Bogoliubov-de Gennes equation and the Andreev equation—that is obtained in the quasi-classical limit—for the domain wall problem. We also have introduced the quasi-classical Green’s function, the quasi-classical Gorkov equations (Eilenberger) and the Zaistev boundary conditions.

We have studied the general properties of the Andreev equation in terms of symmetry and the full Bogoliubov-de Gennes equation in terms of topology. On the one hand, we have discussed the charge-conjugation symmetry of the Andreev equation and shown the presence of zero-energy chiral edge states under the assumption of specular reflection. On the other hand, we have reviewed the concepts related to the topological structure of the full Bogoliubov-de Gennes equation: bulk Chern number, spectral flow, index theorem, and Fermi points in regard to the zero-energy bound states. This conceptual framework will be very important in the next chapter.

We have then derived the analytical solution of the Andreev equation for two simplified (non-self-consistent) domain wall configurations assuming (i) a sharp domain wall, and (ii) a smooth ansatz of the gap function. We have seen that the domain wall spectrum has discontinuities at the singularity points of the Andreev equation, i.e. at the points at which the Andreev approximation (or quasi-classical limit) breaks down. This is in contrast with the spectral structure of the full quantum model as predicted by the index theorem. Incidentally, this represents a limitation of the validity of the demonstration of the index theorem from the quasi-classical Green’s function as proposed by Volovik [95] and Gurarie [96]. Similarly, the Zaitsev boundary conditions that are derived for the quasi-classical Green’s function are only valid as long as the Andreev approximation doesn’t break down. Nevertheless, we found that in the case of the sharp domain wall the use of the continuity condition for the total BdG wave function, i.e. the Blonder Tinkham Klawik boundary conditions, leads to the recovering of the good topology. Unfortunately, this naive approach didn’t work with our analytical solution of the smooth domain wall. Hence it cannot be generalized and it seems to be successful only accidentally in the case of the sharp domain wall. This pleads for the necessity to go beyond the quasi-classical limit, that is the aim of Chapter 6 that treats the lattice approach of the problem.

Furthermore, we have seen that the quasi-classical domain wall spectrum is identical in the two cases (i) and (ii), such that it doesn’t depend essentially on the degree of precision of the solution, i.e. it is
mainly determined by the topology of the problem. We will see that there is even a good qualitative agreement with the domain wall spectrum found from the numerical self-consistent solution. However, the domain wall energy obtained for the smooth ansatz is less accurate (as compared to the full Ginzburg-Landau solution) and it is necessary to solve the full self-consistent problem in order to find the most stable domain wall configuration as a function of the anisotropy of the material and the orientation of the domain wall. This question is addressed in detail in the next chapter where we present the numerical self-consistent solution of the quasi-classical Green’s function equations (Eilenberger equations).
Appendix

4.A Smooth domain wall ansatz

Second order differential equation

In this section we follow the method of resolution of the Andreev equation exposed in [76]. We start by rewriting the Andreev equation as,

\[ iv_x \frac{\partial}{\partial x} \hat{\sigma}_3 + \Delta_1(x) \hat{\sigma}_1 - \Delta_2(x) \hat{\sigma}_2 + E \hat{1} \hat{\sigma}_3 \psi(x) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \] (4.94)

with the gap function decomposed into real and imaginary part \( \Delta(x) = \Delta_1(x) + i\Delta_2(x) \), the Cooper pair energy \( E \) and the Andreev wave function,

\[ \psi(x) = \begin{pmatrix} u(x) \\ v(x) \end{pmatrix}. \] (4.95)

Note that we neglect the vector potential.

We can define an auxiliary spinor \( \chi(x) = (\chi_1 \chi_2)^T \) as

\[ \hat{\sigma}_3 \psi(x) = \begin{pmatrix} iv_x \frac{\partial}{\partial x} \hat{\sigma}_3 + \Delta_1(x) \hat{\sigma}_1 - \Delta_2(x) \hat{\sigma}_2 - E \hat{1} \end{pmatrix} \chi(x), \] (4.96)

such that it satisfies the following second order linear differential equation

\[ \left( -v_x^2 \frac{\partial^2}{\partial x^2} + \Delta^2_1(x) + \Delta^2_2(x) - E^2 \right) \hat{1} - v_x \left( \frac{\partial \Delta_1(x)}{\partial x} \hat{\sigma}_2 + \frac{\partial \Delta_2(x)}{\partial x} \hat{\sigma}_1 \right) \chi(x) = 0. \] (4.97)

The complexity of this equation comes for the fact that the differential equations for the two components of \( \chi \) are coupled. We will see that they can be decoupled when one of the components of the gap function is constant.

Ansatz

We introduce the following ansatz for the real and the imaginary parts of the gap function,

\[
\begin{aligned}
\Delta_1 &= \Delta_0 \bar{v}_F(\theta_v) \cos(\theta_v + \alpha/2), \\
\Delta_2(x) &= \Delta_0 \bar{v}_F(\theta_v) \sin(\theta_v + \alpha/2) \tanh(x/\xi),
\end{aligned}
\] (4.98)

(see the definition of the gap function in (4.64)). We show below that since \( \partial_x \Delta_1 = 0 \) the equation can be diagonalized, and the simple ansatz \( \tanh(x/\xi) \) allows to derive an analytical solution to the Andreev equation.

This proceeds as the following. Making a rotation around the \( \hat{\sigma}_2 \)-axis by an angle \( -\pi/2 \) we transform \( \hat{\sigma}_1 \) to \( \hat{\sigma}_3 \). The corresponding unitary matrix is given by

\[ \hat{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}. \] (4.99)
Note that here $\hat{U}^\dagger \hat{U} = \hat{1} = \hat{U}^T \hat{U}$. We define the new spinor under the $\hat{U}$ transformation as

$$
\hat{U} \left( \begin{array}{c} \chi_1 \\ \chi_2 \end{array} \right) = \left( \begin{array}{c} \phi_1 \\ \phi_2 \end{array} \right) .
$$

(4.100)

Transforming the equation (4.97) under the rotation $\hat{U}$ we find

$$
\left[ -v_x^2 \frac{\partial^2}{\partial x^2} + \Delta^2 + \Delta_2^2(x) - E^2 \right] (\hat{1} - v_x \frac{\partial \Delta_2(x)}{\partial x}) \left( \begin{array}{c} \phi_1(x) \\ \phi_2(x) \end{array} \right) = 0 ,
$$

(4.101)

where the two functions $\phi_1$ and $\phi_2$ are now decoupled. The corresponding dimensionless equation can be written as

$$
\phi''_1(\hat{x}) + [\nu (\nu + 1) \text{sech}^2(\hat{x}) - \mu^2] \phi_1(\hat{x}) = 0 ,
$$

(4.102)

where we have defined

$$
\nu = \frac{\sin(\theta_v + \alpha/2)}{l \cos \theta_v} ,
$$

$$
\mu = \frac{\sqrt{1 - E^2}}{l \cos \theta_v} ,
$$

(4.103)

with $\hat{x} = x/\xi$, $\tilde{E} = E/(\Delta_0 \tilde{\nu} F(\theta_v))$, and $l = \xi_0/\xi$ is the ratio between the BCS coherence length and the width of the domain all ($\xi_0 = \hbar v_F/\Delta_0$).

The solution to the equation (4.102) can be expressed in terms of hypergeometric functions or as a sum of associated Legendre polynomials of the first and the second kind $^9$

$$
\phi_{1,2}(\hat{x}) = A_{1,2} P_{s_{\nu} \mu}^{1,2} (\text{tanh} \hat{x}) + B_{1,2} P_{s_{\nu} \mu}^{1,2} (-\text{tanh} \hat{x}) ,
$$

(4.107)

where we have used $s_\mu = \text{sign} \mu \equiv \text{sign}[\cos \theta_v]$.

From (4.100) we have

$$
\left\{ \begin{array}{l}
\chi_1 = \frac{1}{\sqrt{2}} (\phi_1 - \phi_2) , \\
\chi_2 = \frac{1}{\sqrt{2}} (\phi_1 + \phi_2) ,
\end{array} \right.
$$

(4.108)

which inserted in (4.96) gives $u$ and $v$.

We have for $u$ and $v$,

$$
\left( \begin{array}{c} u \\ v \end{array} \right) = \left( i l \cos \theta_v \partial_{\hat{x}} \hat{1} + i \hat{\Delta}_1 \hat{\sigma}_2 + i \hat{\Delta}_2 \hat{\sigma}_1 - \tilde{E} \hat{\sigma}_3 \right) \left( \begin{array}{c} \chi_1 \\ \chi_2 \end{array} \right)
$$

(4.109)

and the dimensionless Andreev equation reads,

$$
\left[ -i l \cos \theta_v \partial_{\hat{x}} \hat{\sigma}_3 + \hat{\Delta}_1 \hat{\sigma}_1 + \hat{\Delta}_2 \hat{\sigma}_2 - \tilde{E} \hat{1} \right] \left( \begin{array}{c} u \\ v \end{array} \right) = 0 .
$$

(4.110)

Then we can express the functions

$$
a(E, \theta_v, x) = \frac{iu(E, \theta_v, x)}{v(E, \theta_v, x)} , \quad b(E, \theta_v, x) = \frac{iv(E, \theta_v, x)}{u(E, \theta_v, x)} ,
$$

(4.111)

$^9$Note that the Legendre function $P_{\mu}^{\nu}$ is defined as the regularized Hypergeometric function

$$
P_{\nu}^{\mu}(z) = \frac{1}{\Gamma(1 - \mu)} \left( \frac{1 + z}{1 - z} \right)^{\mu/2} z^{\nu} \text{F}_1 \left( -\nu, 1 + \mu; 1 - \mu; \frac{1 - z}{2} \right) .
$$

(4.104)

At $z = 0$ we have

$$
P_{\nu}^{\mu}(0) = \frac{2^{\nu + 1/2}}{\Gamma(\nu/2 - \mu/2 + 1) \Gamma(1/2 - \nu/2 - \mu/2)} ,
$$

(4.105)

and at $z = 1$,

$$
P_{\nu}^{\mu}(1) \sim \frac{1}{\Gamma(1 - \mu)} \left( \frac{2}{1 - z} \right)^{\mu/2} .
$$

(4.106)
from which we derive the quasi-classical Green’s function

\[ g = \frac{1 - ab}{1 + ab} . \]  

(4.112)

This is the Riccati parametrization which will be introduced in the next chapter.

The functions \( a \) and \( b \) are determined by the boundary conditions

\[
a(x = \pm \infty) = \frac{\Delta(\pm \infty)}{\omega_m + \sqrt{\omega^2_m + |\Delta(\pm \infty)|^2}} , \quad b(x = \pm \infty) = \frac{\Delta^*(\pm \infty)}{\omega_m + \sqrt{\omega^2_m + |\Delta(\pm \infty)|^2}} ,
\]

(4.113)

where we have set \( E = i\omega_m = i\pi T(2m + 1) \) (Matsubara frequency for fermions).

We can now construct \( a \) (resp. \( b \)) from the condition \( A_{1,2} = 0 \) and the boundary condition \( u(+\infty) \propto \Delta(+\infty) \), which leads to \( B_2 = B_1 \) (\( A_2 = A_1 \)). Writing \( z = \text{tanh} \, \tilde{x} \), and \( \Delta(z) = \cos(\theta_v + \alpha/2) + iz \sin(\theta_v + \alpha/2) \), we eventually find the solution

\[
a(z) = \frac{i u_-(z)}{v_-(z)} , \quad b(z) = \frac{i v_+(z)}{u_+(z)} ,
\]

(4.114)

with

\[
u_-(z) = [\tilde{E} + \Delta(z) - iz \nu l \cos \theta_v]P^{-\nu\mu}_{-\nu\mu}(-z) + i(1 + s_{\mu\nu} + \nu)l \cos \theta_v P^{-\nu\mu}_{1+\nu\nu}(-z) + \tilde{E} - \Delta(z) - i(1 + s_{\mu\nu} + \nu + z(1 + \nu))l \cos \theta_v P^{-\nu\mu}_{-\nu\nu}(-z) ,
\]

\[
u_+(z) = [\tilde{E} + \Delta(z) - iz \nu l \cos \theta_v]P^{-\nu\mu}_{-\nu\mu}(z) - i(1 + s_{\mu\nu} + \nu)l \cos \theta_v P^{-\nu\mu}_{1+\nu\nu}(z) + \tilde{E} - \Delta(z) + i(1 + s_{\mu\nu} + \nu + z(1 + \nu))l \cos \theta_v P^{-\nu\mu}_{-\nu\nu}(z) ,
\]

(4.115)

The spectrum of the bound states is simply given by the poles of the quasi-classical Green’s function \( g(E, \theta_v, x) \) for \( |E| < \Delta_0 \), that are the zeros of \( 1 + ab \). This gives the relation

\[ \sin(\theta_v + \alpha/2)\tilde{E} + \text{sign}[\cos \theta_v] \cos(\theta_v + \alpha/2) \sqrt{1 - \tilde{E}^2} = 0 \]

(4.116)

with the solution

\[
\begin{aligned}
E_0(\theta_v) &= -s_{\theta_v} \frac{\Delta_0}{v_F} \cos(\theta_v + \alpha/2) , \\
s_{\theta_v} &= \text{sign}[\sin(\theta_v + \alpha/2) \cos \theta_v] .
\end{aligned}
\]

(4.117)

We plot the spectrum of the bound states on Fig. 4.9. We see clearly the discontinuities at \( \theta_v = \pm \pi/2 \) due to the singularity of the coefficient \( 1/v_F \) in the Andreev equation. We saw in the previous section that those lead to limitation in the search for a formal proof concerning the existence of zero energy Andreev bound states.

The spectral function is given by

\[ A(E, \theta_k, x) = \text{Re} \{ g(\omega_m, \theta_k, x) \} \big|_{\omega_m \rightarrow E + i0^+} . \]

(4.118)

We plot the spectral function at a \( \pi_0 \)-domain wall in Fig. ???. Since in the exact quantum problem \( k_x \) is not a good quantum number, we will interpret the results from the spectral function obtained by symmetrization through,

\[ A_{\Sigma}(E, \theta_k, x) = A(E, \theta_k, x) + A(E, \pi - \theta_k, x) . \]

(4.119)
Figure 4.9: Fig. A: Spectrum of the Andreev bound states, $E_\theta(\theta_k)$, at a $\pi_\parallel$-domain wall ($s = 1, \bar{\theta} = 0, \alpha = 0$). Fig. B: Spectral function at the domain wall, $\pi_\parallel$-type, $A(\theta_k, E, x = 0)$. 
Chapter 5

Quasi-classical approach

In this chapter we give the numerical self-consistent solution of the Eilenberger equations for a domain wall configuration between two degenerate chiral p-wave superconducting states specified for the material Sr$_2$RuO$_4$. The Fermi surface and gap function anisotropy, as well as the domain wall orientation with respect to the crystal axis are taken into account. We find that for a realistic anisotropy and depending on the domain wall orientation the gap function acquires an additional global phase shift through the domain wall that is in agreement with the Ginzburg-Landau results presented in Part I. We relate this additional phase shift to the topologically protected Andreev bound states present at the domain wall.

Furthermore, we study the effect of a potential barrier added at the domain wall interface in regard of the Andreev bound states: we show the transition of the spectrum of domain wall bound states to chiral edge states as we go smoothly from a domain wall to an edge.

Finally and in agreement with the topological pathology of the Andreev equation discussed in the previous chapter, we show the missing of a fraction of the spectral weight of the domain wall bound states around the zero-energy level (i.e. at the Fermi energy).

5.1 Introduction

In the previous chapter we have derived the general symmetry and topological properties of the domain wall problem obtained from the Andreev and Bogoliubov-de Gennes equations. In the present chapter we want to address the question of the most stable domain wall configuration as a function of the electronic structure of the material and of the orientation of the domain wall with respect to the main crystal directions. For this we have to go beyond the approximated (non-self-consistent) analytical solutions derived in the previous chapter for simplified gap functions (step-like and simple smooth ansatz). Our aim here is to derive numerically the full self-consistent solution of the Eilenberger equations for the quasi-classical Green’s functions. We will see that the most stable domain wall configurations are in very good qualitative agreement with the results obtained from the Ginzburg-Landau theory. We can now show how the macroscopic structure of the domain wall depends on the electronic structure of the material and relate the physics of the domain wall to the Andreev bound states present within it.

Let us remind the following important finding of the previous chapter that will play an important role in the interpretation of the results of this chapter. We found that the violation of the Andreev approximation in the vicinity of the singularity points of the Andreev equation (at \( v_x \rightarrow 0 \)) leads to discontinuities in the spectrum at those points such that the topology of the original problem (formulated for the full BdG equation)—that is number of bound state branches that cross the gap and connect continuously the lower continuum to the upper continuum, as predicted by the index theorem—is "broken". We showed this from the approximated analytical solutions to the Andreev equation. Since this feature
Figure 5.1: Fermi surface’s transversal section. The full line shows the Fermi surface of the \( \gamma \)-band obtained for the tight-binding parameters \((\epsilon_0, t_\gamma, t_\gamma') = (-0.4, 0.4, 0.12)\) \[77\] for which the anisotropy parameter is \(\nu = -0.6\). The dashed line shows the isotropic Fermi surface at the same filling. In the text a point \(k_F\) of the Fermi surface will be referenced through its polar angle \(\theta_k\).

of the quasi-classical limit is at a topological level it doesn’t depend on the degree of precision of the solution and it is present in the self-consistent solution as we will see.

Before to proceed we mention the work by Sigrist and Matsumoto \[62\] that is closely related to this chapter in which they gave the self-consistent solution of a \(\pi_\parallel\)-domain wall in the case of an isotropic system. We note that the missing of a fraction of the domain wall bound states (due to the topological pathology mentioned above) has not been acknowledged before.

### 5.2 Quasi-classical equations

In the introduction we have motivated the fact that we restrict ourself to the \(\gamma\)-band of Sr\(_2\)RuO\(_4\). As we have seen in the introduction the chiral \(p\)-wave state is an equal spin pairing state with \(\Delta(k) = \Delta_{z\bar{z}}(k) = \Delta_{\bar{z}z}(k)\) belonging to the \(E_u\) irreducible representation of \(D_{4h}\) (with spin-orbit coupling) such that the gap function can be expanded in terms of the basis functions of this representation \(\{\phi_x(k), \phi_y(k)\}\). Up to the lowest order we have,

\[
\Delta(k, x) = \phi_x(k) \Delta_x(x) + \phi_y(k) \Delta_y(x),
\]

where we have written the spatial variable explicitly\(^2\). \(x\) corresponds to the center of mass coordinate of the Cooper pair and \(k\) is the Fourier component conjugated to the relative coordinate of the Cooper pair, see the appendix 5.A where we derive the mean field theory for superconductivity within the path integral formalism. In the quasi-classical picture the position and momentum operators are commuting such that \(k\) defines the trajectory of the quasiparticle. In the following we take \(k = k_F\) and we define \(\theta_k\) as the polar angle of the point \(k_F\) of the Fermi surface as shown on Fig. 5.1.

Before to proceed we note that all the equations of this section are derived in details in the appendix 5.B.

Let us assume there is a domain wall in the system. We write the domain wall axes as \((x_\perp, x_\parallel) \equiv (x, y)\) (see Fig. 2.1), such that the system is translationally invariant in the \(y\)-direction and inhomogeneous in

\(^1\)Note that at this phenomenological level we can decompose the gap function with any functions \(\{\phi_x, \phi_y\}\) that satisfy the same symmetry. The specific form of these basis functions can be determined given a microscopic model that takes the fundamental interactions into account (Hubbard model). Here we take the simplest form that incorporates the symmetries of the material.

\(^2\)In order to keep notations simple we omitted the temperature. The bulk gap is given by \(\Delta(T) \equiv |\Delta_x(T, \text{bulk})| = |\Delta_y(T, \text{bulk})|\).
the $x$-direction. Moreover we choose the gauge in which the vector potential is given by $A = (0, A_y(x))$ with $A_y(\pm \infty) = 0$.

The Eilenberger equations Eq. (5.70) in the domain wall axes are given by\(^3\)

$$
\begin{align*}
\omega_m + i \frac{e}{c} v_y(\theta_k) A_y(x) + \frac{1}{2} \omega_v(\theta_k) \nabla_x g(\theta_k, x, \omega_m) &= \Delta^*(\theta_k, x) f(\theta_k, x, \omega_m) - \Delta(\theta_k, x) \bar{g}(\theta_k, x, \omega_m), \\
\omega_m + i \frac{e}{c} v_y(\theta_k) A_y(x) - \frac{1}{2} \omega_v(\theta_k) \nabla_x f(\theta_k, x, \omega_m) &= \Delta(\theta_k, x) g(\theta_k, x, \omega_m),
\end{align*}
$$

(5.2)

where $\omega_m = \pi T(2m + 1)$ is the Matsubara frequency. The functions $g, f$ and $\bar{f}$ are the components of the quasi-classical matrix Green’s function in the Nambu formalism. They are defined for a given trajectory of the quasiparticle, $k_F \leftrightarrow \theta_k$, as defined above, and they satisfy the following symmetries,

$$
g(\theta_k \pm \pi, x, \omega_m) = g^*(\theta_k, x, \omega_m), \quad f(\theta_k \pm \pi, x, \omega_m) = -\bar{f}^*(\theta_k, x, \omega_m),
$$

$$
g(\theta_k, x, -\omega_m) = -g^*(\theta_k, x, \omega_m), \quad f(\theta_k, x, -\omega_m) = \bar{f}^*(\theta_k, x, \omega_m).
$$

(5.3)

Schopohl [76] has shown that the Eilenberger equations can be transformed into a system of two decoupled second order differential equations. Parametrizing the quasi-classical Green’s functions as,

$$
\begin{align*}
g(\theta_k, x, \omega_m) &= \frac{1 - a(\theta_k, x, \omega_m) b(\theta_k, x, \omega_m)}{1 + a(\theta_k, x, \omega_m) b(k_F, x, \omega_m)}, \\
f(\theta_k, x, \omega_m) &= \frac{2a(\theta_k, x, \omega_m)}{1 + a(\theta_k, x, \omega_m) b(k_F, x, \omega_m)}, \\
\bar{f}(\theta_k, x, \omega_m) &= \frac{2b(\theta_k, x, \omega_m)}{1 + a(\theta_k, x, \omega_m) b(k_F, x, \omega_m)},
\end{align*}
$$

(5.4)

we find that the functions $a$ and $b$ satisfy the Riccati equations,

$$
\begin{align*}
v_x(\theta_k) \frac{d}{dx} a &= \Delta(\theta_k, x) - \Delta^*(\theta_k, x) a^2 - 2 \left[ \omega_m + i \frac{e}{c} v_y(\theta_k) A_y(x) \right] a, \\
v_x(\theta_k) \frac{d}{dx} b &= -\Delta^*(\theta_k, x) + \Delta(\theta_k, x) b^2 + 2 \left[ \omega_m + i \frac{e}{c} v_y(\theta_k) A_y(x) \right] b.
\end{align*}
$$

(5.5)

These equations have to be integrated for each trajectory, $\theta_k$. If $\omega_m > 0$, a stable numerical procedure is to integrate the equation for $a$ in the positive $v_x$-direction and $b$ in the negative $v_x$-direction. If $\omega_m < 0$, the direction of integration has to be reversed. We also note that those equations are ill defined when $v_x \rightarrow 0$, that is for $\theta_k = \pm \pi/2$. We seen in the previous chapter that at these directions the quasi-classical approximation is not valid.

The self-consistent gap equation, Eq. (5.77), gives the gap function in terms of the anomalous quasi-classical Green’s function according to,

$$
\left( \begin{array}{c} 
\Delta_x(x) \\
\Delta_y(x)
\end{array} \right) = V_p \pi T \sum_{\omega_m} \frac{d\theta_k}{2\pi} N(\theta_k) \left( \begin{array}{c} 
\phi_x(\theta_k)/\langle \phi_x^2 \rangle \\
\phi_y(\theta_k)/\langle \phi_y^2 \rangle
\end{array} \right) f(\theta_k, x, \omega_m),
$$

(5.6)

where $V_p$ is the norm of the electron pair coupling in the BCS model (see appendix 5.A). Taking the limit $T \rightarrow T_c$, we find the following relation between the dimensionless coupling $\lambda_p = V_p N_0$ and the energy cutoff $\omega_0 = 2\pi T m_0$,

$$
\frac{1}{\lambda_p} = \log \frac{T}{T_c} + \sum_{m=0}^{m_0(T)} \frac{1}{m + 1/2}.
$$

(5.7)

The self-consistent equation for the current density, Eq. (5.78), is given by,

$$
\left( \begin{array}{c} 
J_x(x) \\
J_y(x)
\end{array} \right) = \frac{i e}{\Omega} 2\pi T \sum_{\omega_m} \frac{d\theta_k}{2\pi} N(\theta_k) \left( \begin{array}{c} 
v_x(\theta_k) \\
v_y(\theta_k)
\end{array} \right) g(\theta_k, x, \omega_m),
$$

(5.8)

\(^3\)Note that we have defined the covariant derivative as $\nabla = \frac{\partial}{\partial x} + \frac{e}{c} A$ with $e > 0$, in order to get a current that corresponds to the conventional definition, i.e. positive for positive charge carriers.
where $\Omega$ is the volume of the system.

We get a full self-consistent set of equations by introducing the Maxwell’s equation form which we derive the magnetic induction $B_z$ and the vector potential $A_y$,

$$B_z(x) = -\frac{4\pi}{c} \left( \int_{-\infty}^{x} dx' J_y(x') - \int_{-\infty}^{0} dx' J_y(x') \right), \quad (5.9)$$

$$A_y(x) = \int_{-\infty}^{x} dx' B_z(x'). \quad (5.10)$$

We have chosen the constants of integration such that the following conditions are always satisfied, $B_z(0) = 0$, $A_y(\pm \infty) = 0$.

The spectral function (angle resolved density of states) of the superconducting phase is simply given as,

$$A(\theta_k, x, E) = \Re \{ g(\theta_k, x, \omega_m)_{i\omega_m \to E+i0^+} \} . \quad (5.11)$$

As discussed in the previous chapter, $k_x$ is not a good quantum number in the full quantum model and in the following we will add up the two contributions \{ $k_x(\theta_k), k_x(\pi - \theta_k)$ \} = \{ $k_x, -k_x$ \} (analogous to the wave function approach treated in the previous chapter) such that they become indistinguishable, i.e. we will plot

$$A_\Sigma(\theta_k, x, E) \equiv [A(\theta_k, x, E) + A(\pi - \theta_k, x, E)] . \quad (5.12)$$

The local density of states is given through the sum over all the quasiparticle directions as,

$$D(x, E) = \int \frac{d\theta_k}{2\pi} N(\theta_k) A(\theta_k, x, E) . \quad (5.13)$$

We note that the current density at the Fermi surface point $\theta_k$ can be expressed as,

$$J(\theta_k, x) = \frac{e v(\theta_k) N_0}{\Omega} \int dE A(\theta_k, x, E) \tanh \frac{E}{2T} , \quad (5.14)$$

where, together with Eq. (5.8) and (5.11), we have used the relation,

$$i2\pi T \sum \omega_m g(\theta_k, x, \omega_m) = \int dE \Re \{ g(\theta_k, x, \omega_m)_{i\omega_m \to E+i0^+} \} \tanh \frac{E}{2T} . \quad (5.15)$$

### 5.3 Anisotropy parameters

Following [73] we introduce the anisotropy of the system through the Fermi-surface harmonics. In a two-dimensional system (no dispersion along the $z$-axis) and with the tetragonal symmetry, these are simply given by the components of the Fermi velocity$^5$,

$$\begin{align*}
\cos \theta_k &= \frac{k_x}{k_F} \quad \Rightarrow \quad \phi_x(\theta_k) = \frac{v_x(\theta_k)}{v_F}, \\
\sin \theta_k &= \frac{k_y}{k_F} \quad \Rightarrow \quad \phi_y(\theta_k) = \frac{v_y(\theta_k)}{v_F} .
\end{align*} \quad (5.16)$$

Although we work in the continuous limit we assume an underlying effective tight-binding model in order to have a consistent set of Fermi surface parameters. Taking into account nearest-neighbor ($t_\gamma$) and next-to-nearest-neighbor ($t'_\gamma$) hopping of the $d_{xy}$-Ru-electrons in the Ru-O$_2$ plane, we find the following dispersion relation for the $\gamma$-band$^6$,

$$\epsilon_\gamma(k) = \epsilon_0 - 2t_\gamma (\cos ak_x + \cos ak_y) - 4t'_\gamma \cos ak_x \cos ak_y , \quad (5.17)$$

$^4$We give the plots of a few solutions with the full angle dependence in the appendix 5.D.

$^5$The Fermi velocity is scaled by $v_F := \max v_x(\theta_k)$. We could also use the averaged value $v_{F,av} = [\frac{1}{2\pi} (v_x(\theta_k)^2 + v_y(\theta_k)^2)]^{1/2}$ but at our level (quasi-classical theory) those two definitions are equivalent. We have $v_{F,av}/v_F(\theta = 0) \approx 0.97$ and a change in the definition leads only to minor numerical changes.

$^6$For more details see chapter 6 where we study the lattice model of the system.
with \( \epsilon_0 = \epsilon_{0,\gamma} - \mu \), and \( a \) is the lattice spacing. The Fermi velocity components are given by \( v_i(\theta_k) = \frac{\partial \epsilon_{\gamma}}{\partial k_i} \bigg|_{k_F} \) and we define the normal density of states per spin direction at the Fermi level by

\[
N(\theta_k) = \left[ \frac{S}{2\pi \hbar v_F(\theta_k)} \right],
\]

with \( S \) the surface of the RuO\(_2\) plane. For a given set of parameters \( (\epsilon_0, t_\gamma, t'_\gamma) \) we find a Fermi surface that can be characterized through the anisotropy parameter,

\[
\nu = \frac{\langle v_x^4 \rangle_{FS} - 3\langle v_x^2 v_y^2 \rangle_{FS}}{\langle v_x^2 \rangle_{FS} + \langle v_x^2 v_y^2 \rangle_{FS}}.
\]

(5.19)

Here and in the following \( \langle \cdot \rangle_{FS} \) reads for the average over the Fermi surface weighted by the dimensionless normal density of states, i.e. for some quantity \( O \),

\[
\langle O \rangle_{FS} \equiv \oint \frac{d\theta_k}{2\pi} \frac{N(\theta_k)}{N_0} O,
\]

where \( N_0 \equiv \oint (d\theta_k/2\pi)N(\theta_k) \) is the averaged normal density of states. In the case of an isotropic Fermi surface, i.e. with circular section, we have \( \nu = 0 \). If the Fermi surface has a square section we have \( \nu = \pm 1 \) (+1 if the edges are aligned with the main crystal axes, \(-1\) if they are rotated by an angle \( \theta = \pi/4 \); in general we have \( \nu_{\theta = \pi/4} = -\nu \)). We show in Fig. 5.1 the basal section of the \( \gamma \)-Fermi surface for the isotropic case and for an anisotropic Fermi surface with \( \nu = -0.6 \).

Rotating the domain wall around the \( \hat{z} \)-axis by an angle \( \bar{\theta} \), the reciprocal coordinates attached to the domain wall transform as \((k_{\perp}, k_{\parallel}) = (\cos \bar{\theta}k_x + \sin \bar{\theta}k_y, -\sin \bar{\theta}k_x + \cos \bar{\theta}k_y)\), see Fig. 2.1. In the following we will always work within the domain wall axes and write \((k_{\perp}, k_{\parallel}) \equiv (k_x, k_y)\) (note that the anisotropy parameter is a property of the bulk and it is always defined within the crystal axes). We show in Fig. 5.2 the angular dependence of the bulk gap, \(|\Delta(\theta_k, \text{bulk})| = \Delta(T)v_F(\theta_k)/v_F\), in the domain wall reciprocal axes and for the anisotropy \( \nu = -0.6 \): (a) at \( \bar{\theta} = 0 \), and (b) at \( \bar{\theta} = \pi/4 \).

### 5.4 Domain wall solution

We present here the numerical self-consistent solution of the quasi-classical theory exposed above when a domain wall separates the two degenerate chiral states. All the quantities are scaled according to the scaling factors defined in the appendix 5.C (those are the standard BCS-units).
5.4.1 Gap structure

The structure of a domain wall is defined by the following boundary conditions of the superconducting state (this is fully similar to the definition (2.14) of chapter 2),

\[
(\Delta_x, \Delta_y)_{x=-\infty} = s e^{-i\alpha/2(1, -i)}\Delta(T),
\]

\[
(\Delta_x, \Delta_y)_{x=+\infty} = e^{i\alpha/2(1, i)}\Delta(T),
\]

with the bulk gap defined as \(\Delta(T) \equiv |\Delta_x(T, \text{bulk})| = |\Delta_y(T, \text{bulk})|\) and \(s = \pm 1\) distinguishes between the two types of domain wall: \(s = 1\) for the \(\pi\parallel\)-domain wall (with a \(\pi\)-phase shift of the component \(\Delta_\parallel \equiv \Delta_y\)) and \(s = -1\) for the \(\pi\perp\)-domain wall (with a \(\pi\)-phase shift of the component \(\Delta_\perp \equiv \Delta_x\)). We found in Part I that the \(\pi\parallel\)-domain wall is stable and the \(\pi\perp\)-domain wall is metastable. The phase shift \(\alpha\) is defined as the global gauge-invariant phase shift across the domain wall, i.e. using the parametrization \(\Delta_x = |\Delta_x| e^{i\phi_x}\),

\[
\alpha \equiv \int_{-\infty}^{+\infty} dx \{\partial_x \varphi_x(x) - \gamma A_x(x)\} = \varphi_x(+\infty) - \varphi_x(-\infty),
\]

since in our gauge \(A_x \equiv 0\) (\(\gamma = 2\pi/\Phi_0 = 2e/\hbar c\)). The phase shift of the \(y\)-component is then given by \(\varphi_y(+\infty) - \varphi_y(-\infty) = \pi + \alpha\).

5.4.2 Andreev bound states

The bound states correspond to the poles of the spectral function \(A_{\Sigma}(\theta_k, x, E)\). Since the quasi-classical Eilenberger equations are equivalent to the Andreev equation, we call them the Andreev bound states. We have seen in the previous chapter that, as long as the quasi-classical limit holds, they are related to the topologically protected bound states predicted by the index theorem. In the geometry assumed above, we have on the left hand side of the domain wall the winding number \(c_L = -1\) (Chern number of the ground state), and \(c_R = +1\) on the right hand side. According to the index theorem we expect to find, on the domain wall, a total number of \(|c_R - c_L| = 2\) bound states (per spin direction) that cross the zero-energy line and connect the lower continuum to the upper continuum. However we also found in the previous chapter that the Andreev equation becomes ill-defined in the vicinity of the points at which the quasi-classical limit \((k_\xi \gg 1)\) breaks down. Whenever the important part of the spectrum of the bound states contains those points (depending on the domain wall configuration) we observe spurious discontinuities of the spectrum at those points which can also lead to the disappearance of the zero-energy bound states. We will discuss those features with regard to the numerical solutions presented in the next section.

5.4.3 Numerical results

- \(\nu = 0\)

We show in Fig. 5.3 the self-consistent solution for the two domain wall types (\(\pi\parallel\) and \(\pi\perp\)) in the isotropic case, \(\nu = 0\), i.e. the Fermi surface is circular and the gap is isotropic\(^7\). Fig. 5.3.A shows the \(\pi\parallel\)-domain wall solution and Fig. 5.3.B shows the \(\pi\perp\)-domain wall solution. We found in part I that the \(\pi\parallel\)-domain wall is stable and the \(\pi\perp\)-domain wall is metastable\(^8\). We find for the width of the domain walls, \(\xi_{\pi\parallel}^{(\text{DW})} \approx 4\xi_0\) and \(\xi_{\pi\perp}^{(\text{DW})} \approx 8\xi_0\). We have seen in part I that the narrowest domain wall is in general the most stable. In this case the global phase shift defined above is \(\alpha = 0\). The electromagnetic quantities, \((J_y, A_y, B_z)\), show the well known spontaneous super-current flowing along the domain wall and its screening as we move away from it. As we observed already with the Ginzburg-Landau results the current density in the two domain wall types flows in opposite direction. This will be explained below in terms of the Andreev bound states present at the domain wall.

Before we proceed any further we note the very good qualitative agreement of the full Ginzburg-Landau results presented in chapter 2 with the full self-consistent quasi-classical results presented here.

\(^7\)The results of the \(\pi\parallel\)-domain wall for the isotropic system are identical—up to the scaling factors which we choose differently—with the results presented by Sigrist and Matsumoto in [62].

\(^8\)We can find the metastable solution because our minimization algorithm is not global. Hence if we initiate the program with a gap function configuration that corresponds to the metastable solution we stay locked in this local minimum.
We show the intensity plot of the spectral function at the domain wall in Fig. 5.4, \( A_{\Sigma}(\theta_k, 0, E) \), (the full angle resolution of the spectral function is plotted in Fig. 5.22 (a) of the appendix 5.D). The highest intensity (for instance the poles) corresponds to the dark color range. We clearly see the presence of bound states that we relate to the expected topological Andreev bound states. Furthermore, we see that the spectrum satisfies the symmetry \( A_{\Sigma}(-\theta_k, x, E) = A_{\Sigma}(\theta_k, x, -E) \), which, before summing over the \( \{k_x, -k_x\} \)-contributions, comes from the charge-conjugation symmetry \( A(-k_F, 0, E) = A(k_F, 0, -E) \), see appendix 5.D.

Let us first consider in more details the spectrum of the \( \pi \)-domain wall, shown in Fig. 5.4 (a), together with the local density of states at the domain wall in the bulk, shown in Fig. 5.5 (a). We find Andreev bound states within the sub-gap energy range. However they do not cross the zero-energy line as we would expect from the index theorem! Fig. 5.6 shows the three dimensional plot of the spectral function as a function of \( \theta_k \in [0, \pi] \) and \( E \). We clearly see that the gap does close at \( \theta_k = \pi/2 \), but it is due to the presence of the continuum part of the spectrum (which is very sharp in the \( \theta \)-function as a function of \( \theta \)) and there is no bound states in a finite energy range around zero (Fermi level), i.e. \( E_b \notin [0 - \Delta E, 0 + \Delta E] \). This leads to the fact that the gap remains open in this energy range, as we can see in the local density of states on Fig. 5.5 (a). We note that this feature is also present in the results of Ref. [62] but it was not considered by the authors.

We have seen in the previous chapter that for the trajectories \( \theta_k = \pm \pi/2 \) the Andreev equation is pathological leading to spurious discontinuities in the spectrum of the bound states at those points. We also found that the two Andreev bound state branches touch the zero-energy line if we neglect the vector potential, i.e. \( A_y = 0 \). Hence the gap between the minimum Andreev bound state energy, \( \min(|E_b(\theta_k)|) \) and the zero-energy line is quantified by the value of the vector potential at the domain wall, i.e. \( \Delta E_b \sim A_y(0) \). This is clearly a violation of the topology of the problem and it will be necessary to go beyond the quasi-classical limit in order to find the correct microscopic structure of the domain wall bound states (this is done in the next chapter with the lattice approach).

We consider now the spectrum of the \( \pi_{\perp} \)-domain wall shown in Fig. 5.4 (b). We find that the Andreev bound states reach the zero energy line at \( \theta_k = 0 \), in agreement with our discussion of the Fermi points of the "classical" Hamiltonian of section 4.5. The bound states are clearly seen from the local density of states shown in Fig. 5.5 (b), which shows the complete closing of the gap at the domain wall. Hence there is no breaking of the topology in this case, as we would have expected from the fact that the important part of the spectrum (of the bound states) lies outside the vicinity of the pathological points \( \pm \pi/2 \).

We note that according to the index theorem there should be two crossings of the zero-energy line (per spin). We will see in the section 5.5 of this chapter that the bound state branches of Fig. 5.4 (a) and (b) are in fact doubly degenerated.

The current density can now be well understood in terms of the Andreev bound states and the modulated continuum states at the domain wall. From Eq. (5.14) we can rewrite the current density at an angle \( \theta_k \) as,

\[ J_i(\theta_k, x) = e \delta n(\theta_k, x)v_i(\theta_k), \tag{5.22} \]

with the quasiparticle weight given by,

\[ \delta n(\theta_k, x) = \int_0^{+\infty} dE A(\theta_k, x, E) \tanh \frac{E}{2T} - \int_{-\infty}^0 dE A(\theta_k, x, E) \tanh \frac{|E|}{2T}. \tag{5.23} \]

Considering first the \( \pi_{\parallel} \)-domain wall, Fig. 5.4 (a), we clearly see that for a state in first quadrant, i.e. \( \theta_k \in [0, \pi/2] \), the second term in \( \delta n(\theta_k) \) (that is for \( E < 0 \)) is winning over the first term (for \( E > 0 \)), leading to a negative charge carrier, \( \delta n(\theta_k) < 0 \), and inversely for a state in the fourth quadrant, i.e. \( \theta_k \in [-\pi/2, 0] \). Fig. 5.7 shows the angular dependance of both \( \delta n \) and the quasiparticle velocity. By symmetry the \( x \)-component of the current density vanishes and we get a resultant current density in the negative \( y \)-direction, as we have seen in Fig. 5.3.A.

For the \( \pi_{\perp} \)-domain wall, Fig. 5.4 (b), we see that the situation is inverted : we have for the states \( \theta_k \in [-\pi/2, 0] \), a positive particle weight \( \delta n(\theta_k) > 0 \), and a negative particle weight for the states \( \theta_k \in [0, \pi/2] \). This gives a positive current density in the \( y \)-direction as seen in Fig. 5.3.B. The local density of states at \( x = 0 \) in this case is finite and mostly constant all over the gap.
Figure 5.3: Self-consistent quasi-classical solutions in the isotropic case, \( \nu = 0 \): the gap function components \( \{ \text{Re}\Delta_x, \text{Im}\Delta_x, \text{Re}\Delta_y, \text{Im}\Delta_y \} \), the current density \( J_y \), the vector potential \( A_y \), and the magnetic induction \( B_z \). All the quantities are scaled according to the standard BCS-units defined the appendix 5.C. Fig. A shows the \( \pi_\parallel \)-domain wall solution and Fig. B shows the \( \pi_\perp \)-domain wall solution. The remaining external parameters are chosen \( \kappa_0 = 3.5 \), \( T = 0.2T_c \) and \( \omega_0/2\pi = 10T_c \).
Figure 5.4: Spectral function (angle resolved density of states) at the domain wall, $A_\Sigma(\theta_k, 0, E) \equiv [A(\theta_k, 0, E) + A(\pi - \theta_k, 0, E)]$ (adding up the $\{k_x, -k_x\}$-contributions), for $\nu = 0$.

Figure 5.5: Local density of states, $D(E, x)$, in the bulk (dashed line) and at the domain wall (full line).

• $\nu = -0.6$

We now consider the anisotropic $\gamma$-band of Sr$_2$RuO$_4$ with the tight-binding parameters $(\epsilon_0, t, t') = (-0.4, 0.4, 0.12)$ [77] for which the anisotropy parameter defined in Eq. (5.19) is $\nu = -0.6$. In the following we look at the two following configurations of the domain wall : when it is aligned along one of the main crystal axes, i.e. $\bar{\theta} = 0$; when it is rotated by 45 degrees, i.e. $\theta = \pi/4$.

We start with the case $\bar{\theta} = 0$ shown on Fig. 5.8. The $\pi_\parallel$-domain wall solution is plotted in Fig. A and the $\pi_\perp$-domain wall solution is plotted in Fig. B. We observe a broadening of the domain wall with the widths $\xi_{\text{DW}}^{(\pi_\parallel)} \approx 6\xi_0$ and $\xi_{\text{DW}}^{(\pi_\perp)} \approx 10\xi_0$. The global phase shift is still zero, $\alpha = 0$. Except for a slight suppression, the general features of the electromagnetic quantities are conserved.

Fig. 5.9. (a) and (b) show the corresponding spectral function, $A_\Sigma(\theta_k, 0, E)$ (the full angle resolution is showed in Fig. 5.22 (b) in the appendix 5.D). Except for the orbital anisotropy of the continuum
Figure 5.6: Three dimensional plot of the spectral function at the domain wall, \( A(\theta_k, 0, E) \), of the \( \pi_\parallel \)-domain wall, for \( \nu = 0 \). We take here \( \theta_k \in [0, \pi] \).

Figure 5.7: Angle dependance of the quasiparticle weight \( \delta n(\theta_k) \) in \( J_i(\theta_k) = e\delta n(\theta_k)v_i(\theta_k) \), computed from the spectral function, Eq. (5.23), for the \( \pi_\parallel \)-domain wall and for \( \nu = 0 \). The origin of the radial direction is taken at the dashed circle such that the red (blue) line is for positive (negative) values and corresponds to a hole-like (resp. electron-like) quasiparticle current.
A : $\pi_\parallel$-domain wall, $(\nu, \bar{\theta}) = (-0.6, 0)$  
B : $\pi_\perp$-domain wall, $(\nu, \bar{\theta}) = (-0.6, 0)$

Figure 5.8: Self-consistent quasi-classical solutions for an anisotropic system with $\nu = -0.6$ and for the domain wall’s angle $\bar{\theta} = 0$: the gap function components $\{\text{Re}\Delta_x, \text{Im}\Delta_x, \text{Re}\Delta_y, \text{Im}\Delta_y\}$, the current density $J_y$, the vector potential $A_y$, and the magnetic induction $B_z$. Fig.A shows the $\pi_\parallel$-domain wall solution and Fig.B the $\pi_\perp$-domain wall solution. All the quantities are scaled according to the standard BCS-units defined in the appendix 5.C. The external parameters are $\kappa_0 = 3.5$, $T = 0.2T_c$ and $\omega_0/2\pi = 10T_c$.

spectrum, the main features are the same as discussed above for the isotropic case. The local density of states is shown on Fig. 5.10 (a) and (b), in the bulk (dashed line) and at the domain wall (full line). We find a narrowing of the gap due to the anisotropy. As for the isotropic case, the breaking of the topology is explicit in the $\pi_\parallel$-domain wall (with the missing of a part of the spectral weight from the domain wall bound states), and, the gap is fully closed at the $\pi_\perp$-domain wall.

The results for a rotated domain wall with the angle $\bar{\theta} = \pi/4$ is shown in Fig. 5.11. In this case, the $\pi_\perp$-domain wall is unstable and we only find the $\pi_\parallel$-domain wall solution. We see that the components $\{\text{Im}\Delta_x, \text{Re}\Delta_y\}$ acquire now a spatial structure. In particular, we observe a global phase shift of the gap function across the domain wall, i.e. $\alpha(\bar{\theta} = \pi/4) \neq 0$. Specially at the angles $\bar{\theta} = \pm\pi/4$, the solution is doubly degenerated with $\alpha = \pm|\alpha|$. This result is in agreement with the Ginzburg-Landau findings presented in chapter 2. We list in Tab. 5.1 the values of the global domain wall phase shift for different tight-binding parameters taken from Ref. [82, 77, 80, 81]. We will come back to this below.
(a) $\pi_\parallel$-domain wall, $(\nu, \tilde{\theta}) = (-0.6, 0)$  
(b) $\pi_\perp$-domain wall, $(\nu, \tilde{\theta}) = (-0.6, 0)$

Figure 5.9: Spectral function at the domain wall, $A_\Sigma(\theta_k, 0, E)$, for $\nu = -0.6$ and $\tilde{\theta} = 0$.

(a) $\pi_\parallel$-domain wall, $(\nu, \tilde{\theta}) = (-0.6, 0)$  
(b) $\pi_\perp$-domain wall, $(\nu, \tilde{\theta}) = (-0.6, 0)$

Figure 5.10: Local density of states $D(E, x)$, in the bulk (dashed line) and at the domain wall (full line).

<table>
<thead>
<tr>
<th>Ref.</th>
<th>$(\epsilon_0, t_\gamma, t'_\gamma)$</th>
<th>$\nu$</th>
<th>$\alpha(\tilde{\theta} = \pi/4)$</th>
<th>[rad]</th>
</tr>
</thead>
<tbody>
<tr>
<td>[82]</td>
<td>$(-0.62, 0.42, 0.17)$</td>
<td>-0.23</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>[77]</td>
<td>$(-0.4, 0.4, 0.12)$</td>
<td>-0.6</td>
<td>0.183</td>
<td></td>
</tr>
<tr>
<td>[80, 81]</td>
<td>$(0.5, 0.44, 0.14)$</td>
<td>-0.62</td>
<td>0.1994</td>
<td></td>
</tr>
</tbody>
</table>

Table 5.1: Global gauge-invariant phase shift across a rotated domain wall for selected tight-binding parameters found in the literature.

The electromagnetic functions, $(J_y, B_z, A_y)$, have the same general features as for the previous cases. Fig. 5.12 (a) shows the spectral function at the domain wall, $A_\Sigma(\theta_k, 0, E)$ (the full angle resolution is showed in Fig. 5.22 (c)). In this case the Andreev bound states are split into two branches that cross the zero-energy line at the points $\theta_0 \approx \pm \pi/4$. As we did in the section 4.5, we can relate the position of
the zero-energy states to the structure of the self-consistent gap function. From the definition (5.1), we find that the gap function of a $\pi_\parallel$-domain wall vanishes under the following condition,

$$0 < \frac{\phi_y(\theta_0)}{\phi_x(\theta_0)} = \frac{|\text{Re}\Delta_x(0)|}{|\text{Re}\Delta_y(0)|} < +\infty,$$

(5.24)

from which we find that the Andreev bound states have to cross the zero-energy line at the points $\pm\theta_0$ with $0 < \theta_0 < \pi/2$. Note that taking the vector potential into account, $A_y(0) \neq 0$, there is a small correction to the equation (5.24).

The density of states in the bulk and at the domain wall is shown in Fig. 5.12 (b). We clearly see the closing of the gap at the domain wall.

Comparing Fig. 5.9 (a) and Fig. 5.12 (a), we see that the zero-energy Andreev bound states are driven towards the vicinity of the bulk gap minima (we will see in the chapter 6 that those points of the Fermi surface are the closest to the van Hove singularity points—or the zeros of the gap—in a lattice model).

Let us now come back to the phase shift across the domain wall, $\alpha$. We find a phase transition driven by the anisotropy with a critical value $\nu_c$ (with the value $\nu_c = -0.52$ at $\bar{\theta} = \pi/4$) above which $\alpha = 0$, and below which the zero-energy Andreev bound states lie at $\theta_k = \pm\theta_0$ ($0 < \theta_0 < \pi/2$) such that $\alpha \neq 0$ : see Fig. 5.13 with the spectral function for $\bar{\theta} = \pi/4$ potted (a) for $\nu = -0.51$, and (b) for $\nu = -0.53$.

We summarize the domain wall structure discussed in this section with the phase diagram shown in Fig. 5.14 that contains both the results of the quasi-classical theory (dots) and the Ginzburg-Landau theory (full line). We observe a good qualitative agreement between the two approaches. The fluctuations in the dots are due to the fact that the quasi-classical solution is not only determined by the anisotropy parameter which is an averaged quantity over the Fermi surface. Different anisotropy parameters correspond to different Fermi surface parameters, such that the dots in the phase diagram represent systems with different microscopic structures and we do not expect the values of $\alpha$ to be smooth as a function of $\nu$. On the other hand, the microscopic information is averaged out in the Ginzburg-Landau approach and we do not expect a quantitative agreement with the quasi-classical approach. To be taken into account is also the fact that the two approaches have different typical temperature ranges : we took $T = 0.2T_c$ in the quasi-classical approach, whereas $T \lesssim T_c$ in the Ginzburg-Landau approach.
Figure 5.11: Self-consistent quasi-classical solutions for an anisotropic system with \( \nu = -0.6 \) and with the domain wall rotated by an angle \( \theta = \pi/4 \): the gap function components \( \{ \text{Re}\Delta_x, \text{Im}\Delta_x, \text{Re}\Delta_y, \text{Im}\Delta_y \} \), the current density \( J_y \), the vector potential \( A_y \), and the magnetic induction \( B_z \). Only the \( \pi_\parallel \)-domain wall solution is stable. All the quantities are scaled according to the standard BCS-units given in the appendix 5.C. The external parameters are \( \kappa_0 = 3.5, T = 0.2T_c \) and \( \omega_0/2\pi = 10T_c \).
\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig5.12.pdf}
\caption{(a) Spectral function at the domain wall, \(A_\Sigma(\theta_0, 0, E)\), for \(\nu = -0.6\) and \(\bar{\theta} = \pi/4\).\newline
Fig. (b) : Local density of states \(D(E, x)\), in the bulk (dashed line) and at the domain wall (full line).}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig5.13.pdf}
\caption{(a) \((\nu, \bar{\theta}) = (-0.51, \pi/4)\) \quad (b) \((\nu, \bar{\theta}) = (-0.53, \pi/4)\)}
\end{figure}

\section{5.5 Effect of a barrier at the domain wall}

In this section we look at the effect of introducing a potential barrier at the domain wall. This allows us to show how the smooth transition from a domain wall configuration to an edge and show how it relates
Figure 5.14: Phase diagram of the global gauge-invariant phase shift across a domain wall, $\alpha$, and the anisotropy of the Fermi surface, $\nu$. The dots represent the quasi-classical solution and the full line the Ginzburg-Landau solution at $\bar{\theta} = \pi/4$. The dashed line gives the results at $\bar{\theta} = 0$, i.e. $\alpha = 0$.

to the Andreev bound states and the predictions of the index theorem.

We assume that the quasiparticles are scattered specularly at the interface, i.e. the momentum parallel to the surface is conserved, $k_{F,x} = k_{F,x}^{\text{out}}$. For each direction $\theta_k$, we define the four momenta that contribute to a scattering process at the interface as \{${k_{l,\text{in}}, k_{l,\text{out}}, k_{r,\text{in}}, k_{r,\text{out}}}$\}, see Fig. 5.15. For specular scattering, the explicit solution of the Zaitsev’s boundary conditions [85] for the functions $a$ and $b$ (in the Riccati parametrization) is given by [86, 87],

$$ a_{l}^{1/r} d_{out}^{1/r} = \frac{a_{l}^{1/r} T (1 + a_{l}^{1/r} b_{out}^{1/r}) + a_{l}^{1/r} R (1 + a_{l}^{1/r} b_{out}^{1/r})}{T (1 + a_{l}^{1/r} b_{out}^{1/r}) + R (1 + a_{l}^{1/r} b_{out}^{1/r})}, $$

$$ b_{l}^{1/r} d_{in}^{1/r} = \frac{b_{l}^{1/r} T (1 + a_{l}^{1/r} b_{in}^{1/r}) + b_{l}^{1/r} R (1 + a_{l}^{1/r} b_{in}^{1/r})}{T (1 + a_{l}^{1/r} b_{in}^{1/r}) + R (1 + a_{l}^{1/r} b_{in}^{1/r})}, $$

where $T = T(\theta_k)$ is the angle dependent transparency of the interface, and the reflectivity is simply given by $R(\theta_k) = 1 - T(\theta_k)$. For a $\delta$-barrier at the interface with the potential $U_0 \delta(x)$, the transparency

$\Delta^* = e^{-i\alpha/2(1, -i)}$ \quad $\Delta = e^{i\alpha/2(1, i)}$

Figure 5.15: Scattered states at a domain wall with a potential barrier.
Figure 5.16: Self-consistent quasi-classical solutions at \((\nu, \bar{\theta}) = (-0.6, \pi/4)\) for different barrier transparencies, \(T_0\).

is given by [88],

\[
T(\theta_k) = T_0 \frac{\cos^2 \theta_k}{1 - T_0 \sin^2 \theta_k},
\]

with \(T_0 = Z^2/(1 + Z^2) \in [0, 1]\) and \(Z = mU_0/(\hbar^2 k_F)\).

We first consider the physical case \((\nu, \bar{\theta}) = (-0.6, \pi/4)\). We show in Fig. 5.16 the self-consistent quasi-classical solutions for \((\nu, \bar{\theta}) = (-0.6, \pi/4)\) at different values of the transparency: \(T_0 = 0.9, 0.5, 0\). We find that in the two limiting cases \((T_0 = 1 \text{ and } 0)\) the role played by the \(x\)- and \(y\)-components of the gap function is inverted, and accordingly the current density changes sign. Furthermore we find that the global phase shift, \(\alpha\), is suppressed as we decrease the transparency.

Fig. 5.17 shows the corresponding spectral function on the right side of the interface, i.e. \(A_\Sigma(\theta_k, 0^+, E)\). We find that the zero-energy Andreev bound states are shifted from \(\theta_k = \pm \pi/2\) towards \(\theta_k = 0\) as we increase the barrier potential. The limit of an infinite barrier is equivalent to the edge configuration: we found in the previous chapter that, as a result of the charge-conjugation symmetry and the specular scattering condition, there is one bound state, the chiral edge state, crossing the zero-energy line at \(\theta_k = 0^9\). In agreement with the index theorem we find two bound states branches that cross the zero-energy line which eventually merge at \(T_0 = 0\). We will come back to this below.

We finally note that as we decrease the transparency, according to the expression (5.23) the negative-energy states in the third and forth quadrants become more populated and we expect the current density to change sign, as we have just seen in Fig. 5.16.

\[9\text{This is goes as the following. From the charge-conjugation symmetry of the system we have (i) } E(-k_F) = -E(k_F). \text{ Furthermore the states } k_{F\perp} \text{ and } -k_{F\perp}, \text{ where } k_{F\perp} \text{ is the direction perpendicular to the surface, are connected through the specular scattering, such that (ii) } E(-k_{F\perp}) = E(k_{F\perp}). \text{ Taking (i) and (ii) together we find } E(-k_{F\perp}) = -E(k_{F\perp}) = E(k_{F\perp}), \text{ that is } E(k_{F\perp}) = 0 !\]
Figure 5.17: Spectral function on the right hand side of the interface, $A_{\Sigma}(\theta_k, 0^+, E)$, for different values of the transparency, $T_0 = 0.9, 0.5, 0$, for $(\nu, \bar{\theta}) = (-0.6, \pi/4)$.

Figure 5.18: Local density of states in the bulk (dashed line) and at the domain wall (full line), $D(E, 0)$.

Figure 5.19: Global phase shift across the domain wall, $\alpha$, as a function of the barrier transparency, $T_0$, for $\nu = -0.6$ and $\bar{\theta} = \pi/4$. At zero transparency all values of $\alpha$ are allowed due to the gauge invariance.
Figure 5.20: Spectral function on the right hand side of the interface, $A\Sigma(\theta_k, 0^+, E)$, at different values of the transparency $T_0$, for $\nu = 0$.

Figure 5.21: Local density of states at the interface, $D(0, E)$, at different values of the transparency $T_0$, for $\nu = 0$.

We show the local density of states in Fig. 5.18 for the same values of the transparency. We find two sub-gap peaks coming from the higher concentration of Andreev bound states as we can see in Fig. 5.17.

Fig. 5.19 gives the diagram of the global gauge-independent phase shift across the domain wall, $\alpha$, at fixed $\nu = -0.6$ and $\theta = \pi/4$, as a function of the barrier transparency, $T_0$. We find a critical value of the transparency $T_{0,c}$ under which $\alpha$ is completely suppressed. We note that, whereas the gauge phase is arbitrary for an infinite barrier, i.e. $T_0 = 0$ (represented by the dashed vertical line), it becomes unstable as soon as the transparency is non zero and the self-consistent solution relaxes to the $\pi_{||}$-domain wall solution.
5.5.1 From a domain wall to an edge

We finish this section by discussing the transition from a domain wall to an edge in the case of an isotropic system ($\nu = 0$) from a topological point of view (we only consider the $\pi_0$-domain wall type). We show the spectral function at the right hand side of the interface, $A_C(\theta_k, 0^+, E)$, and the local density of states, $D(E, x)$, in Fig. 5.20 and Fig. 5.21, respectively.

On the one hand, we find that as soon as we introduce a finite barrier potential—starting at $T_0$ with the spectral function of Fig. 5.4 (a)—the two Andreev bound state branches split into two branches, such that one branch in each region of the Fermi surface (for $\theta_k \in [-\pi/2, 0]$ and $\theta_k \in [0, \pi/2]$ respectively) crosses the zero-energy line. Hence we recovered the topological structure of the full quantum model, i.e. we have two crossings as predicted by the index theorem. From this we can conclude that there is a quantum phase transition in the Andreev model at $T_0 = 1$. We note that this is absent of the exact quantum model for which the zero energy bound states (and the number of crossings) are conserved.

On the other hand, as we increase further the barrier we find that the two Andreev bound state branches that cross the zero-energy line get closer, till we reach an infinite barrier for which they merge. Actually when the barrier is infinite the two sides of the interface are disconnected and we still have two bound state branches crossing the zero-energy line with one on each side of the interface. Hence the total number of crossings is conserved. We note that the bound state spectrum of Fig. 5.20 (d) corresponds to the chiral edge states found on the left edge that separates the bulk from the vacuum. If we remove one half of the system (say the left side) we are then left with only one crossing (the single chiral edge state at the left edge) as we expect from the index theorem, $|C_L - C_R| = |0 - 1| = 1$.

We finish this section by noting that, as we have shown in the sections 4.3.1 and 4.3.1, the Zaitsev boundary conditions are derived for the quasi-classical Green’s functions such that they hold only when the Andreev approximation is valid (i.e. the quasi-classical limit $k_F \xi_{DW} \gg 1$). As we expect from this and as we explained in the previous chapter, the Zaitsev boundary conditions do not guarantee the correct topological structure of the spectrum. Is then necessary to go beyond the quasi-classical approximation.

5.6 Conclusions

We have found a very good qualitative agreement with the domain wall structure obtained with the Ginzburg-Landau theory. This allowed us to explain several important features of the domain walls. (1) We have seen that the spontaneous current flowing along the domain wall is carried by the bound states present at the domain wall. This was first reported by Sigrist and Matsumoto in [62]. We also show here how this current depends on the domain wall type: the change of configuration of the bound states leads to the reversal of the current’s flow. (2) We have studied the effect of the anisotropy of the electronic structure of the material (electronic band and gap function) as well as the effect of the orientation of the domain wall. We have shown that for a realistic electronic anisotropy we find a non-zero global phase shift through the domain wall in its most stable configuration, assuming that it is tilted from the main crystal axes (see chapter 2). (3) We have given the electronic signature of the Andreev bound states of the different domain walls. However those results have to be taken with cautiousness as we have seen that the topology of the full quantum problem can be broken in the quasi-classical limit. (4) Finally we have shown that the introduction of a strong potential barrier at a domain wall leads to the suppression of the phase shift across the domain wall. However a soft barrier between the two opposite chiral states might lead to the possibility to observe unconventional Josephson effects as a function of the external magnetic field.

We conclude this chapter with the two important following remarks. First, by assuming the same angular dependence of the electronic band dispersion and the gap function (by taking $\phi_i = \bar{v}_F \xi$ for $i = x, y$) we cannot disentangle the effect of the anisotropy of the Fermi surface from the anisotropy of the gap function. Their microscopic origin is intrinsically different (hopping versus pairing) and it is interesting to know what of the two is the leading factor on the domain wall structure. This question can be easily solved within a lattice model where the anisotropy of the material comes naturally in the problem (we will see that the gap function anisotropy is the leading factor).

Second, we have seen that depending on the domain wall configuration the topology of the problem can be broken in the quasi-classical limit. Indeed, there are discontinuities in the spectrum of the Andreev bound states, i.e. the lower energy continuum is not connected smoothly to the upper continuum.
the top of that, we have seen that in the case of a $\pi_\parallel$-domain wall in an isotropic system, a fraction of
the spectral weight of the domain wall bound states is missing, leaving the gap opened at the domain
wall. This violation of the index theorem is clearly a spurious effect due to the breaking down of the
Andreev (quasi-classical) approximation. As a consequence, even if the macroscopical structure of the
domain wall looks reasonable, this approach should be taken with cautiousness in studying the spectral
signature of the bound states.

For those two reasons it is necessary to go beyond the quasi-classical limit. In the next chapter we
study the lattice model of the system which constitutes the full quantum version of the problem and
overcomes the limitations that we have encountered with the quasi-classical theory.
Appendix

5.A Free energy from the path integral formalism

We start with the BCS Hamiltonian

\[ \hat{H} = \hat{H}_0 + \hat{H}_{\text{int}} \]

\[ \hat{H}_0 = \int_\Omega d^3r \sum_\sigma \psi_\sigma^\dagger(r, \tau) \left( -\nabla^2 \frac{1}{2m} - \mu \right) \psi_\sigma(r, \tau) \]

\[ \hat{H}_{\text{int}} = -\frac{1}{2} \int_0^\beta d\tau \int_\Omega d^3r_1 \int_\Omega d^3r_2 \sum_{\sigma_1, \sigma_2} [V_{\sigma_1, \sigma_2}(r_1-r_2)] \Phi_{\sigma_1, \sigma_2}^\dagger(r_1, r_2; \tau) \Phi_{\sigma_1, \sigma_2}(r_1, r_2; \tau), \]

where we consider an attractive interaction, i.e. \( V > 0 \), and where

\[ \Phi_{\sigma_1, \sigma_2}^\dagger(r_1, r_2; \tau) := \psi_{\sigma_1}^\dagger(r_1, \tau) \psi_{\sigma_2}^\dagger(r_2, \tau) \quad (5.27) \]

\[ \Phi_{\sigma_1, \sigma_2}(r_1, r_2; \tau) := \psi_{\sigma_2}(r_2, \tau) \psi_{\sigma_1}(r_1, \tau) \quad (5.28) \]

5.A.1 Grassmann path integral

We define the partition function as

\[ Z := \text{Tr} \left\{ e^{-\beta \hat{H}} \right\}. \quad (5.29) \]

We define now the partition function in the path integral formalism with the \( c \)-numbers (Grassmann numbers)

\[ \Phi_{\sigma_1, \sigma_2}^\dagger(r_1, r_2; \tau) := \psi_{\sigma_1}^\dagger(r_1, \tau) \psi_{\sigma_2}^\dagger(r_2, \tau) \quad (5.30) \]

\[ \Phi_{\sigma_1, \sigma_2}(r_1, r_2; \tau) := \psi_{\sigma_2}(r_2, \tau) \psi_{\sigma_1}(r_1, \tau) \quad (5.31) \]

that is

\[ Z_{\beta, \mu} = \int \mathcal{D}[\psi^\dagger] \mathcal{D}[\psi] e^{-S_{\beta, \mu}} \]

\[ S_{\beta, \mu} = S_0 + S_{\text{int}} \]

\[ S_0 = \int_0^\beta d\tau \int_\Omega d^3R \sum_\sigma \psi_\sigma^\dagger(R, \tau) \left( \frac{\partial}{\partial \tau} - \frac{\nabla^2}{2m} - \mu \right) \psi_\sigma(R, \tau) \]

\[ S_{\text{int}} = -\frac{1}{2} \int_0^\beta d\tau \int_\Omega d^3r_1 \int_\Omega d^3r_2 \sum_{\sigma_1, \sigma_2} V_{\sigma_1, \sigma_2}(r_1-r_2) \Phi_{\sigma_1, \sigma_2}^\dagger(r_1, r_2; \tau) \Phi_{\sigma_2, \sigma_1}(r_2, r_1; \tau). \]

Performing the Hubbard Stratonovitch transformation we get (with Einstein summation convention
for the spin)

\[ e^{-S_{\text{int}}} = \exp \left[ \frac{1}{2} \int_{0}^{\beta} d\tau \int_{\Omega} d^{3}r_{1} \int_{\Omega} d^{3}r_{2} V_{\sigma_{1},\sigma_{2}}(r_{1},r_{2}) \Phi_{\sigma_{1,\sigma_{2}}}(r_{1}) \Phi_{\sigma_{2,\sigma_{1}}}(r_{2}) \right] \]

\[ \propto \int \mathcal{D}[\Delta^{*}, \Delta] \exp \left[ -\frac{1}{2} \int_{0}^{\beta} d\tau \int_{\Omega} d^{3}r \int_{\Omega} d^{3}r V_{\sigma_{1},\sigma_{2}}^{-1}(r_{1},r_{2}) \Delta_{\sigma_{1},\sigma_{2}}(r_{1},r_{2};\tau) \Delta_{\sigma_{2},\sigma_{1}}(r_{2},r_{1};\tau) \right] \times \exp \left[ \frac{1}{2} \int_{0}^{\beta} d\tau \int_{\Omega} d^{3}r_{1} d^{3}r_{2} \Delta_{\sigma_{1},\sigma_{2}}^{*}(r_{1},r_{2};\tau) \Phi_{\sigma_{2,\sigma_{1}}}(r_{2},r_{1};\tau) \right] + \frac{1}{2} \int_{0}^{\beta} d\tau \int_{\Omega} d^{3}r_{1} d^{3}r_{2} \Delta_{\sigma_{2},\sigma_{1}}(r_{2},r_{1};\tau) \Phi_{\sigma_{1,\sigma_{2}}}(r_{1},r_{2};\tau) \]

or in relative and center of mass coordinates

\[ e^{-S_{\text{int}}} = \exp \left[ \frac{1}{2} \int_{0}^{\beta} d\tau \int_{\Omega} d^{3}R \int_{\Omega} d^{3}r V_{\sigma_{1},\sigma_{2}}(R + r/2, R - r/2) \right. \]

\[ \Phi_{\sigma_{1,\sigma_{2}}}(R + r/2, R - r/2;\tau) \Phi_{\sigma_{2,\sigma_{1}}}(R - r/2, R + r/2;\tau) \]

\[ \propto \int \mathcal{D}[\Delta^{*}, \Delta] \exp \left[ -\frac{1}{2} \int_{0}^{\beta} d\tau \int_{\Omega} d^{3}R \int_{\Omega} d^{3}r V_{\sigma_{1},\sigma_{2}}^{-1}(R + r/2, R - r/2) \right. \]

\[ \left. \Delta_{\sigma_{1},\sigma_{2}}(R + r/2, R - r/2;\tau) \Delta_{\sigma_{2},\sigma_{1}}(R - r/2, R + r/2;\tau) \right] \times \exp \left[ \frac{1}{2} \int_{0}^{\beta} d\tau \int_{\Omega} d^{3}R \int_{\Omega} d^{3}r \left( \Delta_{\sigma_{1},\sigma_{2}}^{*}(R + r/2, R - r/2;\tau) \Phi_{\sigma_{2,\sigma_{1}}}(R - r/2, R + r/2;\tau) \right. \right. \right. \]

\[ \left. \left. \left. + \Delta_{\sigma_{2},\sigma_{1}}(R - r/2, R + r/2;\tau) \Phi_{\sigma_{1,\sigma_{2}}}(R + r/2, R - r/2;\tau) \right) \right) \right) \]

where we have introduced relative and center of mass coordinates and wave vectors

\[ r = r_{1} - r_{2} \quad ; \quad R = \frac{r_{1} + r_{2}}{2}, \] (5.32)

We have the Fourier expansions

\[ \Phi^{*}(r_{1}, r_{2};\tau) = \psi^{*}(r_{1},\tau) \psi^{*}(r_{2},\tau) \]

\[ = \frac{1}{\beta^{3}} \sum_{\omega_{m},\omega_{m}'} \sum_{k_{1},k_{2}} e^{i(\omega_{m} + \omega_{m}')\tau - i(k_{1} r_{1} + k_{2} r_{2})} \psi^{*}(k_{1},\omega_{m}) \psi^{*}(k_{2},\omega_{m}') \]

\[ = \frac{1}{\beta^{3}} \sum_{\omega_{m},\omega_{m}'} \sum_{k_{q}} e^{i(\omega_{m} + \omega_{m}')\tau - i(k \cdot r + q \cdot R)} \psi^{*}(k + q/2,\omega_{m}) \psi^{*}(-k + q/2,\omega_{m}') \]

\[ \Phi(r_{2}, r_{1};\tau) = \frac{1}{\beta^{3}} \sum_{\omega_{m},\omega_{m}'} \sum_{k_{q}} e^{-i(\omega_{m} + \omega_{m}')\tau + i(k \cdot r + q \cdot R)} \psi(-k + q/2,\omega_{m}) \psi(k + q/2,\omega_{m}') \]

\[ \Delta^{*}(r_{1}, r_{2};\tau) = \Delta^{*}(R + r/2, R - r/2;\tau) \]

\[ = \frac{1}{\Omega} \sum_{\omega_{l}} \sum_{k} e^{i\omega_{l} \tau - i k \cdot R} \Delta^{*}(k, R, \omega_{l}) \]

\[ \Delta(r_{2}, r_{1};\tau) = \Delta(R - r/2, R + r/2;\tau) \]

\[ = \frac{1}{\Omega} \sum_{\omega_{l}} \sum_{k} e^{-i\omega_{l} \tau + i k \cdot R} \Delta(k, R, \omega_{l}) \]

where we have defined

\[ \Delta^{*}(k, R, \omega_{l}) := \frac{1}{\beta} \int_{0}^{\beta} d\tau \int d^{3}r e^{-i\omega_{l} \tau + i k \cdot R} \Delta^{*}(R + r/2, R - r/2;\tau) \]

\[ \Delta(k, R, \omega_{l}) := \frac{1}{\beta} \int_{0}^{\beta} d\tau \int d^{3}r e^{i\omega_{l} \tau - i k \cdot R} \Delta(R - r/2, R + r/2;\tau) \]
where we have introduced relative and center of mass coordinates and wave vectors

$$q = k_1 + k_2; \quad k = \frac{k_1 - k_2}{2},$$

$$k_1 = k + q/2; \quad k_2 = -k + q/2$$

and with the bosonic and fermionic Matsubara frequencies

$$\omega_l = \frac{2\pi l}{\beta}, \quad l \in \mathbb{Z}$$

$$\omega_m = \frac{\pi}{\beta}(2m + 1), \quad m \in \mathbb{Z}.$$  

We write now the result

$$Z_{\beta, \mu} = \int \mathcal{D} [\psi^\dagger] [\psi] e^{-S_{\beta, \mu}}$$

where the modified action is given by

$$-S'_{\beta, \mu} = \left( \frac{1}{\Omega} \int d^3R \right) \sum_k \sum_{\sigma_1, \sigma_2} \psi^\dagger_{\sigma_1}(k, \omega_m) \delta_{\sigma_1, \sigma_2} \left( -i\omega_m + \frac{k^2}{2m} - \mu \right) \psi_{\sigma_2}(k, \omega_m)$$

$$- \frac{\beta}{2\Omega} \int d^3R \sum_k \sum_{\sigma_1, \sigma_2} \tilde{V}^{-1}_{\sigma_1, \sigma_2}(k, k') \Delta^*_{\sigma_1, \sigma_2}(k, R, \omega_l) \Delta_{\sigma_2, \sigma_1}(k', R, \omega_l)$$

$$+ \frac{1}{2\Omega} \int d^3R \sum_k \sum_{\sigma_1, \sigma_2} \left( e^{-iqk R} \Delta_{\sigma_2, \sigma_1}(k, R, \omega_l) \psi^*_{\sigma_1}(k + q/2, \omega_m) \psi^*_{\sigma_2}(-k + q/2, \omega_l - \omega_m) \right.$$

$$+ e^{iqk R} \Delta^*_{\sigma_1, \sigma_2}(k, R, \omega_l) \psi_{\sigma_2}(-k + q/2, \omega_l - \omega_m) \psi_{\sigma_1}(k + q/2, \omega_m)).$$

We have substituted the Fourier transform of the potential

$$\tilde{V}^{-1}_{\sigma_1, \sigma_2}(k, k') := \frac{1}{\Omega} \int_{2\Omega} d^3r \tilde{V}^{-1}_{\sigma_1, \sigma_2}(k + r / 2, R - r / 2) e^{i(k' - k) \cdot r}$$

In the following we only consider particle pairs with time independent gap field \(\omega_l = 0\). (For a homogeneous system we have a vanishing total moment, i.e. \(q = 0\))

### 5.A.2 Nambu Spinor

Introducing the Nambu spinor

$$\Psi(k, \omega_m) = \begin{pmatrix}
\psi_1(k, \omega_m) \\
\psi_1^*(k, \omega_m) \\
\psi^*_1(-k, -\omega_m) \\
\psi^*_1(-k, -\omega_m)
\end{pmatrix}; \quad \Psi^\dagger(k, \omega_m) = \begin{pmatrix}
\psi^*_1(k, \omega_m) & \psi^*_1(k, \omega_m) & \psi_1(-k, -\omega_m) & \psi_1(-k, -\omega_m)
\end{pmatrix}$$

we can rewrite the modified action \(S'_{\beta, \mu}\) as

$$-S'_{\beta, \mu}(\omega_l = 0) = - \frac{\beta}{2\Omega} \int d^3R \sum_k \sum_{\sigma_1, \sigma_2} \tilde{V}^{-1}_{\sigma_1, \sigma_2}(k, k') \Delta^*_{\sigma_1, \sigma_2}(k, R) \Delta_{\sigma_2, \sigma_1}(k', R)$$

$$+ \frac{1}{2\Omega} \int d^3R \sum_k \Psi^\dagger(k, \omega_m) \tilde{G}^{-1}_{\beta, \mu}(R, k, \omega_m) \Psi(k, \omega_m)$$

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with the matrix

\[
-\hat{G}^{-1}_{\beta,\mu}(k, R, \omega_m) := \begin{pmatrix}
-i\omega_m + \xi_k & 0 & \Delta_{\uparrow \downarrow}(k, R) & \Delta_{\uparrow \uparrow}(k, R) \\
0 & -i\omega_m + \xi_k & \Delta_{\downarrow \uparrow}(k, R) & \Delta_{\downarrow \downarrow}(k, R) \\
\Delta_{\uparrow \downarrow}(k, R) & \Delta_{\downarrow \uparrow}(k, R) & -i\omega_m - \xi_k & 0 \\
\Delta_{\uparrow \uparrow}(k, R) & \Delta_{\downarrow \downarrow}(k, R) & 0 & -i\omega_m - \xi_k
\end{pmatrix}.
\]

5.A.3 Free energy

We integrate now the Fermionic fields. We have

\[
Z_{\beta,\mu} = \int D[\psi^*][\psi] e^{-S_{\beta,\mu}} 
\]
\[
\propto \int D[\Delta^*, \Delta] D[\psi^*][\psi] e^{-S'_{\beta,\mu}} 
\]
\[
\propto \int D[\Delta^*, \Delta] e^{-S''_{\beta,\mu}}
\]

We define now the free energy as

\[
\exp\{ -\beta F_{\beta,\mu}[\Delta^*, \Delta] \} := \int D[\psi^*][\psi] \exp\{ -S'_{\beta,\mu} \} 
\]

\[
F_{\beta,\mu}[\Delta^*, \Delta] := \frac{1}{\beta} S''_{\beta,\mu}
\]

we find the free energy per unit volume

\[
F_{\beta,\mu}[\Delta^*, \Delta] = \frac{1}{2\Omega} \int d^3R \sum_{k,k'} \sum_{\sigma_1, \sigma_2} \bar{V}_{\sigma_1, \sigma_2}(k,k') \Delta^*_{\sigma_1, \sigma_2}(k,R) \Delta_{\sigma_2, \sigma_1}(k',R) 
\]
\[
+ \frac{1}{2\beta\Omega} \int d^3R \sum_{\omega_m} \sum_{k} \text{Tr} \log \hat{G}^{-1}_{\beta,\mu}(k, R, \omega_m)
\]

For the chiral p-wave state we have

\[
\hat{\Delta}(k, R) = \begin{pmatrix}
0 & \Delta(k, R) \\
\Delta(k, R) & 0
\end{pmatrix}
\]

where \(\Delta_{\uparrow \downarrow}(k, R) = \Delta_{\downarrow \uparrow}(k, R) := \Delta(k, R) \equiv d_z(k, R)\).

We then have

\[
F_{\beta,\mu}[\Delta^*, \Delta] = \frac{1}{\Omega} \int d^3R \sum_{k,k'} \bar{V}^{-1}(k,k') \Delta^*(k,R) \Delta(k',R) 
\]
\[
+ \frac{1}{\beta} \sum_{\omega_m} \sum_{k} \text{Tr} \log \hat{G}^{-1}(k, R, \omega_m)
\]

where we have used \(\log \det \hat{G}^{-1} = \text{Tr} \log \hat{G}^{-1}\) and where the matrix is now given by

\[
-\hat{G}^{-1}(k, R, \omega_m) = \begin{pmatrix}
-i\omega_m + \hbar^2 (\frac{-i\nabla_R - eA}{2m})^2 - \mu & \Delta(k, R) \\
\Delta^*(k, R) & -i\omega_m - \hbar^2 (\frac{i\nabla_R - eA}{2m})^2 + \mu
\end{pmatrix}.
\]

5.B Derivation of the quasi-classical equations

We start from the BCS-mean field theory for superconductivity within the path integral method (in the weak coupling limit). Then we derive the quasi-classical equations that are used in this section. We eventually derive the Ginzburg-Landau functional of the system giving the expression of all the coefficients in terms of the microscopic parameters. For an other approach based on the wave function solution of the Bogoliubov-de Gennes equation see [78].
5.B.1 Free Energy Functional

The BCS Hamiltonian reads

\[ \mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{int}} \]

\[ \mathcal{H}_0 = \int \Omega d^3R \sum_{\sigma} \psi_1^\dagger(R, \tau) \left( \frac{\nabla_R \cdot \mathbf{e} + e \mathbf{A}}{2m} \right)^2 - \mu + U_{\text{int}}(R) \psi_{\sigma}(R, \tau) \]

\[ \mathcal{H}_{\text{int}} = \frac{1}{2} \int \Omega d^3r_1 \int \Omega d^3r_2 \sum_{\sigma_1,\sigma_2} \tilde{V}_{\sigma_1,\sigma_2}(r_1 - r_2) \psi_{\sigma_1}^\dagger(r_1, \tau) \psi_{\sigma_2}^\dagger(r_2, \tau) \psi_{\sigma_2}(r_2, \tau) \psi_{\sigma_1}(r_1, \tau), \]

where we consider an attractive pair interaction, i.e. \( \tilde{V} < 0 \), (note that \( e > 0 \)). From the path integral method we derive the free energy functional\(^{10}\)

\[ F_{\beta,\mu}[\Delta^*, \Delta, \mathbf{A}] = \frac{1}{2} \int_S d^2R \left\{ \frac{1}{2} \sum_{k,k'} \sum_{\sigma_1,\sigma_2} \tilde{V}_{\sigma_1,\sigma_2}^{-1}(k,k') \Delta^*_{\sigma_1,\sigma_2}(k,R) \Delta_{\sigma_2,\sigma_1}(k',R) \right. \]

\[ + \frac{1}{\beta S} \sum_{\omega_m} \sum_k \det \text{tr} \tilde{G}^{-1}_{\beta,\mu}(k, \mathbf{R}, \omega_m) \right\} \tag{5.48} \]

with \( \beta = 1/k_B T \), and where

\[ \tilde{V}_{\sigma_1,\sigma_2}^{-1}(k,k') = \frac{1}{\Omega} \int_{2\Omega} d^3r \tilde{V}_{\sigma_1,\sigma_2}^{-1}(R + r/2, R - r/2) \psi(k' - k) \cdot r \tag{5.49} \]

is the Fourier transform of the inverse potential between electron pairs, \( \Delta_{\sigma_1,\sigma_2}(k, R) \) is the gap function (introduced through a Hubbard Stratonovitch transformation) and \( \omega_m = \pi T (2m + 1) \) are the Matsubara frequencies. We used the mixed representation, i.e. \( \mathbf{R} = (r_1 + r_2)/2 \) is the center of mass coordinate obtained after Fourier transforming with respect to the relative coordinate of the electron pair \( \mathbf{r} = r_1 - r_2 \). For the chiral p-wave state we have \( \Delta_{\uparrow \downarrow}(k, \mathbf{R}) = \Delta_{\downarrow \uparrow}(k, \mathbf{R}) \equiv \Delta(k, \mathbf{R}) \) (\( \equiv d_\uparrow \)) and \( \Delta_{\uparrow \downarrow}(k, \mathbf{R}) = \Delta_{\downarrow \uparrow}(k, \mathbf{R}) = 0 \). In the following we assume a weak coupling limit such that the interaction is non-zero only in the finite range around the Fermi energy \( (\epsilon_F - \omega_0, \epsilon_F + \omega_0) \), with \( \omega_0 \) the energy cutoff. We thus can rewrite the free energy functional as

\[ F_{\beta,\mu}[\Delta^*, \Delta, \mathbf{A}] = \int_S d^2R \left\{ \frac{1}{2} \sum_{k,k'} \tilde{V}^{-1}(k,k') \Delta^*(k,R) \Delta(k',R) \right. \]

\[ + \frac{1}{\beta S} \sum_{\omega_m} \sum_k \text{tr} \log \tilde{G}^{-1}(k, \mathbf{R}, \omega_m) \right\}, \tag{5.50} \]

with the inverse matrix Green’s function given by

\[ \tilde{G}^{-1}(k, \mathbf{R}, \omega_m) = \begin{pmatrix} i\omega_m - \epsilon & \frac{\Delta(k, \mathbf{R})}{c} - \mu \\ \frac{-\Delta^*(k, \mathbf{R})}{c} & i\omega_m + \epsilon \end{pmatrix} \] \tag{5.51} \]

This is found after we reorganized the action according to the Nambu formalism as

In the quasi-classical limit we assume that the characteristic length scale of the spatial variation of the fields \( \Delta(R) \) and \( \mathbf{A}(R), \xi_0 \), is much larger than the microscopic length scale, i.e. \( \xi_0 \gg 1/k_F \), and we

---

\(^{10}\)The system is assumed to be homogeneous in the z-direction with the volume \( \Omega \equiv L_x L_y \) and the basal section \( S = L_x L_y \) such that the integral over the volume can be simplified as \( \int_\Omega d^3R \equiv L_x \int_0^\Omega d^2R \) with \( \mathbf{R} = (R_x, R_y) \) and in the thermodynamic limit \( \sum_k \rightarrow S \int d^2k/(2\pi)^2 \).

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can linearize the dispersion relation as\(^{11}\)

\[
\epsilon \left( k - i \nabla_R + \frac{e}{c} A(R) \right) - \mu = \xi(k) - i \hbar v(k) \cdot \nabla_R + \frac{\hbar e}{c} v(k) \cdot A(R) + \frac{\hbar^2 c^2}{2m_e^2} A^2(R) + \mathcal{O} \left( |k_F \xi_0|^{23} \right)
\]

\((e > 0),\) where the velocity was defined as \(v(k) = \partial \xi / \hbar \partial \delta k,\) with \(\delta k = -i \nabla_R + \frac{e}{c} A(R).\) In the following we will assume that the reduced energy is smaller than the cutoff \(|\xi| < \omega_0 \ll \epsilon_F\) which allows us to neglect the second order term in \(A\) and to set \(v(k) \approx v(k_F).\) The equation of motion (Gorkov’s equation) for \(\hat{G}\) then reads

\[
[i \omega_m \mathbb{1} - \hat{T}(\xi, \nabla_R, A) - \hat{\Delta}(k, R)] \hat{G}(k, R, \omega_m) = \mathbb{1}
\]

(5.52)

where we introduced the following parametrization

\[
\hat{G} = \begin{pmatrix} G & F \\ F & \hat{G} \end{pmatrix}
\]

(5.53)

with

\[
\hat{T}(\xi, \nabla_R, A) = \begin{pmatrix} \xi - i \hbar v(k_F) \cdot \nabla_R + \frac{\hbar e}{c} v(k_F) \cdot A(R) & 0 \\ 0 & -\xi + i \hbar v(k_F) \cdot \nabla_R + \frac{\hbar e}{c} v(k_F) \cdot A(R) \end{pmatrix}
\]

(5.54)

and with

\[
\hat{\Delta}(k, R) = \begin{pmatrix} 0 & \Delta(k, R) \\ \Delta^*(k, R) & 0 \end{pmatrix}
\]

(5.55)

### 5.3.2 Self-consistent Gap Equation and Current density

We derive the self-consistent gap equation from the minimization of the free energy functional with respect to the gap function, i.e.

\[
\frac{\delta F[\Delta, \Delta, A]}{\delta \Delta^*(k'', R'')} = 0.
\]

(5.56)

In the second term we have to compute

\[
\frac{\delta \log \hat{G}^{-1}(k, R, \omega_m)}{\delta \Delta^*(k'', R'')} = \text{tr} \left\{ \frac{\delta \left[ i \omega_m \mathbb{1} - \hat{T}(\xi, \nabla_R, A) - \hat{\Delta} \right]}{\delta \Delta^*(k'', R'')} \hat{G}(k, R, \omega_m) \right\}
\]

\[
= \frac{\delta F(k, R, \omega_m)}{\delta \Delta^*(k'', R'')}.\]

Noting that

\[
\frac{\delta \Delta^*(k, R)}{\delta \Delta^*(k'', R'')} = \delta_{k, k''} \delta(R - R'') = \delta_{k, k''} \delta(R_x - R_x') \delta(R_y - R_y'),
\]

it reduces to the following equation

\[
\sum_{k'} \hat{V}^{-1}(k'', k') \Delta(k', R'') = -\frac{1}{\beta} \sum_{\omega_m} F(k'', R', \omega_m).
\]
The second term gives

\[ \Delta(k, R''') = -\frac{1}{\beta} \sum_{\omega_m} \sum_{k'''} V(k, k''') F(k''', R''', \omega_m), \]

since \( \sum_{k'''} \hat{V}(k, k''') \hat{V}^{-1}(k''', k') = \delta_{k, k'} \) and we finally get

\[ \Delta(k, R) = -\frac{1}{\beta} \sum_{\omega_m} \sum_{k'} \hat{V}(k, k') F(k', R, \omega_m), \quad (5.57) \]

after substituting \( R'' \to R \) and \( k''' \to k' \). This is the self-consistent gap equation.

We now derive the self-consistent equation for the current density that is obtained through the minimization of the free energy functional with respect to the vector potential. For this we add the magnetic term \( F_{mag} = \int_\Omega \delta \hat{R} \cdot B^2(R)/8\pi \) to the free energy functional. The minimization condition reads

\[ \frac{\delta F[\Delta^*, \Delta, A]}{\delta A(R')} = 0. \quad (5.58) \]

The second term gives

\[
\begin{align*}
\text{tr} \frac{\delta \log \hat{G}^{-1}(k, R, \omega_m)}{\delta A(R')} &= \frac{\delta \log \left[ \omega_m \frac{1}{\hat{G}} - \frac{\hat{\zeta}(\xi, \hat{\nabla} R, A) - \hat{\Delta}}{\hat{G}} \right]}{\delta A(R')}, \\
&= -\text{tr} \left\{ \frac{\delta \hat{\zeta}(\xi, \hat{\nabla} R, A(R))}{\delta A(R')} \hat{G} \right\}, \\
&= -\frac{\hbar e}{c} \left[ \left( \hat{v}(kF) + \frac{\hbar e}{mc} A \right) G - \hat{g}(kF) - \frac{\hbar e}{mc} \hat{G} \right] \hat{G} \frac{\delta A(R)}{\delta A(R')} \\
&= -\frac{\hbar e}{c} \hat{v}(kF) [G - \hat{G}] - \frac{\hbar^2 e^2}{mc} A[G + \hat{G}] \frac{\delta A(R)}{\delta A(R')}. 
\end{align*}
\]

Note that here we have taken the second order term in \( A \) into account.

Since \( \frac{\delta A(R)}{\delta A(R')} = \delta(R - R''') \), the magnetic term gives

\[ \frac{\delta F_{mag}[A]}{\delta A(R''')} = -\frac{L_z}{4\pi} \nabla \times B(R''') = -\frac{L_z}{e} j(R'''). \quad (5.59) \]

We finally have the following equation for the current density

\[ j(R) = -\frac{2\hbar e}{\beta \Omega} \sum_{\omega_m} \sum_{k} \hat{v}(kF) [G(k, R, \omega_m) - \hat{G}(k, R, \omega_m)] - \frac{\hbar^2 e^2}{mc} n A(R), \quad (5.60) \]

where we have introduced the particle density

\[ n(R) = \frac{1}{\beta \Omega} \sum_{\omega_m} \sum_{k} [G(k, R, \omega_m) + \hat{G}(k, R, \omega_m)] = n_0, \quad (5.61) \]

i.e. in the quasi-classical limit the particle density is always identical to the normal particle density \( n_0 \).

### 5.B.3 Quasiclassical equations

We start from the Grokov’s equation

\[ \left[ (\imath \omega_m - \frac{\hbar e}{c} \hat{v}(kF) \cdot A(R)) \hat{i} + (-\xi + i \hat{v}(kF) \cdot \hat{\nabla} R) \hat{\sigma}_3 - \Re \Delta \hat{\sigma}_1 + \Im \Delta \hat{\sigma}_2 \right] \hat{G}(k, R, \omega_m) = \hat{i}, \quad (5.62) \]

\[ ^{12}\text{We will derive it explicitly in the next section.} \]

\[ ^{13}\text{See Introduction to the Microscopic Theory of Superconductivity, N. Kopnin, 1997.} \]
and solution integrated equation, along a closed loop in the complex plane that comprises the real axis, has the

\[ \oint d\xi \tilde{G}_E = \begin{pmatrix} G & F \\ -F & G \end{pmatrix}, \]

where we have introduced the new matrix

and the vector defined by

\[ \vec{w} := (3\Delta, \Re\Delta, \tilde{\omega}_m), \]

with \( \tilde{\omega}_m := \omega_m + i e^{-v_F \cdot A} \) and the Pauli matrices \( \vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3) \). Eilenberger showed that the energy-integrated equation, along a closed loop in the complex plane that comprises the real axis, has the solution

\[ \oint d\xi \tilde{G}_E = -2\pi i \vec{w} \cdot \vec{\sigma}, \]

where \( \vec{a}(k_F, R, \omega_m) \) is determined through the following equation (Eilenberger’s equation)

\[ -i v(k_F) \cdot \nabla_R \vec{a} = 2\vec{\sigma} \times \vec{w}. \]

By doing so it is assumed that the energy-integrated Green’s functions are determined by the poles of the Green’s functions that lie near the Fermi energy. This is the case whenever the quasi-classical limit is valid. Indeed, the characteristic wave vector associated with the fields’ spatial variation is much smaller than the Fermi momentum, i.e. \( k = \xi_\theta^{-1} \ll k_F = a^{-1} \). The quantities obtained, called quasi-classical Green’s functions, do not depend on energy anymore but only on the orientation of the quasiparticle momentum and the pair center-of-mass coordinate. The components of the quasi-classical matrix Green’s function in Eq. (5.62) are defined as

\[ \oint d\xi \hat{G}(k, R, \omega_m) := \hat{g}(k, R, \omega_m) = \begin{pmatrix} -g(k_F, R, \omega_m) & -i f(k_F, R, \omega_m) \\ -i f(k_F, R, \omega_m) & -g(k_F, R, \omega_m) \end{pmatrix}, \]

where we have used the fact that \( \hat{g}(\theta, x, \omega_m) = -g(\theta, x, \omega_m) \), and we can rewrite the equations of motion for \( \hat{g} \) as

\[ -i v(k_F) \cdot \nabla_R \hat{g}(k_F, R, \omega_m) = \begin{pmatrix} i\tilde{\omega}_m & -\Delta(k_F, R) \\ \Delta^*(k_F, R) & -i\tilde{\omega}_m \end{pmatrix} \hat{g}(k_F, R, \omega_m), \]

or

\[ v_F \cdot \nabla_R \hat{g}(k_F, R, \omega_m) = \Delta^*(k_F, R) f(k_F, R, \omega_m) - \Delta(k_F, R) f(k_F, R, \omega_m) \]

\[ (2\tilde{\omega}_m + v_F \cdot \nabla_R) \hat{f}(k_F, R, \omega_m) = 2\Delta(k_F, R) g(k_F, R, \omega_m) \]

\[ (2\tilde{\omega}_m - v_F \cdot \nabla_R) \hat{f}(k_F, R, \omega_m) = 2\Delta^*(k_F, R) g(k_F, R, \omega_m). \]

In the following we use explicit expressions for the coupling and the gap function for the chiral \( p \)-wave state. We expand the coupling and the gap function in terms of Fermi-surface harmonics that have the \( l = 1 \) symmetry\footnote{We can now show the following relation used in the previous section. Using the orthogonality of the basis functions we have}

\[ \sum_{k''} \hat{V}^{-1}(\theta_k, \theta_k') \hat{V}(\theta_k', \theta_k') = \sum_{k''} \frac{(\phi_x \phi_x' + \phi_y \phi_y')(\phi_x \phi_x' + \phi_y \phi_y')}{\langle \phi_x' \phi_x' \rangle} = (\phi_x \phi_x' + \phi_y \phi_y') \sum_{k''} \phi_{k''}^2 \phi_{k''} = \phi_x \phi_x' + \phi_y \phi_y', \]

and

\[ \sum_{k''} \hat{V}^{-1}(\theta_k, \theta_k') \hat{V}(\theta_k', \theta_k') \Delta(\theta_k', R) = \sum_{k''} \frac{\phi_x \phi_x' + \phi_y \phi_y'}{\langle \phi_x' \phi_x' \rangle} \Delta(\theta_k', R) = \sum_{k'} \frac{\phi_x \phi_x' \Delta_x + \phi_y \phi_y' \Delta_y}{\langle \phi_x' \phi_x' \rangle} = \Delta(\theta_k, R), \]

and

\[ \sum_k \phi_x^2(\theta_k) = \langle \phi_x^2 \rangle = \langle \phi_y^2 \rangle. \]
In the corp of the paper we take the two components of the Fermi velocity, i.e. \( \phi_i(\theta_k) = v_{F,i}(\theta_k)/v_F \). The bracketing of a quantity \( \langle A \rangle \) means the average over the Fermi surface weighted by the density of state: \( \langle A \rangle = \int (d\theta_k/2\pi) N(\theta_k) A \) with \( N(\theta_k) = N(\theta_k)/N_0 \) and \( N_0 = \int (d\theta_k/2\pi) N(\theta_k) \).

**Free energy functional**

Using the orthogonality property of the \( \phi_i \) it is easy to show that we can rewrite the free energy per unit surface as\(^{15} \) (in the following we assume only inhomogeneity along the \( x \)-direction)

\[
\frac{F_{\beta,\mu}}{L_y L_z} = \int dx \int_0^{2\pi} \frac{d\theta_k}{2\pi} N(\theta_k) \left[ \frac{|\Delta(\theta_k, x)|^2}{\lambda_p} + \frac{1}{\beta} \sum_{\omega_m} \int d\xi_k \text{tr} \log \tilde{G}^{-1}(k, x, \omega_m) \right]
\]

with \( \lambda_p \equiv V_p N_0 \) and where we have introduced the normal density of states for one spin direction at the Fermi energy

\[
N(\theta_k, \xi_k = 0) = \frac{S k}{2\pi} \left( \frac{d\xi_k}{dk} \right)^{-1} \Bigg|_{k = k_F} = \frac{S k_F(\theta_k)}{2\pi v_F(\theta_k)}.
\]

We perform the \( \xi \)-integration using the following trick (see [74]): We define the function

\[
h(z) := \text{tr} \int d\xi_k \log \left[ \frac{1}{z} i \omega_m \frac{1}{z} \tilde{\zeta}(\xi, \nabla_R, A) - \tilde{\Delta} \right]
\]

\[
h'(z) = \text{tr} \int d\xi_k \frac{-i\omega_m}{z^2} \tilde{G}(k) = -\frac{i\omega_m}{z^2} \text{tr} \tilde{g}(z)
\]

\[
= \frac{\pi\omega_m}{z^2} (g(z) - \tilde{g}(z)) = \frac{2\pi\omega_m}{z^2} g(z),
\]

and the physical quantity (for \( z = 1 \)) is given by

\[
h(1) = h(0) + 2\pi\omega_m \int_0^1 dz \frac{g(z)}{z^2}.
\]  

(5.73)

Here \( \tilde{G}(k, R, \omega_m; z) \) is the solution of the modified Gro'kov equation

\[
\left[ \frac{1}{z} i \omega_m \frac{1}{z} \tilde{\zeta}(\xi, \nabla_R, A) - \tilde{\Delta} \right] \tilde{G}(k, R, \omega_m; z) = 1
\]

(5.74)

and \( \tilde{g}(\theta_k, x, \omega_m; z) \) is the solution of the correspondingly modified Eilenberger equations. We can finally rewrite the free energy as

\[
\frac{F_{\beta,\mu}}{L_y L_z} = \int dx \int_0^{2\pi} \frac{d\theta_k}{2\pi} N(\theta_k) \left[ \frac{|\Delta(\theta_k, x)|^2}{\lambda_p} + \frac{1}{\beta} \sum_{\omega_m} \int dz \frac{g(\theta_k, x, \omega_m; z)}{z^2} \right] + Cst,
\]

(5.75)

in which the constant \( Cst \) contains the contribution from \( h(0) \).

\(^{15}\)We give here an alternative expression for the free energy functional. Substituting the inverted gap equation (5.57)

\[
-\sum_{k'} \tilde{V}^{-1}(k, k') \Delta(k', R) = F(k, R; \tau = 0) = \frac{1}{\beta} \sum \omega_m e^{-i\omega_m 0^+} F(k, R, \omega_m),
\]

we can write the free energy functional as

\[
\frac{F_{\beta,\mu}}{L_y L_z} = \int dx \int_0^{2\pi} \frac{d\theta_k}{2\pi} N(\theta_k) \sum_{\omega_m} \int d\xi_k \left[ \Delta^*(\theta_k, x) F(k, x, \omega_m) + \text{tr} \log \tilde{G}^{-1}(k, x, \omega_m) \right].
\]  

(5.71)
Gap equation and current density

We derive now the quasiclassical version of the self-consistent gap equations. We start from the gap equation derived above

\[ \Delta(k, R) = -T \sum_{\omega_m} \sum_{k'} \tilde{V}(k, k') F(k', R, \omega_m) \]

\[ = -T \sum_{\omega_m} S \int \frac{d^2k'}{(2\pi)^2} \tilde{V}(k, k') F(k', R, \omega_m) \]

\[ = -T \sum_{\omega_m} \int \frac{d\theta'_k}{2\pi} \int d\xi'_k N(\theta'_k, \xi'_k) \tilde{V}(k, k') F(k', R, \omega_m) \]

\[ \approx -T \sum_{\omega_m} \int \frac{d\theta'_k}{2\pi} N(\theta'_k) \tilde{V}(k, k') \int d\xi'_k F(k', R, \omega_m). \]

We then have, using the definition of the anomalous quasiclassical Green’s function \( \int d\xi_k F = \pi f \),

\[ \Delta(\theta_k, R) = V_p \pi \sum_{\omega_m} \int \frac{d\theta'_k}{2\pi} N(\theta'_k) \phi_x(\theta'_k) \phi_y(\theta'_k) f(\theta'_k, R, \omega_m), \]

which can be rewritten as

\[ \left( \frac{\Delta_x(R)}{\Delta_y(R)} \right) = V_p \pi T \sum_{\omega_m} \int \frac{d\theta_k}{2\pi} N(\theta_k) \left( \frac{\phi_x(\theta_k)/\langle \phi_x^2 \rangle}{\phi_y(\theta_k)/\langle \phi_y^2 \rangle} \right) f(\theta_k, R, \omega_m). \]

From the expression of the current density derived above we have (see [?])

\[ j(R) = -\frac{eT}{\Omega} \sum_{\omega_m} \int \frac{d\theta_k}{2\pi} N(\theta_k) v_F(\theta_k) \int d\xi_k (G(k, R, \omega_m) - \bar{G}(k, R, \omega_m)) \]

\[ = eT \sum_{\omega_m} \int \frac{d\theta_k}{2\pi} N(\theta_k) v_F(\theta_k) (i\pi g(k, R, \omega_m) - i\pi \bar{g}(k, R, \omega_m)) \]

\[ = i2\pi \frac{eT}{\Omega} \sum_{\omega_m} \int \frac{d\theta_k}{2\pi} N(\theta_k) v_F(\theta_k) g(k, R, \omega_m). \]

Component-wise we finally have

\[ \left( \frac{j_x(R)}{j_y(R)} \right) = \frac{i2\pi eT}{\Omega} \sum_{\omega_m} \int \frac{d\theta_k}{2\pi} N(\theta_k) \left( \frac{v_x(\theta_k)}{v_y(\theta_k)} \right) g(\theta_k, R, \omega_m). \]

5.5 Ginzburg-Landau functional

Following [79] we expand \( f, \tilde{f} \) and \( g \) in \( z \). The Eilenberger equations now read

\[ \left( \frac{1}{z} + \frac{2\omega_m}{\omega_m + D} \right) f = 2\Delta g \]

\[ \left( \frac{1}{z} - \frac{2\omega_m}{\omega_m - D^*} \right) \tilde{f} = 2\Delta^* g \]

\[ g^2 + f \tilde{f} = 1 \]

with \( D \equiv v_F \cdot \left( \nabla + i \frac{2e}{c} A \right) \). We finally get the superconducting free energy per unit of surface

\[ \frac{\Delta F}{L_y L_z} = \int dx \int_0^{2\pi} \frac{d\theta_k}{2\pi} N(\theta_k) \left\{ \frac{|\Delta(\theta_k, x)|^2}{\lambda_p} + \pi \sum_{0 < \omega_m < \omega_c} \left( -2 \frac{|\Delta|^2}{\omega_m} + \frac{1}{2\omega_m^3} [ |\Delta|^4 + (D\Delta)(D\Delta)^* ] \right) \right\}. \]
where $\Delta F := F_s - F_n$. Substituting

$$
\log t = \frac{1}{\lambda} - \frac{2\pi}{\beta} \sum_{\omega_m > 0} \frac{1}{\omega_m} \tag{5.79}
$$

$$
\sum_{\omega_m > 0} \frac{1}{\omega_m} = \frac{7\zeta(3)}{(\pi T_c)^3} \tag{5.80}
$$

with $t = 1 - \frac{T}{T_c}$ we finally find the Ginzburg-Landau free energy functional

$$
\frac{F_s}{L_y L_z} = \int dx \int_0^{2\pi} d\theta_k \frac{N_0}{\Omega} \log \left( \frac{T}{T_c} \right) |\Delta|^2 + B_{\text{BCS}} \left[ |\Delta|^4 + (D\Delta)(\Delta^*)^2 \right],
$$

with

$$
\begin{align*}
\Delta(x, \theta_k) &= \phi_x(\theta_k)\Delta_x(x) + \phi_y(\theta_k)\Delta_y(x) \\
D &= v_x(\theta_k)D_x + v_y(\theta_k)D_y \\
D_i &= \nabla_i + i2eA_i \\
B_{\text{BCS}} &= \frac{7\zeta(3)N_0}{16\pi^2 T_c^2 \Omega},
\end{align*}
$$

from which we find (energy per unit surface)

$$
\frac{F_s - F_n}{L_y L_z} = \int dx \left[a_p(T) \left( |\Delta_x|^2 + |\Delta_y|^2 \right) + b_1 |\Delta|^4 + \frac{b_2}{2} (\Delta_x^2 \Delta_y^2 + 2\Delta_x \Delta_y^2) + b_3 |\Delta_x|^2 |\Delta_y|^2 \\
+ K_1 \left( |D_x \Delta_x|^2 + |D_y \Delta_y|^2 \right) + K_2 \left( |D_x \Delta_y|^2 + |D_y \Delta_y|^2 \right) \\
+ \{K_3(D_x \Delta_x)(D_y \Delta_y)^* + K_4(D_y \Delta_x)(D_x \Delta_y)^* + \text{c.c.} \} \right], \tag{5.81}
$$

with

$$
\begin{align*}
a_p(T) &= \log \left( \frac{T}{T_c} \right) \frac{N_0}{\Omega} \langle \phi_x^2 \rangle \approx -(1-t) \frac{N_0}{\Omega} \langle \phi_x^2 \rangle \\
b_1 &= B_{\text{BCS}} \langle \phi_x^4 \rangle \\
b_2 &= 2B_{\text{BCS}} \langle \phi_x^2 \phi_y^2 \rangle \\
b_3 &= 2B_{\text{BCS}} \left( 2\langle \phi_x^2 \phi_y^2 \rangle - \langle \phi_x^4 \rangle \right) \\
K_1 &= B_{\text{BCS}} \langle \phi_x^2 v_x^2 \rangle \\
K_2 &= B_{\text{BCS}} \langle \phi_y^2 v_y^2 \rangle \\
K_3 = K_4 &= B_{\text{BCS}} \langle \phi_x \phi_y v_x v_y \rangle.
\end{align*}
$$

and where we used the average over the Fermi surface $\langle \cdot \rangle \equiv \frac{1}{(2\pi)^3} \hat{N}(\theta_k) \langle \cdot \rangle$.

From the solution of the homogeneous case we find $a_p(T) = -\Delta(T)^2 (4b_1 - b_2 + b_3)$ with $\Delta(T) \equiv |\Delta_x(T, \text{bulk})| = |\Delta_y(T, \text{bulk})|$. Defining the two parameters,

$$
b = 2B_{\text{BCS}} \left( \langle \phi_x^4 \rangle + \langle \phi_x^2 \phi_y^2 \rangle \right) \\
\nu &= \frac{\langle \phi_x^4 \rangle - 3\langle \phi_x^2 \phi_y^2 \rangle}{\langle \phi_x^2 \rangle + \langle \phi_y^2 \phi_y^2 \rangle},
$$

we can rewrite

$$
\begin{align*}
b_1 &= b \frac{3 + \nu}{8} \\
b_2 &= b \frac{1 - \nu}{4} \\
b_3 &= -b \frac{1 + 3\nu}{4}.
\end{align*}
$$

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If we take \((\phi_x, \phi_y) = (v_x/v_F, v_y/v_F)\) we have
\[
K_1 = K \frac{3 + \nu}{4},
\]
\[
K_2 = K_3 = K_4 = K \frac{1 - \nu}{4},
\]
with \(K = B_{\text{BCS}} v_F^2 (\langle \phi_x^4 \rangle + \langle \phi_y^2 \phi_x^2 \rangle)\). We rotate the domain wall by an angle \(\bar{\theta}\) around the \(\hat{z}\)-axis and we express all the quantities in the domain wall axis. Setting \(p = \sin^2(2\bar{\theta})\), we find
\[
b_1 = \frac{b}{8} (3 + \nu - 2\nu p) \\
b_2 = \frac{b}{4} (1 - \nu + 2\nu p) \\
b_3 = -\frac{b}{4} (1 + 3\nu - 6\nu p),
\]
and
\[
K_1 = \frac{K}{\langle \phi_x^4 \rangle + \langle \phi_y^2 \phi_x^2 \rangle} \left[ \left( 1 - \frac{p}{2} \right) \langle \bar{v}_x^2 \phi_x^2 \rangle + \frac{p}{2} \langle \bar{v}_x \bar{v}_y \phi_x \phi_y \rangle \right],
\]
\[
K_2 = \frac{K}{\langle \phi_x^4 \rangle + \langle \phi_y^2 \phi_x^2 \rangle} \left[ \frac{p}{2} \langle \bar{v}_x^2 \phi_x^2 \rangle + \left( 1 - \frac{p}{2} \right) \langle \bar{v}_y^2 \phi_y^2 \rangle - \langle \bar{v}_x \bar{v}_y \phi_x \phi_y \rangle \right],
\]
\[
K_3 = K_4 = \frac{K}{\langle \phi_x^4 \rangle + \langle \phi_y^2 \phi_x^2 \rangle} \left[ \frac{p}{2} \langle \bar{v}_x^2 \phi_x^2 \rangle - \frac{p}{2} \langle \bar{v}_y^2 \phi_y^2 \rangle + (1 - p) \langle \bar{v}_x \bar{v}_y \phi_x \phi_y \rangle \right].
\]

We also get the extra terms given in the section 2.2.1, with the coefficient,
\[
b_{\bar{\theta}} = \frac{b \nu}{4} \sin 4\bar{\theta} \\
K_{\bar{\theta}} = \frac{K \sin 4\bar{\theta}}{4} \frac{\langle \bar{v}_y^2 \phi_y^2 \rangle - \langle \bar{v}_y \bar{v}_x \phi_x \phi_y \rangle - 2 \langle \bar{v}_x \bar{v}_y \phi_x \phi_y \rangle}{\langle \phi_x^4 \rangle + \langle \phi_y^2 \phi_x^2 \rangle}. 
\]

We see that the coefficients satisfy the following symmetry \(f(\nu, \bar{\theta} = \pi/4) = f(-\nu, \bar{\theta} = 0)\) for \(f \in \{b_1, b_2, b_3, K_1, K_2, K_3, K_4\}\).

### 5.C Scaling factors

All along this paper we use the Gauss units. The quasiclassical results are presented in the natural BCS units:

\[
\Delta_0 := \Delta_c(T = 0, \text{bulk}) = \Delta_y(T = 0, \text{bulk}) \\
\xi_0 := \frac{\hbar v_F}{\pi \Delta_0} \\
\lambda_0^2 := \frac{mc^2}{4\pi e^2 n_2} = \frac{\Omega}{\pi \hbar^2 \gamma^2 v_F^2 N_0} \\
\kappa_0 := \frac{\lambda_0}{\xi_0} \\
B_0^2 := 8\pi \frac{F_{\text{cond}}}{\Omega} = 8\pi \frac{\langle \phi_x^4 \rangle N_0}{\Omega} \Delta_0^2 \\
J_0 := 2ev_F N_0 T_c \\
A_0 := \frac{\Phi_0}{2\pi \xi_0} = \frac{1}{\gamma \xi_0}
\]

where \(\Omega\) is the volume of the system, \(\gamma = \frac{2e}{\hbar c} = \frac{2\pi}{\Phi_0}\) and the density of particle is (for the two spin species and 2 dimensional system) \(n_2 = \epsilon_F N_0/\Omega = \pi m v_F^2 N_0/\Omega\) using the quasiclassical relation \(m = \hbar k_F/v_F\).
Note that in the paper we set $h = 1$ and $k_B = 1$. Note that we can rewrite the magnetic induction in the standard form $B_0 = \sqrt{2\langle \phi_x^2 \rangle} \frac{2}{\pi \gamma \xi_0 A_0}$, where the factor $\sqrt{2\langle \phi_x^2 \rangle}$ just gives 1 for an isotropic Fermi surface. From those definitions we can rewrite all the equations of this paper in their dimensionless form. For instance considering the equations (5.9) we find

\[
\begin{align*}
    b_z(x) &= -\frac{4\pi \xi_0 J_0}{c B_0} \left( \int_{-\infty}^{\bar{x}} d\bar{x}' j_y(\bar{x}') - \int_{-\infty}^{0} d\bar{x}' j_y(\bar{x}') \right), \\
    a_y(x) &= \frac{\xi_0 B_0}{A_0} \int_{-\infty}^{\bar{x}} d\bar{x}' b_z(\bar{x}'),
\end{align*}
\]

($\bar{x} = x/\xi_0$) where the scaling factors can be reduced to

\[
\begin{align*}
    \frac{4\pi \xi_0 J_0}{c B_0} &= \frac{1}{\sqrt{2\langle \phi_x^2 \rangle}} \frac{2C}{\kappa_0}, \\
    \frac{\xi_0 B_0}{A_0} &= \frac{\sqrt{2\langle \phi_x^2 \rangle}}{\pi \kappa_0}.
\end{align*}
\]

The factor $C := T_c/\Delta_0$ is determined through the gap equation (5.6) solved for $T = 0$ (in practice we solve it numerically taking $T = 0.005T_c$) and the energy cutoff is fixed at $(\omega_0/2\pi T_c) = 10T_c$. All along the paper we take $\kappa_0 = 3.5$.

The two sets of scaling factors differ. We choose to use them because they are natural in each method and our aim is not to make a quantitative but a qualitative comparison of the results from the two methods. Anyway those methods are used in two different ranges of temperature : in the paper we take $t_{QC} = 0.2$ whereas for the Ginzburg-Landau theory $t_{GL} \lesssim 1$, and it makes no sense to a make quantitative comparison between them.

(In Maeno they only give the values $\kappa$ for GL with a scalar order parameter $\eta = \psi$ !!!!)

5.D Spectral function : full angular resolution

We give in Fig.5.22 the plots of the full angular dependency of the spectral function, $A(\theta_k, x, E)_{x=0}$, that we present in the paper.
Figure 5.22: Spectral function at the domain wall, $A(\theta_k, E, x = 0)$. 

(a) $\nu = 0$

(b) $(\nu, \bar{\theta}) = (-0.6, 0)$

(c) $(\nu, \bar{\theta}) = (-0.6, \pi/4)$

(d) $(\nu, \bar{\theta}, T_0) = (-0.6, \pi/4, 0.9)$
Chapter 6

Lattice approach

We present in this chapter the numerical self-consistent solution of the lattice Bogoliubov-de Gennes equation for a ribbon geometry without domain wall and with a domain wall that separates the two degenerate chiral $p$-wave superconducting states, specifying our model to the $\gamma$-band of Sr$_2$RuO$_4$. We consider the two following geometries: (i) the edges are aligned with one main crystal axis of the basal plane, i.e. the ribbon has straight edges; (ii) the edges are rotated by 45° with respect to the main crystal axes, i.e. the ribbon has zigzag edges.

The main results are: (1) at high band filling we find extra Fermi level crossings by the chiral edge states (other than $k_y = 0$) for the edges rotated by 45°; (2) we give an explanation of those extra zero-crossings based on a simple quasi-classical picture; (3) the self-consistent results fully confirm the macroscopic structure of the domain walls derived from Ginzburg-Landau and quasi-classical theory, i.e. depending on the domain wall orientation the anisotropy of the gap-function induces a non-zero global phase shift through the domain wall; (4) contrary to the quasi-classical approach we find the consistent topological structure of the bound states at the domain wall; (5) we relate those domain wall bound states to the macroscopic structure of the self-consistent solution; (6) we give the electronic signature of the chiral edge states and the domain wall bound states (in terms of the density of states) which provides a clear-cut frame for future STM experiments.

6.1 Introduction

Although we have found a good agreement between the quasi-classical and the Ginzburg-Landau results regarding the macroscopic structure of the domain walls, we have also pointed the fact that (i) the quasi-classical limit introduces some arbitrariness in the angular dependence of the orbital structure of the gap function (i.e. anisotropy), and (ii) it leads to spurious effects on the spectrum—discontinuities in the spectral flow and breaking of the topology—in the vicinity of the points where the quasi-classical limit breaks down.

In this chapter we present the study of the lattice version of the Bogoliubov-de Gennes equations for the $\gamma$-band of Sr$_2$RuO$_4$ assuming the chiral $p$-wave state. This approach allows to overcome the difficulties encountered before. First, it incorporates naturally the anisotropy of the system, that is intrinsic to the lattice structure, such that we can distinguish between the effect of the band anisotropy (determined by the hopping terms of the tight-binding model) from the effect of the gap-function’s anisotropy (pairing terms). Furthermore the pathology of the Andreev equation is completely removed since all the high order terms beyond the quasi-classical limit are automatically included. As a consequence the numerical findings are now in agreement with the index theorem. Therefore this chapter constitutes the most complete treatment of the domain wall problem at the mean-field and single-band level.
6.2 Lattice equations

In this chapter we study the one-band tight-binding model with \( p \)-wave spin-triplet interaction that describes the \( \gamma \)-band of Sr\(_2\)RuO\(_4\). Like in the rest of this thesis and as it has been motivated in the introduction, we neglect the spin-orbit coupling term and assume the chiral \( p \)-wave superconducting state with a \( \mathbf{d} \)-vector pointing in the crystal \( c \)-direction (see the introduction).

We consider a ribbon geometry with Dirichlet boundary conditions \([112]\) in the direction perpendicular to the edges, \( x_\perp \in (0, L) \), and assume translational invariance with periodic boundary conditions in the direction parallel to the edges, \( x_\parallel \). We will consider the two following configurations: (i) the surfaces correspond to \((100)\) crystal planes (in the Milner indices), i.e. the edges are parallel to the main crystal \( x \)-axis; (ii) the surfaces correspond to \((110)\) crystal planes, i.e. the edges are rotated by \(45^\circ\) around the main crystal \( z \)-axis. For those two cases we study the effect of the presence of a domain wall parallel to the surfaces crossing the system in the center, i.e. at \( x_\perp = L/2 \). In the following we work within the edge axes and set \((x, y) \equiv (x_\perp, x_\parallel)\). Technical details concerning the derivation of the lattice equations are given in the appendix \(6.B\).

### 6.2.1 Straight edges

In this section we assume that the edges are parallel to the crystal \( x \)-axis. The system is then inhomogeneous in the \( x \)-direction and translationally invariant in the \( y \)-direction. Working within the edge axes, we set \((x, y) \equiv (x_\parallel, x_\perp) = (\bar{x}, \bar{y})\).

Performing the Fourier transform along the \( y \)-direction, the equations are written in terms of the mixed coordinates \((x_i, k_y)\): \(x_i\) is the lattice coordinate in the \( x \)-direction, i.e.

\[
x_i \in \{0, \ldots, (N - 1)a = L\}, \quad \text{for} \ i = 1, \ldots, N,
\]

where \(N\) is the number of lattice sites in the \( x \)-direction and \(a = x_{i+1} - x_i\) is the lattice spacing; \(k_y\) is the reciprocal coordinate in the \( y \)-direction, i.e.

\[
k_y \in (-\pi/a, \pi/a) \equiv \text{B.Z.}, \quad \text{for} \ k_y L_y/(2\pi) = n_y \in \{(N_y - 1)/2 + 1, \ldots, (N_y - 1)/2\},
\]

with \(N_y\) the number of sites in the \( y \)-direction such that \(L_y = (N_y - 1)a\). Note that due to the periodicity in the \( y \)-direction, the two sites at the opposite edges of the lattice are matched and we have \(N_y - 1\) independent points covering the first Brillouin zone.

**Bogoliubov-de Gennes equation**

The tight-binding mean-field Hamiltonian of the system is given by,

\[
\mathcal{H}_\text{MF} = \frac{1}{2} \sum_{i,j,k} \begin{pmatrix} a_{i,k} & a_{i,-k} \end{pmatrix} \begin{pmatrix} \epsilon_{ij}(k_y) & \Delta_{ij}(k_y) \\ \Delta^*_j(k_y) & -\epsilon_{ij}(-k_y) \end{pmatrix} \begin{pmatrix} a_{j,k} \cr a_{j,-k} \end{pmatrix} + K + C_0,
\]

for \(i, j = 1, \ldots, N\) and \(k_y \in (\pi/a, \pi/a)\), and where \(K\) and \(C_0\) are constants. The diagonal elements are given by,

\[
\epsilon_{ij}(k_y) = \left[ \epsilon_{0, \gamma} - \mu - t_{\gamma} \cos a \left( k_y + \frac{\pi}{\Phi_0} A_y(i) \right) \right] \delta_{ij} - \left[ t_{\gamma} + t_{\gamma}' \cos a \left( k_y + \frac{\pi}{2\Phi_0} [A_y(i) + A_y(j)] \right) \right] \delta_{j,i+1} + \delta_{j,i-1}.
\]

The off diagonal elements are given in terms of the anomalous Green’s function, \(F_{ij}(k_y) := \langle a_{i,k_y} a_{j,-k_y} \rangle\), that is

\[
\Delta_{i,i\pm 1} = g_{p,x} \frac{1}{N_y} \sum_{k_y \in \text{B.Z.}} F_{i,i+1}(k_y),
\]

for \(i \neq j\), and

\[
\Delta_{i}(k_y) = 2g_{p,y} \sin ak_y \frac{1}{N_y} \sum_{k_y' \in \text{B.Z.}} \sin ak_y' F_i(k_y'),
\]

\[114\]
for \( i = j \). Those are the self-consistent gap equations. We note that in general when \( N_y \neq N \), we have \( g_{p,x} \neq g_{p,y} \). From the definition of the anomalous Green’s function we have \( F_{ij}(-k_y) = -F_{ji}(k_y) \), and we find that the off diagonal elements transform as,

\[
\Delta_{ij}(-k_y) = -\Delta_{ji}(k_y) \tag{6.7}
\]

This relation will be important for the charge-conjugation symmetry of the system discussed in the section 6.3.

The Hamiltonian can be diagonalized through the following unitary transformation,

\[
\begin{align*}
 a_{i,k_y} &= \sum_{n=1}^{N} \left[ u_{i,n,k_y}^{n} c_{n,k_y} + (u_{i,-n,k_y}^{n})^* c_{n,-k_y}^+ \right], \\
 a_{i,k_y}^+ &= \sum_{n=1}^{N} \left[ v_{i,n,k_y}^{n} c_{n,-k_y} + (v_{i,-n,k_y}^{n})^* c_{n,k_y}^+ \right],
\end{align*}
\]

where the functions \( \{ u_{i,k_y}^{n}, v_{i,k_y}^{n} \} \) are the components of the eigenvectors with the eigenvalue \( E_{n,k_y} \) of the associated lattice Bogoliubov-de Gennes (BdG) equation,

\[
\sum_{j=1}^{N} \left( \epsilon_{ij}(k_y) \Delta_{ij}(k_y) - \epsilon_{ji}(-k_y) \right) \begin{pmatrix} u_{j,k_y}^{n} \\
v_{j,k_y}^{n} \end{pmatrix} = E_{n,k_y} \begin{pmatrix} u_{i,k_y}^{n} \\
v_{i,k_y}^{n} \end{pmatrix},
\]

for the quantum number \( n = 1, \ldots, 2N \). We note that the form of the transformation (6.8) is a consequence of the charge-conjugation symmetry discussed in the section 6.3.1, as it is shown in the appendix 6.B.

**Gap function, current density, density of states and electron density**

We can now express the different quantities in terms of the eigenvectors of the BdG equation. According to the transformation Eq. (6.8), we find for the anomalous Green’s function,

\[
\begin{align*}
 F_{ij}(k_y) &= \langle a_{i,k_y} a_{j,-k_y}^\dagger \rangle = \frac{2N}{\sum_{n=1}^{2N}} \left[ U_{i,n,k_y}^{n} \left( V_{j,n,k_y}^{n}\right)^* \right] \left[ 1 - f_F(E_{n,k_y}) \right], \\
 F_{ij}(-k_y) &= \langle a_{i,-k_y} a_{j,k_y}^\dagger \rangle = \frac{2N}{\sum_{n=1}^{2N}} \left[ U_{i,n,k_y}^{n} \left( V_{j,n,k_y}^{n}\right)^* \right] f_F(E_{n,k_y}),
\end{align*}
\]

where we have introduced the Fermi distribution function \( f_F(E_{n,k_y}) = \langle \epsilon_{n,k_y}^{\dagger} c_{n,k_y} \rangle \). We then define the \( x \) and \( y \) components of the gap function as,

\[
\begin{align*}
\Delta_x(x_i) &= i (\Delta_{i,i+1} - \Delta_{i,i-1}), \\
\Delta_y(x_i) &= 2g_{p,y} \sum_{k_y \in B.Z.} \sin a k_y F_{ii}(k_y).
\end{align*}
\]

Taking the limit \( T \rightarrow T_c \) in the self-consistent gap equations (6.5) and (6.6) for a homogeneous system, we can relate the critical temperature \( T_c \) to the pairing potentials \( g_{p,x} \) and \( g_{p,y} \) through the following equations, with \( \beta_c = 1/T_c \) (\( k_B = 1 \)),

\[
\begin{align*}
\frac{1}{g_{p,x}} &= \frac{1}{N_x N_y} \sum_{k'} \left( \sin a k'_x \right)^2 \frac{\tanh (\beta_c |\epsilon_{k'}|/2)}{|\epsilon_{k'}|}, \\
\frac{1}{g_{p,y}} &= \frac{1}{N_x N_y} \sum_{k'} \left( \sin a k'_x \right)^2 \frac{\tanh (\beta_c |\epsilon_{k'}|/2)}{|\epsilon_{k'}|}.
\end{align*}
\]

We note that when \( N = N_y \), we find \( g_{p,x} = g_{p,y} \).

The total current density that flows along the bond \( i \leftrightarrow i + 1 \) is given by \( J_y = \langle J_{i,i+1,y} \rangle - \langle J_{i+1,i,y} \rangle \), where \( J_{ij} \) is the lattice current density operator given in Eq. (6.88) of the appendix\(^1\). We find from Eq.\(^1\)

\[1\]We note that we only consider here the nearest-neighbor contributions to the current density. The next-to-nearest-neighbor contributions scale as \( t'_s \sim 0.3 t_x \) and at the time of the redaction of this thesis we thought it would give only small corrections to the current density. In a latter work we have shown that taking the second-neighbor terms for the current has very important implications, see Ref. [114].

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(6.89),

\[
J_y(x_i) = -\frac{2J_0}{N_y} \left[ \sum_{k_y \geq 0} \sin a \left( k_y + \frac{\pi}{p_0} A_y(x_i) \right) \langle a_{i,k_y} \rangle \right.
+ \left. \sum_{k_y \geq 0} \sin a \left( -k_y + \frac{\pi}{p_0} A_y(x_i) \right) \langle a_{i,-k_y} \rangle \right].
\] (6.15)

The total current density that flows along the bond \( \mathbf{i} \mapsto \mathbf{i} + 1_\mathbf{z} \) is given by \( J^{(i \mapsto i+1)}_x = \langle J_{i,i+1} \rangle - \langle J_{i+1,i} \rangle \), and we find from Eq. (6.89),

\[
J^{(i \mapsto i+1)}_x = -i \frac{J_0}{N_y} \sum_{k_y} \left[ \langle a_{i+1,k_y} \rangle - \langle a_{i+1,k_y} \rangle \right].
\] (6.16)

The current density is then determined by the following expecting values,

\[
\begin{align*}
\langle a_{i,k_y}^+ \rangle &= \sum_{n=1}^{2N} u_{i,k_y}^n u_{i,k_y}^n f_F(E_{n,k_y}), \\
\langle a_{i,-k_y}^+ \rangle &= \sum_{n=1}^{2N} v_{i,k_y}^n v_{i,k_y}^n [1 - f_F(E_{n,k_y})].
\end{align*}
\] (6.17)

The Maxwell’s equations on the lattice read,

\[
B_z(x_i) = -\frac{4\pi}{c} \sum_{j=1}^{i} J_y(x_j) + C_0,
\] (6.18)

\[
A_y(x_i) = \sum_{j=1}^{i} B_z(x_j) + C'_0,
\] (6.19)

where we fix the integration constants such the functions \( B_z \) and \( A_y \) vanish in the bulk.

The electron occupation number is given by

\[
\begin{align*}
n_p(x_i, k_y) &= \langle a_{i,k_y}^+ a_{i,k_y} \rangle = \sum_{n=1}^{2N} |u_{i,k_y}^n|^2 f_F(E_{n,k_y}), \\
n_p(x_i, -k_y) &= \langle a_{i,-k_y}^+ a_{i,-k_y} \rangle = \sum_{n=1}^{2N} |v_{i,k_y}^n|^2 [1 - f_F(E_{n,k_y})].
\end{align*}
\] (6.20)

and the hole occupation number by

\[
\begin{align*}
n_h(x_i, k_y) &= \langle a_{i,-k_y}^+ a_{i,-k_y} \rangle = \sum_{n=1}^{2N} |v_{i,k_y}^n|^2 f_F(E_{n,k_y}), \\
n_h(x_i, -k_y) &= \langle a_{i,k_y}^+ a_{i,k_y} \rangle = \sum_{n=1}^{2N} |u_{i,k_y}^n|^2 [1 - f_F(E_{n,k_y})].
\end{align*}
\] (6.21)

The spectral function is given through the particle-hole occupation number as,

\[
n_p(x_i, k_y) + n_h(x_i, k_y) = \int d\omega \ A(x_i, k_y, \omega) f_F(\omega),
\] (6.22)

which can be inverted as,

\[
\begin{align*}
A(x_i, k_y, \omega) &= \sum_{n=1}^{2N} \left( |u_{i,k_y}^n|^2 + |v_{i,k_y}^n|^2 \right) \delta (\omega - E_{n,k_y}), \\
A(x_i, -k_y, \omega) &= \sum_{n=1}^{2N} \left( |u_{i,k_y}^n|^2 + |v_{i,k_y}^n|^2 \right) \delta (\omega + E_{n,k_y}).
\end{align*}
\] (6.23)
Figure 6.1: Edge axes $r_e = (x_\parallel, x_\perp) = R_{\theta}^{-1}\hat{r}$. The unit cell contains two rows, $\Lambda_1$ and $\Lambda_2$, which coordinates are labeled as $i^1 \in \Lambda_1$ and $i^2 = i^1 + 1/2 \in \Lambda_2$.

The local density of states is then simply given by,

$$D(x_i, \omega) = \frac{1}{N_y} \sum_{k_y \in B.Z.} A(x_i, k_y, \omega).$$

Finally the local electron occupation number at the site $i$ is given by,

$$n_i = \langle a^\dagger_i a_i \rangle_{y=0} = \frac{1}{N_y} \sum_{k_y \in B.Z.} \sum_{n=1}^{2N} |u_{i,k_y}|^2 f(E_{n,k_y}),$$

where we have chosen $y_i = 0$, since the system is translationally invariant in the $y$-direction. The charge accumulation is then given by,

$$\delta n(x_i) = n(x_i) - n_{\text{bulk}}.$$

Contrary to the quasi-classical limit, for which we find $n = n_0$, this function is not necessarily constant and it can give rise to a local electric field $E_x(x_i)$ and electric potential $\phi_0(x_i)$. In a self-consistent scheme, this would induce a spatially dependent renormalization of the chemical potential through $\mu \rightarrow \mu - e\phi_0(x_i)$. However the effect is small and we don’t include it here.

### 6.2.2 Zigzag edges

We assume in this section that the surfaces form $(\bar{1}10)$ crystal planes, e.g. we assume the edges are rotated by $45^\circ$ anti-clockwise around the $\hat{z}$-axis, as illustrated on Fig. 6.1. The coordinates in the edge axes are then given by,

$$\begin{align*}
x_\perp &= \frac{1}{\sqrt{2}}(\hat{x} + \hat{y}) , \\
x_\parallel &= \frac{1}{\sqrt{2}}(-\hat{x} + \hat{y}).
\end{align*}$$

The edge coordinates are in general given by $r_e = (x_\parallel, x_\perp) = R_{\theta}^{-1}\hat{r}$, where $\hat{r} = (\hat{x}, \hat{y})$ are the crystal coordinates and $R_{\theta}$ is the $\theta$-rotation matrix. Note that the new reciprocal coordinates are given in the same way, $k_e = (k_\parallel, k_\perp) = R_{\theta}^{-1}\hat{k}$. From now on we work in the edge axes and we write $(x, y) \equiv (x_\perp, x_\parallel)$.

As shown on Fig. 6.1 there are two rows of lattice points in each unit cell: $\Lambda_1 \in \mathbb{Z}$ and $\Lambda_2 \in \mathbb{Z} + 1/2$. We set the number of sites to $N_1$ and $N_2 = N_1 - 1$ respectively. The lattice Bogoliubov-de Gennes equation is again given by Eq. (6.9) but the sum now runs over all $j \in \Lambda_1 \cup \Lambda_2 = \{1, 3/2, 2, \ldots, N_1 - 1\}$.
where we used the notation $\epsilon_{ij}(k_y) = \left(\epsilon_{0,y} - \mu - 2t_y \cos \frac{\sqrt{2}a}{2} \left(k_y + \frac{\pi}{\Phi_0}A_y(i)\right)\right)\delta_{j,i} - t_y'[\delta_{j,i+1} + \delta_{j,i-1}]
- 2t_y \cos \frac{a}{\sqrt{2}} \left(k_y + \frac{\pi}{2\Phi_0}[A_y(i) + A_y(j)]\right)[\delta_{j,i+1/2} + \delta_{j,i-1/2}].$ \hfill (6.27)

We find for the off diagonal elements,

$$\Delta_{ij}(k_y) = \left(\cos \frac{ak_y}{\sqrt{2}} \Delta_i^c + \cos \frac{ak_y}{\sqrt{2}} \Delta_i^s\right) \left[\delta_{j,i+1/2} + \delta_{j,i-1/2}\right],$$ \hfill (6.28)

using the definitions,

$$\Delta_i^c := \frac{2q_{p,x}}{N_y} \sum_{k_y} \cos \frac{ak_y}{\sqrt{2}} F_{ij}(k_y'),$$

$$\Delta_i^s := \frac{2q_{p,y}}{N_y} \sum_{k_y} \sin \frac{ak_y}{\sqrt{2}} F_{ij}(k_y').$$

The anomalous Green’s function $F_{ij}(k_y) = (a_{i,k_y}a_{j,-k_y})$ is given as in the previous section but now with $(i,j) \in \Lambda_1 \times \Lambda_2$ or $(i,j) \in \Lambda_2 \times \Lambda_1$ (i.e. there is no $i = j$ term). The anomalous Green’s function still satisfies $F_{ij}(-k_y) = -F_{ji}(k_y)$, and we again find that the off diagonal elements transform as,

$$\Delta_{ij}(-k_y) = -\Delta_{ji}(k_y).$$ \hfill (6.29)

We define the $x$ and $y$ components of the gap function as,

$$\Delta_x(x_i) := \frac{i}{\sqrt{2}} \left(\Delta_{i,i+1/2}^c + \Delta_{i-1/2,i}^c\right),$$ \hfill (6.30)

$$\Delta_y(x_i) := \frac{1}{\sqrt{2}} \left(\Delta_{i,i+1/2}^s + \Delta_{i-1/2,i}^s\right).$$ \hfill (6.31)

The current density in the edge axes is now given by $J = R_x^{-1} \hat{J}$, and the total current density flowing along the $i \mapsto i + 1_x/2$ bond is then given by

$$\left\{\begin{array}{l}
J_{x}^{(i\mapsto i+1/2^2)} = \frac{1}{\sqrt{2}} \left(J_{x}^{(i\mapsto i+1/2^2)} + J_{y}^{(i\mapsto i+1/2^2)}\right), \\
J_{y}^{(i\mapsto i+1/2^2)} = \frac{1}{\sqrt{2}} \left(-J_{x}^{(i\mapsto i+1/2^2)} + J_{y}^{(i\mapsto i+1/2^2)}\right),
\end{array}\right.$$ \hfill (6.32)

where we used the notation $i^2 \equiv i + 1/2$, with

$$\left\{\begin{array}{l}
J_{x}^{(i\mapsto i+1/2^2)} = \langle J_{i,i+1/2+1/2} \rangle - \langle J_{i+1/2,i+1/2} \rangle, \\
J_{y}^{(i\mapsto i+1/2^2)} = \langle J_{i,i+1/2+1/2} \rangle - \langle J_{i+1/2,i+1/2} \rangle.
\end{array}\right.$$ \hfill (6.33)

Using Eq. (6.89) we finally find

$$J_{y}^{(i\mapsto i+1/2^2)} = -\frac{J_0}{\sqrt{2}N_y} \sum_{k_y} \sin \frac{a}{\sqrt{2}} \left(k_y + \frac{\pi}{\Phi_0} [A_y(x_i) + A_y(x_{i+1/2})] \left[a_{i,k_y}^\dagger a_{i+1/2,k_y} + a_{i+1/2,k_y}^\dagger a_{i,k_y}\right]\right)$$ \hfill (6.34)

All the other quantities are given analogously to the previous section.
6.3 Symmetries

In this section we derive all the symmetries of the lattice equations derived above. For this we first introduce some useful notations. We can rewrite the edge Hamiltonian, Eq. (6.3), successively as,

$$
\mathcal{H}^{\text{edge}} = \sum_{i,j,k_y} \left( a_{i,j,k_y}^\dagger a_{i,-k_y,\downarrow} \right) H_{ij}(k_y) \left( \begin{array}{c} a_{j,k_y,\uparrow} \\ a_{j,-k_y,\downarrow} \end{array} \right)
$$

$$
= \sum_{k_y} \mathcal{H}^{\text{edge}}_{k_y} = \sum_{k_y} a_{i,k_y}^\dagger H_{k_y} a_{k_y} = \sum_{i,j,k_y} a_{i,k_y}^\dagger H_{ij}(k_y) a_{j,k_y}.
$$

(6.35)

We directly note that we have the following symmetry,

$$
\sum_{i,j,k_y} a_{i,k_y}^\dagger H_{ij}(k_y) a_{j,k_y} = \sum_{i,j,k_y} a_{i,k_y}^\dagger H_{ij}(k_y) \left( \Delta_{ij}^*(k_y) \right) a_{j,k_y},
$$

(6.36)

which simply means that the two chiral states, \( \Delta = (\Delta_x, \Delta_y) \) and \( \Delta^* = (\Delta_x^*, \Delta_y^*) \), are degenerated.

The Hamiltonian of the homogeneous ("bulk") system is given by (imposing periodic boundary conditions and Fourier transforming along the \( x \)-direction),

$$
\mathcal{H}^{\text{bulk}} = \sum_{k} \left( a_{k,\uparrow}^\dagger \mathcal{H}_{k_{\|}} a_{k,\downarrow} \right) \left( \begin{array}{c} \xi_k \\ \Delta_k \end{array} \right) \left( \begin{array}{c} \Delta_k^* \\ -\xi_k^* \end{array} \right)
$$

$$
= \sum_{k} \mathcal{H}^{\text{bulk}}_k = \sum_{k} a_{k,\uparrow}^\dagger h_{k} a_{k}.
$$

(6.37)

The dispersion relation \( \xi_k \) and the gap function \( \Delta_k \) depend on the orientation of the axes. From now on we use the notation \( \epsilon_0 \equiv \epsilon_{0,\gamma} = \mu \).

**Aligned axes**

In the unrotated coordinates, \( k = \hat{k} = (\hat{k}_x, \hat{k}_y) \), we find for the bulk Hamiltonian,

$$
\begin{align*}
\xi_{\gamma}(k) &= \epsilon_0 - 2t_{\gamma}(\cos ak_x + \cos ak_y) - 4t'_{\gamma} \cos ak_x \cos ak_y, \\
\Delta(k) &= \phi_x(k) \Delta_{x}^{(\text{bulk})} + \phi_y(k) \Delta_{y}^{(\text{bulk})},
\end{align*}
$$

(6.38)

with the lattice basis functions\(^2\),

$$
\begin{align*}
\phi_x(k) &= \sin ak_x, \\
\phi_y(k) &= \sin ak_y.
\end{align*}
$$

(6.39)

We show on Fig. 6.2 (a) the corresponding Fermi surface obtained for the parameters \( (\epsilon_0, t_{\gamma}, t'_{\gamma}) = (-0.4, 0.4, 0.12) \) (with \( \epsilon_0 \equiv \epsilon_{0,\gamma} = \mu \)). The black thick line is the reduced Brillouin zone of the edge system.

**Rotated axes**

In the rotated coordinates, \( k = k_{\gamma} = (k_{\perp}, k_{\|}) \), we find for the bulk Hamiltonian,

$$
\begin{align*}
\xi_{\gamma}(k) &= \epsilon_0 - 4t_{\gamma} \cos ak_x / \sqrt{2} \cdot \cos ak_y / \sqrt{2} - 2t'_{\gamma} \cos \sqrt{2} ak_x + \cos \sqrt{2} ak_y, \\
\Delta(k) &= \phi_x(k) \Delta_{x}^{(\text{bulk})} + \phi_y(k) \Delta_{y}^{(\text{bulk})},
\end{align*}
$$

(6.40)

with the lattice basis functions\(^3\),

$$
\begin{align*}
\phi_x(k) &= \sqrt{2} \sin ak_x / \sqrt{2}, \\
\phi_y(k) &= \sqrt{2} \sin ak_y / \sqrt{2}.
\end{align*}
$$

(6.41)

\(^2\)They are basis functions of the odd-parity two dimensional irreducible representation \( E_{\gamma} \) (or \( \Gamma_{\gamma}^- \)) of the tetragonal point group \( D_{4h} \) when we include spin-orbit coupling. The chiral \( p \)-wave state corresponds to \( (\Delta_x, \Delta_y)_{\text{bulk}} = \Delta_{\gamma}(1, \pm i) \).

\(^3\)An alternative derivation goes as the following. We write the bulk gap function in the crystal coordinates,

$$
\Delta(k) = \phi_x(k) \Delta_{x} + \phi_y(k) \Delta_{y},
$$

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We show on Fig. 6.2 (b) the Fermi surface (the same as above) with the reduced Brillouin zone of the edge system with rotated edges.

### 6.3.1 Charge-conjugation symmetry

In this section we show that the edge system satisfies the charge-conjugation symmetry and we derive the consequences for the eigenvalues of the Bogoliubov-de Gennes equation. The results of this section are valid for the both geometries, i.e. (100)- and (110)-edges.

**Second quantization level**

Let us consider the following charge-conjugation transformation in real space,

\[
T_{cc} : \begin{cases} 
    a^\dagger_{i,\uparrow(\downarrow)} & \rightarrow a^\dagger_{\bar{\imath},\downarrow(\uparrow)}, \\
    a^\dagger_{\bar{\imath},\uparrow(\downarrow)} & \rightarrow -a^\dagger_{i,\downarrow(\uparrow)}, \\
    h^\dagger_{ij} & \rightarrow h^\dagger_{\bar{i}\bar{j}},
\end{cases}
\]

(note that the last line is equivalent to the following transformation of the vector potential \(A \rightarrow -A\)), that is, in reciprocal space,

\[
T_{cc} : \begin{cases} 
    a^\dagger_{\bar{k},\uparrow(\downarrow)} & \rightarrow a^\dagger_{-\bar{k},\downarrow(\uparrow)}, \\
    a^\dagger_{-\bar{k},\uparrow(\downarrow)} & \rightarrow -a^\dagger_{\bar{k},\downarrow(\uparrow)}.
\end{cases}
\]  

(6.43)

The gap function, \(\Delta_{\bar{k}} \sim \left(\langle a_{\bar{k},\uparrow} a_{-\bar{k},\downarrow}\rangle + \langle a_{\bar{k},\downarrow} a_{-\bar{k},\uparrow}\rangle\right)\), transforms accordingly as,

\[
T_{cc} : \Delta_{\bar{k}} \rightarrow \Delta^*_{\bar{k}}.
\]

(6.44)

with \((\phi_x(\bar{k}), \phi_y(\bar{k})) = (\sin \bar{k}_x, \sin \bar{k}_y)\). Now we rewrite it in terms of the edge coordinates after a rotation by \(\bar{\theta} = \pi/4\). Performing the transformations, \(\bar{r} = R_{\pi/4}r\) and \(\bar{k} = R_{\pi/4}k\), we find

\[
\Delta(k) = \phi_x \left(\frac{k_x - k_y}{\sqrt{2}}\right) \frac{\Delta_x - \Delta_y}{\sqrt{2}} + \phi_y \left(\frac{k_x + k_y}{\sqrt{2}}\right) \frac{\Delta_x + \Delta_y}{\sqrt{2}}
\]

\[
= \phi_x(k) \Delta_x + \phi_y(k) \Delta_y,
\]

with the functions \((\phi_x(k), \phi_y(k))\) given in (6.41).
Since here $\xi_{k,\uparrow} = \xi_{k,\downarrow}$, the bulk Hamiltonian is invariant under this transformation, which is equivalent to

$$\hat{\sigma}_y h_k^T \hat{\sigma}_y = -h_k.$$  

(6.45)

It follows that for each $k$ the eigenstates of the bulk Hamiltonian come in pair with the eigenvalues $E(k)$ and $-E(k)$. This is the “particle-hole” symmetry for spin triplet states discussed in the literature on topological insulators, see for instance Ref. [83].

Let us now consider the edge Hamiltonian. In this case, the transformation above is given by

$$\mathcal{T}_cc : \begin{cases} a_{i,k_y,\uparrow}^{\dagger} \rightarrow a_{i,-k_y,\downarrow}^{\dagger}, \\
 \quad a_{i,k_y,\downarrow} \rightarrow -a_{i,-k_y,\uparrow}, \\
 \quad A_y \rightarrow -A_y. 
\end{cases}$$

(6.46)

The gap function, $\Delta_{ij}(k_y) \sim (a_{i,k_y,\uparrow} a_{j,-k_y,\downarrow} + a_{i,k_y,\downarrow} a_{j,-k_y,\uparrow})$, transforms accordingly as

$$\mathcal{T}_cc : \Delta_{ij}(k_y) \rightarrow \Delta_{ji}^*(k_y) = \Delta_{ji}(k_y).$$

(6.47)

It is easy to show that the edge Hamiltonian, $H_{k_y}^{\text{edge}}$, is invariant under this transformation since we have,

$$\hat{\sigma}_x h_{ij}^{*}(-k_y) \hat{\sigma}_x = -h_{ij}(k_y).$$

(6.48)

We see that it connects the two sectors with opposite $k_y$. We also note that this is a global symmetry in the sense that it holds for every couples $(ij)$. We derive the consequences of this symmetry below after rephrasing the charge-conjugation symmetry in regard of the BdG equation.

**First quantization level**

It is convenient to rewrite the BdG equations (6.9) in the following matrix form,

$$H_{k_y} V_{k_y}^n = E_{n,k_y} V_{k_y}^n,$$

(6.49)

with the matrix Hamiltonian and the eigenvectors,

$$H_{k_y} = \begin{pmatrix} e_{k_y} & \Delta_{k_y} \\
 \Delta_{k_y}^* & -e_{-k_y} \end{pmatrix},$$

$$V_{k_y}^n = \begin{pmatrix} u_{k_y}^n \\
 v_{k_y}^n \end{pmatrix} = \begin{pmatrix} u_{1,k_y}^n \cdots u_{N,k_y}^n \\
 v_{1,k_y}^n \cdots v_{N,k_y}^n \end{pmatrix}^T,$$

where the elements of the matrix are given by $(e_{k_y})_{ij} = \epsilon_{ij}(k_y)$ and $(\Delta_{k_y})_{ij} = \Delta_{ij}(k_y)$.

We have shown in the appendix 6.B that the BdG equation (6.49) satisfies the following symmetry: if the eigenvector $V_{k_y}^{n_1}$ with the eigenvalue $E_{n_1,k_y}$ constitute a solution of the BdG equation for the Matrix $H_{k_y}$—let us write this as the following,

$$\left\{ H_{k_y}, V_{k_y}^{n_1}, E_{n_1,k_y} \right\} \equiv \left( V_{k_y}^{n_1} \right)^*,$$

(6.50)

—then the following eigenvector and eigenvalue also constitute a solution of the same equation,

$$\left\{ H_{k_y}, V_{k_y}^{n_2} = \left( V_{k_y}^{n_1} \right)^*, E_{n_2,k_y} = -E_{n_1,-k_y} \right\}.$$  

(6.51)

This is the generic charge-conjugation symmetry of the Bogoliubov-de Gennes equation. We illustrate the constraint of the charge-conjugation symmetry on the spectrum on Fig. 6.3.

---

4Given the inverse Fourier transform,

$$a_{i,1,2,k_y} = \frac{1}{\sqrt{N_y}} \sum_{y_{1/2}} e^{-i k_y y_{1/2}^2} a_{i,1,2}.$$  

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This symmetry is identical to the charge-conjugation symmetry derived above at the second quantization level. Indeed, it is easy to show that the relation Eq. (6.48) is equivalent to the following symmetry relation for the BdG matrix,

\[ T_{cc} \{ H_{k_y} \} = \left[ \hat{\sigma}_x \otimes 1_{N \times N} \right] H_{k_y} \left[ \hat{\sigma}_x \otimes 1_{N \times N} \right] = -H^*_{-k_y}, \quad (6.52) \]

which leads to nothing but (6.50) and (6.51). The fact that the charge-conjugation symmetry holds globally is related to the fact that the operator \( \hat{\sigma}_x \otimes 1_{N \times N} \) is local, i.e. it doesn’t exchange the lattice sites (as we have seen above).

**Consequences**

We first note the important fact that at \( k_y = 0 \) the charge-conjugation symmetry leads to the particle-hole symmetry of the spectrum at this point: the eigenvalues \( E_{n,0} \) and \( -E_{n,0} \) come in pair. This property will play an important role, combined with the index theorem (see section 6.E), in the demonstration of the existence of a zero-energy bound state at the edges.

Another consequence of the charge-conjugation symmetry goes as the following. We want to know how does the solution of the BdG equation transform under the exchange of the chirality of the superconducting state, that is under the transformation \( \Delta \mapsto \Delta^* \). We note that according to the definition of the gap function in Eq. (6.11-6.12), this corresponds to the transformation \( \Delta_{ij}(k_y) \mapsto \Delta_{ji}^*(k_y) \) for the off diagonal elements of the BdG matrix.

Let us take \( (\Delta, A_y) \mapsto (\Delta^*, -A_y) \) in the BdG equation (6.49). After some algebra we get the equation,

\[ H_{k_y} (\Delta, A_y) \left( \begin{array}{c} u^n_{k_y} \\ -v^n_{-k_y} \end{array} \right) = E_n(-k_y) \left( \begin{array}{c} u^n_{-k_y} \\ -v^n_{k_y} \end{array} \right)^*. \]

Using now the charge-conjugation symmetry we know that the following set ”solves” the BdG equation— in the sense of the relation (6.50) and (6.51)—i.e.

\[ \left\{ H_{k_y} (\Delta, A_y), \left( \begin{array}{c} -v^n_{k_y} \\ u^n_{k_y} \end{array} \right), -E_{n,k_y} \right\}. \]

We then have that the BdG equation is invariant under the following transformation,

\[ \left\{ H_{k_y} (\Delta, A_y), \left( \begin{array}{c} u^n_{k_y} \\ v^n_{k_y} \end{array} \right), E_{n,k_y} \right\} \mapsto \left\{ H_{k_y} (\Delta^*, -A_y), \left( \begin{array}{c} -v^n_{k_y} \\ u^n_{k_y} \end{array} \right), -E_{n,k_y} \right\}, \quad (6.53) \]
where \( T \{ H_{b \nu} (\Delta, A_{\nu}) \} = -H_{b \nu} (\Delta^*, -A_{\nu}) \), i.e. the time reversal of the BdG matrix. We deduce then that the spectrum of the time reversal transformed system is simply the reversed spectrum of the system, i.e. \( T \{ \{ E_{n,k \nu} | n,k \} \} = \{-E_{n,k \nu} | n,k \} \), and with all the time dependent quantities reversed as well, i.e. \( T \{ \{ A_{\nu}, J_{\nu}, B_{\nu} \} \} = \{-A_{\nu}, -J_{\nu}, -B_{\nu} \} \).

We note that the relation (6.53) connecting the system and its time reversal can equivalently be written as,

\[
T_{\nu} \{ H_{b \nu} \} = [\hat{\sigma}_{y} \otimes 1_{N \times N}] H_{b \nu} [\hat{\sigma}_{y} \otimes 1_{N \times N}]^\dagger = -H_{b \nu} (\Delta^*, -A_{\nu}) .
\] (6.54)

### 6.3.2 Chiral symmetry

It is well known that the tight-binding Hamiltonian of a bipartite lattice (say with the sub-lattices \( \Lambda_1 \) and \( \Lambda_2 \)) and with only nearest-neighbor terms satisfies the following chiral symmetry\(^5\) (we drop the spin indices here):

\[
T_{ch} : \begin{cases} 
  a_{i}^{\dagger} &\rightarrow a_{i} , & \text{for } i \in \Lambda_1 , \\
  a_{j}^{\dagger} &\rightarrow -a_{j} , & \text{for } j \in \Lambda_2 , \\
  h_{i j} &\rightarrow h_{i j}^* .
\end{cases}
\] (6.55)

In reciprocal space this transformation corresponds to\(^6\)

\[
T_{ch} : \begin{cases} 
  a_{k} &\rightarrow a_{-k-Q} , \\
  a_{k}^{\dagger} &\rightarrow a_{-k-Q} , \\
  \xi_{k} &\rightarrow -\xi_{k} , & \text{or equivalently } \xi_{k}^{0,2} = 0 , \\
  \Delta_{k} &\rightarrow -\Delta_{k} .
\end{cases}
\] (6.56)

with \( Q = (\pi/a, \pi/a) \) in the unrotated axes, or \( Q = (\sqrt{2}\pi/a, 0) \) in the rotated axes. As a consequence the gap function transforms as,

\[
T_{ch} : \Delta_{k} \rightarrow \Delta_{k+Q} .
\] (6.57)

It is easy then to show that the bulk Hamiltonian is invariant under this transformation if the following conditions are satisfied\(^7\),

\[
\xi_{k+Q} = -\xi_{k} , \quad \text{or equivalently } \xi_{k}^{0,2} = 0 , \\
\Delta_{k+Q} = -\Delta_{k} ,
\] (6.58)

where \( \xi_{k}^{i} \) is the \( i \)-th order hopping term. We note that this symmetry is more constraining then the charge-conjugation symmetry of the bulk Hamiltonian discussed in the previous section. Since there are onsite and next-to-nearest-neighbor terms in our model this symmetry is not satisfied. Nevertheless there are special points that satisfy the chiral symmetry : the points of intersection between the Fermi surface and the small square of Fig. 6.2 (b), which we denote \( k_{F,0} \). Indeed, we have for those states, \( \xi_{k_{F,0}} - Q = -\xi_{k_{F,0}} = 0 \). Although the chiral symmetry is not satisfied by the system we are studying we will see that those special points play an important role for the rotated-edge Hamiltonian (see the section 6.7).

---

\(^5\)This was early noticed in Ref. [107].

\(^6\)We have introduced the bounding–anti-bonding basis,

\[
\begin{align*}
  a_{k} &:= a_{k+} = \frac{1}{\sqrt{N \nu}} \left( \sum_{R_{1} \in \Lambda_{1}} e^{-ik_{1}a_{1}^{\dagger}} + \sum_{R_{2} \in \Lambda_{2}} e^{-ik_{2}a_{1}^{\dagger}} \right) , \\
  a_{k+Q} &:= a_{k-} = \frac{1}{\sqrt{N \nu}} \left( \sum_{R_{1} \in \Lambda_{1}} e^{-ik_{1}a_{1}^{\dagger}} - \sum_{R_{2} \in \Lambda_{2}} e^{-ik_{2}a_{1}^{\dagger}} \right) .
\end{align*}
\]

Note that \( a_{k+} a_{k-} = a_{k-} a_{k+} \).

\(^7\)In the bonding–anti-bonding basis the bulk Hamiltonian is,

\[
\begin{pmatrix}
  a_{k}^{\dagger} & a_{-k} & a_{k+Q} & a_{-k-Q}
\end{pmatrix}
\begin{pmatrix}
  \xi_{k}^{0} + \xi_{k}^{1} & \Delta_{k} & 0 & 0 \\
  \Delta_{k} & -\xi_{k}^{0} - \xi_{k}^{1} & 0 & 0 \\
  0 & 0 & -\xi_{k}^{0} - \xi_{k}^{1} & \Delta_{k} \\
  0 & 0 & \Delta_{k}^{*} & -\xi_{k}^{0} + \xi_{k}^{1}
\end{pmatrix}
\begin{pmatrix}
  a_{k} \\
  a_{-k} \\
  a_{k+Q} \\
  a_{-k-Q}
\end{pmatrix},
\]

where \( \xi_{k}^{i} \) is the \( i \)-th order hopping term.
For completeness we consider now the edge Hamiltonian with the rotated edges. The chiral transformation introduced above is given now by\(^8\),

\[
\mathcal{T}_c : \begin{cases} 
  a_{i1,k_y}^{\dagger} & \rightarrow a_{i1,-k_y}, \text{ for } i^1 \in \Lambda_1, \\
  a_{i2,k_y}^{\dagger} & \rightarrow -a_{i2,-k_y}, \text{ for } i^2 \in \Lambda_2, \\
  A_y & \rightarrow -A_y. 
\end{cases} 
\]

(6.59)

Accordingly the gap function transforms as,

\[
\mathcal{T}_c : \Delta_{ij}(k_y) \rightarrow -\Delta_{ji}^*(k_y). 
\]

(6.60)

We can then easily show that the rotated-edge Hamiltonian satisfies the following relation,

\[
\mathcal{T}_c \{H_{k_y}\} = [1_{N \times N} \otimes \hat{\sigma}_z] H_{k_y} \{\epsilon_0, t'_y\} [1_{N \times N} \otimes \hat{\sigma}_z] = -H_{k_y} \{-\epsilon_0, -t'_y\}, 
\]

(6.61)

from which we conclude that a system with zero onsite and next-to-nearest-neighbor terms, i.e. \(\epsilon_0 = t'_y = 0\), would satisfy the chiral symmetry. This is not the case here.

6.3.3 Inversion symmetry

When there is no domain wall in the system and the edges (at \(x = 0\) and \(x = L\)) are symmetric under inversion, the edge Hamiltonian satisfies the following symmetry\(^9\),

\[
h_{i,j}(k_y) = h_{N-j+1,N-i+1}(k_y). 
\]

(6.62)

It is easy to show that this guarantees the inversion symmetry with, as the inversion center, the center of the ribbon \(N_c = (N - 1)/2\). Indeed, inversion transformation is given by,

\[
\mathcal{I} : \begin{cases} 
  i & \rightarrow N - i + 1, \\
  k_y & \rightarrow -k_y, \\
  A^y(i) & \rightarrow -A^y(N - i + 1) = A^y(i). 
\end{cases} 
\]

(6.63)

The diagonal and off-diagonal elements transform then under inversion as,

\[
\mathcal{I} : \begin{cases} 
  \epsilon_{ij}(k_y) & \rightarrow \epsilon_{N-i+1,N-j+1}(k_y) = \epsilon_{ij}(-k_y), \\
  \Delta_{ij}(k_y) & \rightarrow \Delta_{N-i+1,N-j+1}(-k_y) = \Delta_{ij}(-k_y), 
\end{cases} 
\]

(6.64)

where we have used Eq. (6.62). We then have the relation \(\mathcal{I}\{H_{k_y}\} = H^T_{-k_y}\), and applying successively the inversion and the charge-conjugation transformations, we get

\[
\mathcal{T}_{c\mathcal{C}} \mathcal{I}\{H_{k_y}\} = -H^\dagger_{k_y} = -H_{k_y}, 
\]

(6.65)

where we have used the fact that the Hamiltonian is hermitian. We then have that if \(\{E_{n,k_y}\}_{n,k_y}\) is the spectrum of the inversion and charge-conjugation symmetric system, then \(\{-E_{n,k_y}\}_{n,k_y}\) is also spectrum of the system, i.e. the spectrum is particle-hole symmetric. This is clearly observed in the numerical results when there is no domain wall.

6.3.4 Global gauge symmetry

For completeness we mention the generic global \(U(1)\) gauge symmetry of the BdG Hamiltonian. It is easy to show that,

\[
\mathcal{T}_U \{H_{k_y}\} = \left[ \begin{pmatrix} e^{i\theta} & 0 \\
0 & e^{-i\theta} \end{pmatrix} \otimes 1_{N \times N} \right] H_{k_y} (\Delta) \left[ \begin{pmatrix} e^{i\theta} & 0 \\
0 & e^{-i\theta} \end{pmatrix} \otimes 1_{N \times N} \right]^\dagger = H_{k_y} (e^{i\theta} \Delta), 
\]

(6.66)

from which conclude that the spectrum of the gauge transformed system is identical to the spectrum of the original system.

\(^8\)Since \(g^1 = n\sqrt{2}a\) and \(g^2 = (2n + 1)a/\sqrt{2}\), we have for \(Q_y = \sqrt{2}\pi/a\),

\[
\begin{cases} 
  a_{i1,k_y+Q_y}^{\dagger} & = a_{i1,-k_y}^{\dagger}, \\
  a_{i2,k_y+Q_y}^{\dagger} & = -a_{i2,-k_y}^{\dagger}, 
\end{cases} 
\]

and the edge Hamiltonian for the rotated edges is invariant under a translation by \(Q_y = (0, Q_y)\).

\(^9\)Matrices with this property are called persymmetric, however here the elements \(h_{ij}\) are two-by-two matrices and we cannot apply the results concerning persymmetric matrices and their spectrum [106].
6.4 Domain wall configuration

In the following we will assume that a domain wall between the two chiral states crosses the ribbon in the center, in parallel with the surfaces. The angle of the domain wall with respect to the main crystal axes is then (i) $\theta = 0$ for the unrotated surfaces, and (i) $\theta = \pi/4$ for the rotated surfaces, see Fig. 6.1. We will use the letter ‘L’ for the bulk on the left hand side of the domain wall (that is $x < L/2$), and ‘R’ for the bulk on the right hand side ($x > L/2$). The global phase shift across the domain wall, $\alpha$, is defined as,

$$\alpha \equiv \int_L^R dx \{ \partial_x \varphi_x(x) - \gamma A_x(x) \} = \varphi_x(R) - \varphi_x(L),$$

with in our gauge $A_x = 0$, and where we have used the parametrization $\Delta_x = |\Delta| e^{i\varphi_x}$. We can then define the general domain wall structure as,

$$\Delta_L = \Delta_\perp \equiv s \Delta(T) e^{-i\alpha/2}(1, -i) \longleftrightarrow \Delta_R = \Delta_\parallel \equiv \Delta(T) e^{i\alpha/2}(1, i),$$

where we have introduced the bulk gap $\Delta(T) \equiv \Delta_x$(bulk) = $\Delta_y$(bulk). When there is a $\pi$-phase shift in the $\Delta_y$ component of the gap function—that is the component parallel to the domain wall—we call it a $\pi_\parallel$-domain wall. We call a $\pi_\perp$-domain wall when it is the component $\Delta_x$ that acquires a $\pi$-phase shift. We note that with our notation we have the simple relation, $\Delta_\perp = \Delta_\parallel$. In general the global phase shift across the domain wall, $\alpha$, depends on the orientation of the domain wall, i.e. $\theta$.

6.5 Topological defects and index theorem

As already introduced in chapter 4, the chiral $p$-wave state is a topological superconductor for which we can define a Z topological invariant associated to the bulk of the material. Then we can use an index theorem in order to predict the existence of bound states at the topological defects, i.e. in the regions where there is a jump in the value of the bulk invariant. The index theorem for quantum Hall systems, i.e. systems without time reversal symmetry, has been proven for lattice models by Hatsugai [111], Graf and Porta [112], see also Ref. [113]. The approach by Graf and Porta [112] can be generalized to the case of the chiral $p$-wave topological superconductor.$^{10}$

The bulk Hamiltonian of the system can be parametrized as [110],

$$h_k = m(k) \cdot \hat{\sigma},$$

with the vector

$$m(k) = (\text{Re}\Delta_k, -\text{Im}\Delta_k, \xi_k).$$

The following topological invariant, or Chern number, for broken time reversal systems has been proposed by Volovik [95],

$$C = \frac{1}{4\pi} \int_{B.Z} d^2k \ m \cdot \left( \frac{\partial m}{\partial k_x} \times \frac{\partial m}{\partial k_y} \right).$$

This is the same as the Chern number defined in chapter 4 with the only change that now the integral is taken over the Brillouin zone. Again the only relevant case for us is $\mu > 0$, such that we find $C = \pm 1$ for $\Delta = \Delta_\pm$. In the vacuum we trivially have $C = 0$.

We define $\nu_\sigma$ as the spectral flow of the system, that is the total number (per spin$^{11}$) of signed crossings of the Fermi level $\mu$ by eigenvalues of the edge Hamiltonian. Expanding the eigenvalue branch at the vicinity of the Fermi level as$^{12}$ $E_\nu(k_y) \sim c_0(k_y - k_0)$, with $k_0$ the position of the crossing, we then have $\nu_\sigma = \sum_b \text{sign}[c_b]$. The index theorem then reads [112],

$$C_R - C_L = \nu_\sigma.$$  

\hspace{1cm}$^{10}$Private communication.

\hspace{1cm}$^{11}$Taking into account the fact that $\mathcal{H}_{L} = \mathcal{H}_{L}^\dagger$ all the results are multiplied by two for the full system.

\hspace{1cm}$^{12}$The velocity $c_0$ can always be made non-zero by adiabatically tuning $\mu$.  

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Applying the index theorem to the case of an edge between the bulk and the vacuum (we take the normal vector point outwards as \( n = (1, 0, 0) \)), we find, \( C_{\text{vacuum}} - C_{\text{bulk}} = 0 - 1 = -1 \), that is one bound state branch (per spin) connecting continuously the upper eigenvalue continuum to the lower eigenvalue continuum as we scan \( k_y \) from \(-\Lambda_y\) to \( \Lambda_y\). In the case of a domain wall between the two chiral states we find, \( C(R) - C(L) = +1 - (-1) = 2 \), that is two bound state branches (per spin) connecting continuously the lower eigenvalue continuum to the upper eigenvalue continuum. Taking the spin degrees of freedom into account and the fact that the Bogoliubov quasiparticles obtained from the following spin configuration of the Cooper pairs, \((\uparrow\downarrow), (\downarrow\uparrow)\), are completely equivalent to the quasiparticles \((\downarrow\uparrow)\), we know that the bound state branches are doubly degenerated (hence multiplying the number of crossings by a factor two for the whole system). In the following we show only the results for one half of the system, i.e. for the spin configuration \((\downarrow\uparrow)\).

### 6.6 Numerical results

We present in this section the numerical self-consistent lattice solution for the two geometries, \( \tilde{\theta} = 0 \) and \( \tilde{\theta} = \pi/4 \), and for each case first without and then with a domain wall. We take the number of lattice sites \( N = 120 \) and \( N_y = 120 \). All the quantities are scaled according to the scaling factors defined in the appendix 6.D. The remaining external parameters are chosen \( T_c = 0.27t_0 \), \( T = 0.1T_c \) and \( \kappa = 3 \).

#### 6.6.1 Straight edges

In this section we consider the (100)-surface geometry, i.e. \( \tilde{\theta} = 0 \), see Fig. 6.1. The results are computed for the tight-binding parameters \((\epsilon_0, t_\gamma, t'_0) = (-0.4, 0.4, 0.12)\), as in Ref. [77], which corresponding Fermi surface is shown on Fig. 6.2 (a)\(^{\text{13}}\). The good quantum number for this ribbon geometry is \( k_y \in (-\pi/a, \pi/a) \) (the reduced Brillouin zone is represented by the black thick line on Fig. 6.2 (a)).

**Chiral edge states**

We show on Fig. 6.4 the self-consistent lattice solution for the (100)-surface geometry without domain wall when the bulk is in the state \((\Delta_x, \Delta_y) = \Delta(T)(1, i)\). On Fig. (a) and (b) we see that \( \Delta_x \) vanishes at the edges while \( \Delta_y \) is enhanced. This profile corresponds to the specular scattering boundary conditions at the surfaces, see the solution for an infinite barrier in the section 5.5 of chapter 5. On Fig. (c) we observe a spontaneous current flowing along the edges in opposite directions, i.e. \( J_y(0)/J_y(L) = -1 \). This is the well known chiral edge current carried by the chiral bound states present at the edges (we come back to this below). Furthermore, on Fig. (d), we observe an accumulation of charge at the edges (this quantity is not computed self-consistently here). It has the same profile on both edges and the effect is simply to induce a dipole layer at the surface leaving the system overall charge neutral. As it was shown in Ref. [25], if an external current is driven through the system in the \( y \)-direction, a resultant Hall transverse voltage \( V_{x,H} \) is induced.

We show on Fig. 6.4 (e) the spectrum of the Bogoliubov-de Gennes equation, i.e. \( \{E_{n,k_y}\} \forall n, k_y \}. Due to the charge-conjugation symmetry and the inversion symmetry the spectrum is particle-hole symmetric: for each eigenvalue \( E_{n,k_y} \) there is an other eigenvalue \( E_{\bar{n},k_y} = -E_{n,k_y} \). On top of that we clearly see two bound state branches crossing the Fermi level at \( k_y = 0 \) with opposite slopes, as it was expected from the index theorem presented in the section 6.5. Those are the well known chiral states that appear at the edges of the chiral \( p \)-wave superconductor. They have a linear dispersion at the vicinity of the Fermi level \( E_c(k_y \approx 0) \sim s_c c_n k_y \) (with \( c_n > 0 \)), with the quasiparticle velocity of opposite signs: for the left edge \( s_c = 1 \), and for the right edge \( s_c = -1 \). Fig. (f) and (h) show the spectral function on the right edge \( (x = L) \) and on the left edge \( (x = 0) \), respectively. We can see very well the chiral bound states crossing the gap with opposite slopes and both reaching the zero energy at \( k_y = 0 \). Finally we compare the local density of states at one edge and in the bulk on Fig. 6.4 (g). Due to the presence of the chiral edge states the quasiparticle weight is enhanced inside the gap.

\(^{\text{13}}\)The anisotropy parameter defined in the quasi-classical approach is \( \nu = -0.6 \).
\(\pi||\)-domain wall

We show on Fig. 6.5 the self-consistent lattice solution for the (100)-surface geometry when a \(\pi||\)-domain wall is present at the center of the ribbon. On top of the edge profile discussed above we see on Fig. (a,b) the enhancement of \(\Delta_\perp\) as well as the \(\pi\)-phase shift of \(\Delta_y\) at the domain wall. We stress the fact that this is the most stable domain wall compared to the \(\pi\perp\)-domain wall that discuss below. The width of the domain wall is \(\xi_{\text{DW}}^{(\pi||)}\approx 10a\). As for the Ginzburg-Landau and the quasi-classical results the global phase shift across the domain wall is \(\alpha = 0\). Fig. (c) shows the current density (together with the vector potential and the magnetic induction). We find the spontaneous current flowing in the negative \(y\)-direction at the domain wall. We note the fact that \(J_y\) on the left edge flows now in the opposite direction as compared to the solution on Fig. 6.4 (c). As we will show below, this is a consequence of the charge-conjugation symmetry of the system. We see on Fig. (d) that the effect of the domain wall on the charge accumulation is small compared to the edges.

Fig. 6.5 (e) shows the spectrum. We first note the charge-conjugation symmetry of the spectrum: for each eigenvalue \(E_{n,k_y}\), there exists an other eigenvalue \(E_{\tilde{n}^-,k_y} = -E_{n,k_y}\). This was demonstrated in the section 6.3.1 on the charge-conjugation symmetry of the BdG equation. We first consider the chiral edge states that cross the Fermi level at \(k_y = 0\). We see that the chiral edge states are degenerate as a consequence of changing the chirality of the bulk state on the left hand side. Indeed we showed in the section 6.3.1 that the solution for the chiral \(p\)-wave state \(\Delta_\perp = \Delta^*\) is simply given by \(-E_{n,k_y}, -J_y, -A_y, -B_z\) when \(\{E_{n,k_y}, J_y, A_y, B_z\}\) is the solution for the state \(\Delta_+ = \Delta\). So the eigenvalues of the chiral edge states on the right hand side that we found above (without domain wall) are now reversed. As a consequence the chiral edge states of the both edges go as \(E_c(k_y \approx 0) \sim -c_e k_y\) (with \(c_e > 0\)) at the vicinity of the Fermi level. We can see this on Fig. (f) that shows the spectral function on the right edge (the plot for the left edge is identical).

On top of the chiral edge states we also find the two bound-states located at the domain wall, as predicted by the index theorem. They cross the Fermi level at \(k_y = \pm k_0\) with a positive slope, i.e. \(E_d(k_y \approx \pm k_0) \sim c_d (k_y \pm k_0)\) (\(c_d > 0\)). There are well seen from the spectral function at the domain wall shown on Fig. (h). We finally compare the local density of states at the center of the ribbon with a domain wall (full line) and without domain wall (dashed line). We find an enhancement of the quasiparticle weight inside the gap due the presence of the domain wall bound states.

\(\pi\perp\)-domain wall

We show on Fig. 6.6 the self-consistent solution when a \(\pi\perp\)-domain wall is present in the ribbon with the same geometry, i.e. the \(\pi\)-phase shift occurs now in the \(\Delta_\perp\) component. We stress the fact that this domain wall is metastable and will relaxes with time to the stable \(\pi||\)-domain wall configuration\(^{14}\).

We note the fact that this domain wall is broader with a width \(\xi_{\text{DW}}^{(\pi\perp)}\approx 15a > \xi_{\text{DW}}^{(\pi||)}\). Again there is no global phase shift, \(\alpha = 0\). We find that the spontaneous current flowing at the domain wall is reversed as compared to the \(\pi||\)-domain wall solution. This is easily explained in terms of the domain wall bound states.

The spectrum in shown on Fig. 6.5 (e). The remarks concerning the symmetry of the spectrum of the previous section still apply. The chiral edge states are mainly identical with the previous case, for instance in the vicinity of the Fermi level the edge eigenvalue is linear, \(E_c(k_y \approx 0) \sim -c_e k_y\) with a negative slope. This is clearly seen with the spectral function at the edges on Fig. (f) (right and left edges are identical).

The bound states at the domain wall are now crossing the Fermi level at \(k_y = 0\) with a positive slope, as we can see on Fig. (h) that shows the spectral function at the domain wall, i.e. their eigenvalues at the Fermi level go as \(E_d(k_y \approx 0) \sim c_d k_y\). This explains the change of sign of the current density at the domain wall. Fig. (g) shows the density of states at the domain wall (full line) and in the bulk without domain wall (dashed line). We again see the enhanced quasiparticle weight in the gap due to the presence of the domain wall bound states.

\(^{14}\)As for the quasi-classical approach we find it as a self-consistent solution because our minimization algorithm is non-global, such that initiating the simulation with a \(\pi\perp\)-domain wall, since it is a local minimum, the program remains trapped in this solution.
Figure 6.4: Self-consistent lattice solution for the (100)-surface geometry (without domain wall) : (a,b) Gap function $\{\Delta_x, \Delta_y\}$; (c) Current density $J_y$, vector potential $A_y$, and magnetic induction $B_z$; (d) Charge accumulation $\delta n = n(x) - n_{\text{bulk}}$; (e) Energy eigenvalues; (f) Spectral function on the right edge, $A(L, k_y, E)$, (h) on the left edge, $A(0, k_y, E)$; (g) Local density of states, $D(x, E)$, at the edge (full line) and in the bulk (dashed line).
Figure 6.5: $\pi_1$-domain wall self-consistent lattice solution for the (100)-surface geometry: (a, b) Gap function $\{\Delta_x, \Delta_y\}$; (c) Current density $J_y$, vector potential $A_y$, and magnetic induction $B_z$; (d) Charge accumulation $\delta n = n(x_i) - n_{\text{bulk}}$; (e) Spectrum; (f) Spectral function at the edges (right and left are identical); (g) Local density of states, $D(x_i, E)$, at the domain wall (full line) and in the bulk without domain wall (dashed line); (f) Spectral function at the domain wall, $A(L/2, k_y, E)$. 
Figure 6.6: $\pi_\perp$-domain wall self-consistent lattice solution for the (100)-surface geometry: (a,b) Gap function \{${\Delta}_x, {\Delta}_y$\}; (c) Current density $J_y$, vector potential $A_y$, and magnetic induction $B_z$; (d) Charge accumulation $\delta n = n(x_i) - n_{\text{bulk}}$; (e) Spectrum; (f) Spectral function at the edges (right and left are identical); (g) Local density of states, $D(x_i, E)$, at the domain wall (full line) and in the bulk without domain wall (dashed line); (h) Spectral function at the domain wall, $A(L/2, k_y, E)$. 


6.6.2 Zigzag edges

In this section we consider the $\bar{\langle 110\rangle}$-surface geometry, i.e. $\bar{\theta} = \pi/4$. We fix the following tight-binding parameters $(t_z, t'_z) = (0.4, 0.12)$ and compare the solutions for the different fillings $\epsilon_0 \equiv \epsilon_{0,\gamma} - \mu = -0.4, -0.3, 0, 0.3$ ($\epsilon_0 \equiv \epsilon_{0,\gamma} - \mu$). We show on Fig. 6.7 the corresponding Fermi surfaces. The good quantum number for this ribbon geometry is now $\bar{k}_y = k_y \in (-\pi/\sqrt{2a}, \pi/\sqrt{2a})$ (the reduced Brillouin zone is represented by the black thick line on Fig. 6.7).

Chiral edge states

We show on Fig. 6.8 the self-consistent lattice solution for the $\langle 110\rangle$-surface geometry without domain wall when the bulk is in the state $(\Delta_x, \Delta_y) = \Delta(T)(1,i)$. On Fig. A we show the solution for the filling $\epsilon_0 \equiv \epsilon_{0,\gamma} - \mu = -0.4$, and Fig. B for the filling $\epsilon_0 = -0.3$. We see that we can reach a larger charge accumulation at the edges for $\epsilon_0 = -0.4$. Hence we expect the Hall effect to be larger when we apply a current along the edges in this geometry since $\delta n(0) \approx 0.1 \gg 0.04$ (compared to the $(100)$-surface geometry).

The spectra at those fillings are shown on Fig. 6.9 (a), and (b) respectively. We note again the particle-hole symmetry of the spectrum when there is no domain wall due to the inversion symmetry.

A new feature is the presence of extra crossings of the Fermi level by the edge states: on top of the crossing at $k_y = 0$, we find two other crossings away from zero, i.e. at $\pm k_0 \neq 0$. We will argue in the section 6.7 that the position of those new Fermi-level crossings corresponds in a good approximation to the position of the intersection points between the Fermi surface and the small square of Fig. 6.7 (a) and (b). The spectral function at the right edge, $\mathcal{A}(\ell/\sqrt{2}, k_y, E)$, plotted on Fig. (c) and (d), shows

Figure 6.7: The full blue line shows the transversal section of the $\gamma$-band Fermi surface obtained for the tight-binding parameters $(t_z, t'_z) = (0.4, 0.12)$ at the different fillings $\epsilon_0 \equiv \epsilon_{0,\gamma} - \mu = -0.4, -0.3, 0, 0.3$. The black thick line shows the reduced Brillouin zone when the surfaces are rotated by an angle $\bar{\theta} = \pi/4$ anti-clockwise around the $\hat{z}$-axis. The dashed lines are the corresponding reciprocal edge axes with the coordinates $(k_\perp, k_\parallel)$.
clearly that the crossings happen within the same edge state, i.e. each edge state crosses the Fermi level three times. Fig. (e) and (f) show the density of states at the domain wall (full line) and in the bulk (dashed line). We find that the quasiparticle weight of the chiral edge states for the (110)-edge geometry is enhanced compared to the (100)-edge geometry (shown on Fig. 6.4 (g)).

We show on Fig. 6.10 the same quantities at the lower fillings, \( \epsilon_0 = 0 \) and \( \epsilon_0 = 0.3 \). We see, Fig. (a,b), that there is a critical value of the filling, \( \epsilon_0 \approx 0 \), below which the extra crossings disappear. As we can seen with the spectral function, shown on Fig. (c,d), the dispersion of the edge states becomes flat at this critical value. This is due to the merging of the three zeros as \( \pm k_0 (\epsilon_0 \to 0) \to 0 \). It is accompanied with the appearance of a high peak in the density of states at \( E = 0 \), as we can see on Fig. (e). This peak is suppressed as we decrease further the filling, see Fig. (f).

We note that at the time of the redaction of this thesis we neglected the contribution from the second-neighbor terms in the current density, assuming that they would only lead to minor correction. In a more resent work we show that taking them into account has very important consequences on the edge currents, see Ref. [114].

### \( \pi_\parallel \)-domain wall solution

We show on Fig. 6.11 the self-consistent lattice solution for the (110)-surface geometry with a \( \pi_\parallel \)-domain wall (parallel to the rotated surfaces). In this geometry the \( \pi_\perp \)-domain wall is unstable and it cannot be found as a self-consistent solution (initializing the program with a \( \pi_\perp \)-domain wall configuration, the solution relaxes spontaneously to the stable \( \pi_\parallel \)-domain wall configuration). As we found with the Ginzburg-Landau and the quasi-classical approaches, there is, for this geometry, a non-zero global phase shift through the domain wall, \( \alpha \neq 0 \), which specifically at the angle \( \bar{\theta} = \pi/4 \), is doubly degenerate, i.e. \( \alpha(\bar{\theta} = \pi/4) = \pm |\alpha| \).

In the following we show the solutions for the filling \( \epsilon_0 = -0.3 \) and 0.3. Fig. 6.11 (a) shows the solution for the filling \( \epsilon_0 = -0.3 \) corresponding to phase shift \( \alpha < 0 \). There is another degenerated solution with \( \alpha > 0 \). Fig. 6.11 (b) shows the solution for the filling \( \epsilon_0 = 0.3 \) corresponding to \( \alpha > 0 \) (there is again a degenerated solution with \( \alpha < 0 \)). We note that the filling has an effect on the magnitude of the phase shift and the width of the domain wall, however the results are qualitatively similar.

We plot the spectra for the same fillings on Fig. 6.12 (a,b). It has the charge-conjugation symmetry discussed in the section 6.3.1. The edge states for the two sides are now degenerated since we changed the chirality of the state on left hand side (we showed in section 6.3.1 that it is a consequence of the charge-conjugation symmetry of the system). As in the case without domain wall, the edge states are crossing the Fermi level three times when \( \epsilon_0 < 0 \) : at \( k_y = 0 \) and at \( \pm k_0 \neq 0 \). When \( \epsilon_0 > 0 \) they cross the Fermi level only one time at \( k_y = 0 \). Due to the presence of the domain wall, the spectrum has also two extra bound states localized at the domain wall, as we expect from the index theorem. We see them clearly in the spectral function at the domain wall, shown on Fig. (c,d). Finally we show on Fig. (e,f) the density of states at the domain wall (full line) and in the bulk without domain wall (dashed line). We see the enhancement of the quasiparticle weight in the gap at the domain wall due to the presence of the domain wall bound states.
Figure 6.8: Self-consistent lattice solution for the (110)-surface geometry. A: at the filling $\epsilon_0 = -0.4$. B: at the filling $\epsilon_0 = 0.3$. 

A : $\epsilon_{0,\gamma} - \mu = -0.4$

B : $\epsilon_{0,\gamma} - \mu = 0.3$
Figure 6.9: Self-consistent lattice solution for the (110)-surface geometry (without domain wall). A : at the filling $\epsilon_0 = -0.4$ and B : at the filling $\epsilon_0 = -0.3$. (a,b) Spectrum; (c,d) Spectral function at the right edge $A(L/\sqrt{2}, k_y, E)$; (e,f) Local density of states, $D(x_i, E)$, at the edge (full line) and in the bulk without domain wall (dashed line).
Figure 6.10: Self-consistent lattice solution for the (110)-surface geometry (without domain wall). A : at the filling $\epsilon_0 = 0$ and B : at the filling $\epsilon_0 = 0.3$. (a,b) Spectrum; (c,d) Spectral function at the right edge $A(L/\sqrt{2}, k_y, E)$; (e,f) Local density of states, $D(x, E)$, at the edge (full line) and in the bulk without domain wall (dashed line).
Figure 6.11: $\pi_j$-domain wall self-consistent lattice solution for the $(\bar{1}10)$-surface geometry.  

- **A**: at the filling $\epsilon_0 = -0.3$ and 
- **B**: at the filling $\epsilon_0 = 0.3$. 

**Notes:**

- **A**: $\epsilon_0, \gamma - \mu = -0.3$
- **B**: $\epsilon_0, \gamma - \mu = 0.3$
Figure 6.12: \( \pi \) domain wall self-consistent lattice solution for the \((\overline{110})\)-surface geometry. A : at the filling \( \epsilon_0 = -0.3 \) and B : at the filling \( \epsilon_0 = 0.3 \).
6.7 Zero-energy edge states from a quasi-classical picture

We use the quasi-classical picture in order to find the location of the Fermi-level-crossings by the edge states. It is easy to show that if two bulk states—obtained as asymptotic quasi-classical states—say \( \psi_{k_1} \) and \( \psi_{k_2} \), are connected in the same process (for instance through specular scattering), i.e. \( E(k_1) = E(k_2) \), and are such that the gap function changes sign from one to the other, i.e. \( \Delta(k_2) = -\Delta(k_1) \), then there exists a bound state at the corresponding \( k_y \) in the edge system. In the two geometries we have considered, the argument goes as the following.

- **Straight edges**
  We plot on Fig. 6.13 the asymptotic quasi-classical states \( k_1 = (k_F,0) \) and \( k_2 = (-k_F,0) \) that are connected through the specular reflection on the edge. Since those two states are involved in the same process, we have \( E(k_1) = E(k_2) \). Then, since \( k_2 = -k_1 \), we readily find that they connect two points of the Fermi surface that involve a change of sign of the gap function, i.e. \( \Delta(k_2) = \Delta(-k_1) = -\Delta(k_1) \). Hence we conclude that there is an edge state crossing the Fermi level at \( k_y = k_{1,y} = k_{2,y} = 0 \).

![Figure 6.13: Quasi-classical states connected through a specular reflexion on the (100)-edge.](image)

- **Zigzag edges**
  We work here within the rotated axes \( (k_x,k_y) \equiv (k_\perp,k_\parallel) \). The same argument as above applies here and we also find a zero-energy edge state at \( k_y = 0 \). However we also find two extra zero-energy edge states. We plot on Fig. 6.14 the asymptotic quasi-classical states \( k_1 = (\pi/\sqrt{2}a,-k_{y,0}) \) and \( k_2 = (-\pi/\sqrt{2}a,-k_{y,0}) \) that are connected through the specular reflection on the edge. Since those two states are involved in the same process we have \( E(k_1) = E(k_2) \). Furthermore, the points of intersection between the Fermi surface and the small square satisfy the relation \( \Delta(k_1) = \Delta(k_2 + Q) = -\Delta(k_2) \), i.e. the gap function acquires a sign change in the scattering process. We then expect the presence of a Fermi level crossing by an edge state at the point \( k_y = k_{1,y} = k_{2,y} \). The same argument applies at for the point \( k_y = -k_{1,y} = -k_{2,y} \). We then have two extra Fermi level crossing by the edge states at \( k_0 = \pm k_{1,y} \).

![Figure 6.14: Degenerated quasi-classical states involved in a specular reflexion on the (110)-edge. The states \( \vec{k}_1 \) and \( -\vec{k}_1 + \vec{Q} = -\vec{k}_2 \) are connected through the chiral transformation, with \( \vec{Q} = (\pi/a,\pi/a) \).](image)
6.8 Conclusions

We have given the numerical self-consistent solution of the lattice Bogolyubov-de Gennes equations corresponding to the $\gamma$-band of Sr$_2$RuO$_4$. We have considered a ribbon geometry with straight and zigzag edges. For each case we have given the solution for a system without domain wall, i.e. when there are only two edges, and with one domain wall traversing the system at the center. The solution comprises, on the one hand, the two-component gap function, the current density (with the magnetic induction and the vector potential), and the local charge accumulation, on the other hand, also the following microscopic quantities, the spectrum, the spectral function at the different defects, and the local density of the states. Contrary to the quasi-classical results we have found the fully consistent picture of the edge and domain wall bound states in agreement with the counting of the index theorem.

Peculiarly concerning the edge states, we have found the existence, at the zigzag edges and at high filling, of two additional zero-energy edge states. We studied the effect of the filling and showed that they disappear at low filling. We gave an interpretation in terms of the quasi-classical picture and showed that they are associated to the $\pi$-phase shift acquired by the gap function in the process of specular scattering at a zigzag edge.

Concerning the domain wall structure, we found a very good qualitative agreement of the domain wall profile (in terms of the two-component gap function) comparing with the two other approaches that we have studied in this thesis, Ginzburg-Landau and quasi-classical. Indeed, we find that the system spontaneously acquires a non-zero global phase shift (gauge-invariant) across the domain wall when the domain wall is unaligned with the main crystal axes (we have seen in the first part of this thesis that this corresponds to the most stable configuration of the domain wall). This demonstrates the robustness of our result. From the microscopic structure of the domain wall bound states we could also given an interpretation of the corresponding macroscopic domain wall structure in terms of the gap function and the current densities.

We mention here the two later works, Ref. [114] and Ref. [115], that complete the picture presented in this Chapter.
Appendix

6.A Three-band tight-binding Hamiltonian with spin-orbit coupling derived from the double group

Sr$_2$RuO$_4$ (or Strontium Ruthenate) has a layered perovskite crystal structure corresponding to the body centered tetragonal lattice $I4/mmm$, see Fig. 1.1. The point group is then the tetragonal point group $D_{4h}$. The low energy physics is principally determined by the 4$d^4$ electrons of the ions Ru$^{4+}$ of the RuO$_2$ planes$^{15}$. Due to the tetragonal crystal field surrounding each Ru atoms the $d$-orbitals are split into the \{A$_{1g}$, A$_{2g}$, B$_{2g}$, E$_g$\} irreducible representations of $D_{4h}$. At low energy only the B$_{2g}$ and E$_g$ states are occupied such that the electronic orbitals are described by the basis functions $d_{xy}$ and \{ $d_{yz}$, $d_{zx}$ \} (these are separated by the basal plane reflection symmetry, $\sigma_h$). In the following we assume that there is no dispersion along the c-axis, i.e. the system is two dimensional.

We want here to derive the three-band tight-binding model (single-particle model) with spin-orbit coupling for the \{ $d_{xz}$, $d_{xy}$, $d_{yz}$ \}-electrons on a square lattice (the Ru sites of the RuO$_2$-plane). For this we make use of our method that generalizes the Slater-Koster-Dresselhaus method to the double point group of the system$^{16}$.

We will first work within the point group $C_{4v}$ and then impose the mirror symmetry $\sigma_h$. The decomposition of the angular momentum and spin representations in $C_{4v}$ gives,

$$\Gamma^{d_{xz}, d_{xy}} = \Gamma_5, \quad \Gamma^{d_{xy}} = \Gamma_4, \quad \Gamma^{\uparrow \downarrow} = \Gamma_6.$$  

The coupling of the internal degrees of freedom is done through the direct product as,

$$\Gamma^{d_{xz}, d_{xy}} \otimes \Gamma^{\uparrow \downarrow} = \Gamma_6(\Gamma_5) + \Gamma_7(\Gamma_5), \quad \Gamma^{d_{xy}} \otimes \Gamma^{\uparrow \downarrow} = \Gamma_7(\Gamma_4).$$

$^{15}$See for instance Ref. [4, 5].

$^{16}$For more details see From point group theory with spin-orbit coupling to topological insulators, A. Bouhon and M. Sigrist, in preparation.
The basis functions for each of the three irreducible representations are given by

\[
\begin{align*}
\Gamma_a = \Gamma_6(\Gamma_5) : & \quad \psi_1 = \frac{i}{\sqrt{2}}(d_{yz} + i d_{xz}) \chi^\uparrow \\
& \quad \psi_2 = \frac{i}{\sqrt{2}}(d_{yz} - i d_{xz}) \chi^\downarrow \\
\Gamma_b = \Gamma_7(\Gamma_5) : & \quad \psi_3 = \frac{i}{\sqrt{2}}(d_{yz} - i d_{xz}) \chi^\uparrow \\
& \quad \psi_4 = \frac{i}{\sqrt{2}}(d_{yz} + i d_{xz}) \chi^\downarrow ,
\end{align*}
\]

(6.74)

where we have used the following notation for the spin wave functions \( \chi^\uparrow = \phi(1/2, 1/2) \), \( \chi^\downarrow = \phi(1/2, -1/2) \) [100].

The matrix Hamiltonian can accordingly be decomposed into sub-matrices,

\[
H = \begin{pmatrix}
H_{a,a} & H_{a,b} & H_{a,c} \\
H^\dagger_{a,b} & H_{b,b} & H_{b,c} \\
H^\dagger_{a,c} & H^\dagger_{b,c} & H_{c,c}
\end{pmatrix}.
\]

(6.75)

From the generalized selection rules we find that the sub-matrices decompose as,

\[
\begin{align*}
H_{a,a}^{(\Gamma_1 + \Gamma_2 + \Gamma_3)} &= [a_0 + a_1 f_{11}(k) + a_2 f_{21}] \hat{1} + a_{15} \left[f_{15}^a(k) \hat{\sigma}_y + f_{15}^b(k) \hat{\sigma}_z\right] + a_{25} \left[f_{25}^a(k) \hat{\sigma}_y + f_{25}^b(k) \hat{\sigma}_z\right] , \\
H_{b,b}^{(\Gamma_1 + \Gamma_2 + \Gamma_3)} &= [b_0 + b_1 f_{11}(k) + b_2 f_{21}] \hat{1} + b_{15} \left[f_{15}^a(k) \hat{\sigma}_y + f_{15}^b(k) \hat{\sigma}_z\right] + b_{25} \left[f_{25}^a(k) \hat{\sigma}_y + f_{25}^b(k) \hat{\sigma}_z\right] , \\
H_{c,c}^{(\Gamma_1 + \Gamma_2 + \Gamma_3)} &= [c_0 + c_1 f_{11}(k) + c_2 f_{21}] \hat{1} + c_{15} \left[f_{15}^a(k) \hat{\sigma}_y + f_{15}^b(k) \hat{\sigma}_z\right] + c_{25} \left[f_{25}^a(k) \hat{\sigma}_y + f_{25}^b(k) \hat{\sigma}_z\right] , \\
H_{a,b}^{(\Gamma_1 + \Gamma_2 + \Gamma_3)} &= \alpha_{13} f_{13}(k) \hat{1} + i \alpha_{24} f_{24}(k) \hat{\sigma}_z + \alpha_{15} \left[f_{15}^a(k) \hat{\sigma}_y - f_{15}^b(k) \hat{\sigma}_z\right] + \alpha_{25} \left[f_{25}^a(k) \hat{\sigma}_y - f_{25}^b(k) \hat{\sigma}_z\right] , \\
H_{b,c}^{(\Gamma_1 + \Gamma_2 + \Gamma_3)} &= i \beta_{13} f_{13}(k) \hat{\sigma}_z + \beta_{24} f_{24}(k) \hat{1} + \beta_{15} \left[f_{15}^a(k) \hat{\sigma}_y + f_{15}^b(k) \hat{\sigma}_z\right] + \beta_{25} \left[f_{25}^a(k) \hat{\sigma}_y + f_{25}^b(k) \hat{\sigma}_z\right] , \\
H_{a,c}^{(\Gamma_1 + \Gamma_2 + \Gamma_3)} &= i [\gamma_0 + \gamma_1 f_{11}(k) + \gamma_2 f_{21}(k)] \hat{\sigma}_z + \gamma_{15} \left[f_{15}^a(k) \hat{\sigma}_y - f_{15}^b(k) \hat{\sigma}_z\right] + \gamma_{25} \left[f_{25}^a(k) \hat{\sigma}_y - f_{25}^b(k) \hat{\sigma}_z\right] ,
\end{align*}
\]

where we have written the coefficients such that they are real and the Hamiltonian is time reversal invariant (note that the irrep \( \Gamma_2 \) is not present for hopping up to next-to-nearest-neighbor), with the functions

\[
\begin{align*}
 f_{13}(k) &= \cos ak_x + \cos ak_y , & f_{21}(k) &= 2 \cos ak_x \cos ak_y , \\
f_{15}^a(k) &= \cos ak_x - \cos ak_y , & f_{24}(k) &= 2 \sin ak_x \sin ak_y , \\
f_{15}^b(k) &= \sin ak_x , & f_{25}^a(k) &= 2 \sin ak_x \cos ak_y , \\
f_{25}^b(k) &= \sin ak_y , & f_{25}^a(k) &= 2 \cos ak_x \sin ak_y .
\end{align*}
\]

(6.76)

Since the point group of the system is \( D_{4h} \) we have the mirror symmetry \( \sigma_h \) and we can neglect all the Rashba spin-orbit coupling terms, i.e. \( O_{15,25} = 0 \) with \( O \in \{a, b, c, \alpha, \beta, \gamma\} \). The remaining parameters

\[\text{Note that it is useful to rewrite the cubic harmonics in terms of the spherical harmonics, } Y_l^m, \text{ as,}\]

\[
\begin{align*}
 d_{yz} &= \frac{i}{\sqrt{2}} \left(Y_2^{-1} + Y_2^{1}\right) , \\
 d_{zx} &= \frac{i}{\sqrt{2}} \left(Y_2^{-1} - Y_2^{1}\right) , \\
 d_{xy} &= \frac{i}{\sqrt{3}} \left(Y_2^{-2} - Y_2^{2}\right) .
\end{align*}
\]

The transformation rule is then simply given by,

\[
\mathcal{O}_{\alpha, \beta, \gamma} Y_l^m = \sum_{m=-m}^{+m} Y_l^n D_{nm}^\alpha(\alpha, \beta, \gamma) ,
\]

(6.73)

where \( D_{nm}^\alpha(\alpha, \beta, \gamma) \) are the Wigner functions expressed in the active picture, see for instance Ref. [99]. It goes similarly for the spin functions \( \{\chi^\uparrow, \chi^\downarrow\} \) which can be considered as spherical harmonics for the half integer angular momentum, \( l = 1/2 \).
are set,

\[ \begin{align*}
a_0 &= \epsilon_0 - \lambda_0, \\
b_0 &= \epsilon_0 + \lambda_0, \\
\alpha_{13} &= t_1 - t_1', \\
\alpha_{24} &= -2g, \\
\gamma_1 &= (\lambda_{1b} + \lambda_{1b}' + \sqrt{2})/2, \\
\gamma_2 &= (\lambda_{1b} - \lambda_{1b}')/\sqrt{2}. \\
\end{align*} \] (6.77)

Transforming the Hamiltonian into the basis \( \Psi = (d_{yz}, d_{zx}, d_{xy}, d_{zy}, d_{zy}' d_{xy}, d_{xy}') \), we eventually find

\[ \mathcal{H} = \sum_{s = \pm 1, \mathbf{k}} \left( \begin{array}{c} c_{\mathbf{k},yz,s}^\dagger \ H_{11}(\mathbf{k}) \ H_{12}(\mathbf{k}) \ H_{13}(\mathbf{k}) \\ c_{\mathbf{k},zx,s}^\dagger \ H_{12}(\mathbf{k}) \ H_{22}(\mathbf{k}) \ H_{23}(\mathbf{k}) \\ c_{\mathbf{k},xy,s}^\dagger \ H_{13}(\mathbf{k}) \ H_{23}(\mathbf{k}) \ H_{33}(\mathbf{k}) \end{array} \right) \left( \begin{array}{c} c_{\mathbf{k},yz,s} \\ c_{\mathbf{k},zx,s} \\ c_{\mathbf{k},xy,s} \end{array} \right), \] (6.78)

with

\[ \begin{align*}
H_{11}(\mathbf{k}) &= \epsilon_0 - 2t_1 \cos k_y - 2t_1' \cos k_x - 4t_2 \cos k_x \cos k_y, \\
H_{12}(\mathbf{k}) &= \epsilon_0 - 2t_1 \cos k_x - 2t_1' \cos k_y - 4t_2 \cos k_x \cos k_y, \\
H_{13}(\mathbf{k}) &= \epsilon_0 - 2t_1 \cos k_x - \lambda_1 \cos k_y, \\
H_{22}(\mathbf{k}) &= \epsilon_0 - 2t_1 \cos k_x - 2t_1' \cos k_y - 4t_2 \cos k_x \cos k_y, \\
H_{23}(\mathbf{k}) &= \epsilon_0 - 2t_1 \cos k_x - \lambda_1 \cos k_y, \\
H_{33}(\mathbf{k}) &= \epsilon_0 - 2t_1 \cos k_x - \lambda_1 \cos k_y.
\end{align*} \] (6.79)

where \( s = +1 (-1) \) stands for spin up (resp. spin down), and the parameters \( t_i \) and \( \lambda_i \) stand for the \( i \)-th order hopping and spin-orbit coupling respectively. We note that this is the most general tight-binding model up to next-nearest-neighbor order including spin-orbit coupling.

The following simplified model has been extensively studied (see the references in the next section),

\[ \begin{align*}
H_{11}(\mathbf{k}) &= \epsilon_0 - 2t_1 \cos k_y - 2t_1' \cos k_x, \\
H_{12}(\mathbf{k}) &= \epsilon_0 - 2t_1 \cos k_x - 2t_1' \cos k_y, \\
H_{13}(\mathbf{k}) &= \epsilon_0 - 2t_1 \cos k_x, \\
H_{22}(\mathbf{k}) &= \epsilon_0 - 2t_1 \cos k_x - 2t_1' \cos k_y, \\
H_{23}(\mathbf{k}) &= \epsilon_0 - 2t_1 \cos k_x, \\
H_{33}(\mathbf{k}) &= \epsilon_0 - 2t_1 \cos k_x.
\end{align*} \] (6.80)

We show in Fig. 6.15 the Fermi surfaces generated by this model for typical values of the parameters: \( \epsilon_0 - \epsilon_0 = -0.065t, \ t_1 = 0.1t, \ t_1' = 0.7t, \ t_2 = 0.3t, \ g = 0.1t, \ \lambda = 0.1t \) and \( t_1' = 0 \), taken from Ref. [101]. The hybridization between the \( d_{yz} \) and \( d_{xz} \)-orbitals, through the term \(-4g \sin k_x \sin k_y\), leads to two quasi-one dimensional bands: a hole-like band, called \( \alpha \)-band, and an electron-like band, called \( \beta \)-band. The \( d_{xz} \)-orbital is mainly responsible for the two dimensional \( \gamma \)-band. We can relate them to the two quasi-one dimensional Fermi surfaces, from the \( \{\alpha, \beta\} \)-bands, and the one quasi-two dimensional Fermi surface, from the \( \gamma \)-band, revealed by precise de Haas-van Alphen experiments, reviewed in Ref. [43], and ARPES, see for instance Ref. [1].

### 6.B Lattice model derivation

The two particle Hamiltonian in the second quantized Wannier representation reads

\[ \mathcal{H} = \sum_{ij} \epsilon_{ij,ss'} a_{ij,s}^\dagger a_{ij,s'} + \frac{1}{2} \sum_{ijkl} V_{ijkl} a_{ij,s1}^\dagger a_{ij,s2}^\dagger a_{kl,s3} a_{kl,s4}, \] (6.81)

with \( a_i \equiv a_{(x_i,y_i)} \), where \( i \) refers to a point of a two dimensional lattice. The coefficients are given in the Dirac notation by,

\[ \begin{align*}
\epsilon_{ij,ss'} &= \langle R_{ij,s} | \hat{h}_{ss'} | R_{ij,s'} \rangle, \\
V_{ijkl} &= \langle R_{ij}^{(1)} | s_1 | R_{jk}^{(2)} \rangle s_2 | V_{ijkl} | R_{kl}^{(2)} \rangle | s_3 | R_{il}^{(1)} \rangle s_4. 
\end{align*} \]
with the one particle Hamiltonian operator

\[
\hat{h}_{ss'} = \left[ \delta_{ss'} \left( \frac{1}{2m} \left( \nabla_r + \frac{e}{c} A(r) \right) \right)^2 + U(r) - \mu \right] + g_{ss'}(r),
\]

where \(U(r)\) is the periodic crystal potential, and the Wannier function is given through

\[
\langle \mathbf{r} | \mathbf{R}_i, s \rangle = w_s(\mathbf{r} - \mathbf{R}_i).
\]

As argued at the beginning this chapter we will neglect the spin-orbit coupling term, \(g_{ss'}\), and assume a spin-triplet \(p\)-wave interaction.

In the following we work within the domain wall axes, see Fig. 6.1, and we set \((\tilde{x}, \tilde{y}) \equiv (x, y)\). The system is then translationally invariant along \(y\)-direction and inhomogeneous along the \(x\)-direction. It is convenient to impose periodic boundary conditions in the \(y\)-direction and perform the Fourier transformation,

\[
a_i = \frac{1}{\sqrt{N_y}} \sum_{k_y \in B.Z.} e^{ik_y y} a_{x_i,k_y},
\]

where \(N_y\) is the number of sites along the \(y\)-direction.

### 6.B.1 Tight-binding approximation

The tight-binding approximation for the non-interacting part of the Hamiltonian, taking into account nearest-neighbor \((t_\gamma)\) and next-to-nearest-neighbor \((t'_\gamma)\) hopping of the \(d_{xy}\)-Ru-electrons in the Ru-O\(_2\) plane, is given through,

\[
\epsilon_{ji}^{(\gamma)} = (\epsilon_{0,\gamma} - \mu) \delta_{ij} - t_\gamma \left( \delta_{j,i+1x} + \delta_{j,i-1x} + \delta_{j,i+1y} + \delta_{j,i-1y} \right) - t'_\gamma \left( \delta_{j,i+1x+1y} + \delta_{j,i-1x+1y} + \delta_{j,i-1x+1y} + \delta_{j,i+1x-1y} \right).
\]

We introduce now the vector potential through the Peierls substitution according to the following rule,

\[
\langle \mathbf{R}_i, \alpha | \mathcal{H} \left( \mathbf{r}, \mathbf{p} + \frac{e}{c} \mathbf{A}(\mathbf{r}) \right) | \mathbf{R}_j, \beta \rangle = \exp \left\{ -\frac{ie}{\hbar c} \Phi_{ij} \right\} \langle \mathbf{R}_i, \alpha | \mathcal{H}(\mathbf{r}, \mathbf{p}) | \mathbf{R}_j, \beta \rangle,
\]

see Ref. [102]. Assuming that \(\mathbf{A}(\mathbf{r})\) varies smoothly along the path \(\mathbf{R}_i \mapsto \mathbf{R}_j\), we make the approximation,

\[
\Phi_{ij} \equiv \int_{\mathbf{R}_i}^{\mathbf{R}_j} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{r} \approx \frac{1}{2} \left[ \mathbf{A}(\mathbf{R}_i) + \mathbf{A}(\mathbf{R}_j) \right] \cdot (\mathbf{R}_j - \mathbf{R}_i).
\]
Because of the translational symmetry along the \( y \)-direction, we can choose a gauge in which the vector potential is given by \( \mathbf{A}(x) = (0, A_y(x)) \). Using the notation \((i, j, k, l) \equiv (i_x, j_x, k_y, l_z)/a\), we find for the non-interacting Hamiltonian,

\[
\mathcal{H}_0 = \sum_{ij, k_y, s} \epsilon_{ji}(k_y) a_{j, k_y, s}^\dagger a_{i, k_y, s},
\]

with \( \epsilon_{ji}(k_y) \) given in Eq. (6.4), where \( a \) is the lattice spacing, \( a = x_{i+1} - x_i \) (not to be confused with the annihilation operator \( a_{i, k_y, s} \)). The index \( i = 1, \ldots, N \) labels the site along the \( x \)-direction.

**Lattice current density**

The current density operator from the site \( i \) to the site \( j \) is given by

\[
J_{ij} = -\frac{e}{\hbar c} \sum_{\sigma} \exp\left\{ -i \frac{e}{\hbar c} \Phi_{ij} \right\} a_{j, i, \sigma}^\dagger a_{i, i, \sigma},
\]

where \( d \) is the length of the unit cell in the \( z \)-direction. Performing the Fourier transform and taking the expectation value we get

\[
\langle J_{ij} \rangle = -i J_0 \exp\left\{ -i \frac{e}{\hbar c} \Phi_{ij} \right\} \frac{1}{N_y} \sum_{k_y} e^{i k_y (y_j - y_i)} \langle a_{j, k_y, a_{i, k_y}^\dagger} \rangle,
\]

with \( J_0 = \frac{2 e t_c}{\hbar a d} \).

**6.B.2 Effective interaction**

Following Ref. [103] we split the interaction into its orbital and spin parts as,

\[
V_{ij\,kl}^{s_l,s_k,s_3,s_4} = g_{ij\,kl}^s g_{s_l \, s_k \, s_3 \, s_4}^s,
\]

where for a spin-triplet interaction, the spin part is given by

\[
g_{s_l \, s_k \, s_3 \, s_4}^s = \frac{1}{2} (\sigma_s i \sigma_y)^t_{s_l \, s_k} (\sigma_s i \sigma_y)_{s_3 \, s_4} = \frac{1}{2} \delta_{s_2, -s_1} \delta_{s_4, -s_3}.
\]

Note that this form is invariant under spin rotation and we conserve the \( SU(2) \) symmetry of the Hamiltonian, see Ref. [55]. The effective orbital \( p \)-wave interaction can be written as,

\[
g_{ij\,kl}^p = g_{ij\,k\,l}^p \delta_{k, l} \delta_{i, l} \delta_{j, l} \delta_{i, l},
\]

with, for nearest-neighbor interaction,

\[
g_{ij\,k\,l}^p = -g_p \left[ \delta_{j, i+1} + \delta_{j, i-1} + \delta_{j, i+1} + \delta_{j, i-1} \right],
\]

where we chose \( g_p > 0 \). Assuming that the system is translationally invariant along the \( y \)-direction and imposing periodic boundary conditions, we can perform the Fourier transform (6.83), from which we find

\[
\mathcal{H}_{int} = \frac{1}{2 N_y} \sum_{k_y, k'_y} \sum_{s_l, s_k, s_3, s_4} g_{ij} (k_y, k'_y) a_{i, k_y, s_l}^\dagger a_{j, k'_y, s_k}^\dagger a_{j, k'_y, s_3} a_{i, k_y, s_4},
\]

with the potential

\[
g_{ij} (k_y, k'_y) = -\frac{g_p}{2} \left[ \delta_{j, i+1} + \delta_{j, i-1} + 2 \cos a (k_y - k'_y) \delta_{ij} \right].
\]

We note the fact that in general when the number of lattice sites are no equal in the two directions, \( x \) and \( y \), i.e. \( N \neq N_y \), we have to consider the two potentials \( \{g_{p,x}, g_{p,y}\} \), which have to be determined self-consistently from the gap equations in the limit \( T \to T_c \).
6.B.3 Bogoliubov-de Gennes equation

Performing the standard BCS-mean field approximation we find the following Hamiltonian,

\[ \mathcal{H}^{MF} = \mathcal{H}_{\uparrow\downarrow}^{MF} + \mathcal{H}_{\downarrow\uparrow}^{MF}, \]

(6.96)

where the first term is given by,

\[ \mathcal{H}_{\uparrow\downarrow}^{MF} = \frac{1}{2} \sum_{i,j,k_y} \begin{pmatrix} a_{i,y,k_y} & a_{i,-y,k_y} \end{pmatrix} \begin{pmatrix} \epsilon_{ij}(y) & \Delta_{ij}(k_y) \\ \Delta_{ij}(k_y) & -\epsilon_{ij}(-k_y) \end{pmatrix} \begin{pmatrix} a_{i,y,k_y}^\dagger \\ a_{i,-y,k_y}^\dagger \end{pmatrix} + K + C_0, \]

(6.97)

with the constants,

\[ K = \frac{1}{2} \sum_{i,j,k_y} \Delta_{ij}(k_y) \left( F_{ij}^\dagger(k_y) + F_{ij}^\dagger(k_y) \right), \]

(6.98)

\[ C_0 = \frac{1}{2} \sum_{i,k_y} \epsilon_{ii}(k_y), \]

(6.99)

and similarly for the term \( \mathcal{H}_{\downarrow\uparrow}^{MF} \). The anomalous Green’s functions are defined through,

\[ \begin{cases} F_{ij}^\dagger(k_y) := \langle a_{i,y,k_y} a_{j,-y,k_y} \rangle, \\ F_{ij}^\dagger(k_y) := \langle a_{i,-y,k_y} a_{j,y,k_y} \rangle, \end{cases} \]

(6.100)

and the gap function through,

\[ \Delta_{ij}(k_y) := -\frac{1}{N_y} \sum_{k_y'} g_{ij}(k_y,k_y') \left( F_{ij}^\dagger(k_y') + F_{ij}^\dagger(k_y') \right), \]

(6.101)

\[ \Delta_{ij}(k_y) := -\frac{1}{N_y} \sum_{k_y'} g_{ij}(k_y,k_y') \left( F_{ij}^\dagger(k_y') + F_{ij}^\dagger(k_y') \right). \]

Note that according to this definition the gap function transforms as

\[ \Delta_{ij}(-k_y) = -\Delta_{ji}(k_y), \]

\[ \Delta_{ij}^\dagger(k_y) = \Delta_{ji}^\dagger(k_y). \]

Because of the symmetry of the spin part of the coupling, we have \( F_{\downarrow\uparrow} = F_{\uparrow\downarrow} \), such that \( \mathcal{H}_{\downarrow\uparrow}^{MF} = \mathcal{H}_{\uparrow\downarrow}^{MF} \). In the following we then only consider the term \( \mathcal{H}^{MF} \) and we drop the spin indices.

The mean field Hamiltonian can be diagonalized through the transformation,

\[ \begin{pmatrix} a_{i,y,k_y} \\ a_{i,-y,k_y} \end{pmatrix} = \sum_{n=1}^{N} U_{i,k_y}^{n} \begin{pmatrix} c_{n,k_y} \\ c_{n,-k_y}^\dagger \end{pmatrix}, \]

(6.102)

with the unitary matrices,

\[ U_{i,k_y}^{n} = \begin{pmatrix} u_{i,k_y}^{n_1} & v_{i,k_y}^{n_2} \\ u_{i,k_y}^{n_2} & v_{i,k_y}^{n_1} \end{pmatrix}, \]

(6.103)

where the columns are eigenvectors, with the eigenvalues \( \{ E_{\tilde{n}_1,k_y}, E_{\tilde{n}_2,k_y} \} \), of the Bogoliubov-de Gennes equation,

\[ \sum_{j=1}^{N} \begin{pmatrix} \epsilon_{ij}(k_y) & \Delta_{ij}(k_y) \\ \Delta_{ij}(k_y) & -\epsilon_{ij}(-k_y) \end{pmatrix} \begin{pmatrix} u_{j,k_y}^{n} \\ v_{j,k_y}^{n} \end{pmatrix} = E_{n,k_y} \begin{pmatrix} u_{k_y}^{n} \\ v_{k_y}^{n} \end{pmatrix}, \]

(6.104)

with \( n = 1, \ldots, 2N \). It is easy to show that this equation satisfies the chiral (particle-hole) symmetry. Let us start from the BdG equation in matrix form,

\[ \begin{pmatrix} e_{k_y} & \Delta_{k_y} \\ \Delta_{k_y}^\dagger & -e_{-k_y} \end{pmatrix} \begin{pmatrix} u_{k_y} \\ v_{k_y} \end{pmatrix} = E_{k_y} \begin{pmatrix} u_{k_y} \\ v_{k_y} \end{pmatrix}. \]
It can be rewritten as
\[
\begin{pmatrix}
-e_{-k_y} & \Delta^*_k \\
\Delta_k & e_{k_y}
\end{pmatrix}
\begin{pmatrix}
v_{k_y} \\
u_{k_y}
\end{pmatrix} = E_{k_y}
\begin{pmatrix}
v_{k_y} \\
u_{k_y}
\end{pmatrix}.
\]
Making now the transformation \(k_y \rightarrow -k_y\) and taking the complex conjugate, we find
\[
\begin{pmatrix}
e_{k_y} & \Delta^*_k \\
\Delta_k & -e_{-k_y}
\end{pmatrix}
\begin{pmatrix}
v_{-k_y}^* \\
u_{-k_y}^*
\end{pmatrix} = -E_{-k_y}
\begin{pmatrix}
v_{-k_y}^* \\
u_{-k_y}^*
\end{pmatrix},
\]
where we used \(\Delta_{ij,-k_y} = -\Delta_{ji,k_y}\). We then have that if \((u_{k_y}, v_{k_y})\) is an eigenvector of \(H_{k_y}\) with the eigenvalue \(E_{k_y}\), then \((v_{-k_y}^*, u_{-k_y}^*)\) is also an eigenvector of \(H_{k_y}\) with the eigenvalue \(-E_{-k_y}\). Hence we can rewrite the transformation matrix as,
\[
U_{i,k_y}^\dagger = \begin{pmatrix}
u_{i,k_y}^* & u_{i,-k_y}^* \\
u_{i,k_y} & u_{i,-k_y}
\end{pmatrix},
\]
which, substituted in Eq. (6.102), leads to Eq. (6.8).

### 6.C Homogeneous system

We assume that the system is translationally invariant with periodic boundary conditions. Fourier transforming the Hamiltonian (6.97) in the \(x\)-direction, we find the Bloch Hamiltonian,
\[
\mathcal{H}^{MF}(k) = -K - C_0 = \frac{1}{2} \sum_k \left( a_k^\dagger a_{-k} \right) \left( \begin{array}{c}
\epsilon_y(k) \\
\Delta(k)
\end{array} \right)
\begin{pmatrix}
\epsilon_y(k) \\
\Delta^*(k)
\end{pmatrix}
\begin{pmatrix}
a_k \\
a_{-k}^\dagger
\end{pmatrix},
\]
with, in the non-rotated reciprocal axis \((k = \tilde{k})\),
\[
\begin{align*}
\epsilon_y(k) &= \epsilon_{0,y} - \mu - 2t_y \cos ak_x + \cos ak_y - 4t'_y \cos ak_x \cos ak_y, \\
\Delta(k) &= \Delta_0 (\phi_x(k) \pm i\phi_y(k)),
\end{align*}
\]
when we set \(\Delta_x = \Delta_0\) and \(\Delta_y = \pm i\Delta_0\), with the basis functions
\[
\begin{pmatrix}
\phi_x(k) \\
\phi_y(k)
\end{pmatrix} = \begin{pmatrix}
\sin ak_x \\
\sin ak_y
\end{pmatrix}.
\]
In the rotated axis \((k = \tilde{k})\), we find
\[
\begin{align*}
\epsilon_y(k) &= \epsilon_{0,y} - \mu - 4t_y \cos ak_x / \sqrt{2} : \cos ak_y / \sqrt{2} - 2t'_y \cos \sqrt{2}ak_x : \cos \sqrt{2}ak_y, \\
\Delta(k) &= \Delta_0 (\phi_x(k) \pm i\phi_y(k)),
\end{align*}
\]
when we set \(\Delta_x = \Delta_0\) and \(\Delta_y = \pm i\Delta_0\), with the basis functions
\[
\begin{pmatrix}
\phi_x(k) \\
\phi_y(k)
\end{pmatrix} = \begin{pmatrix}
\sqrt{2} \sin ak_x / \sqrt{2} \cos ak_y / \sqrt{2} \\
\sqrt{2} \sin ak_y / \sqrt{2} \cos ak_x / \sqrt{2}
\end{pmatrix}.
\]
The Hamiltonian can be readily diagonalized and we find the eigenvalues
\[
E(k) = \pm \sqrt{\epsilon_y(k) + |\Delta(k)|^2},
\]
\[
F(k) = \langle a_k a_{-k} \rangle = \frac{\Delta(k)}{2E(k)} \tanh \left( \frac{\beta E(k)}{2} \right),
\]
The condensation energy at \(T = 0\) is found to be,
\[
E_{\text{cond}} = \langle \mathcal{H} \rangle, \\
E_{\text{cond}} = \frac{\Delta}{2} + \sum_k \left[ E(k) - \epsilon_y(k) \right] + K.
\]
6.D Scaling factors

The $y$-component of the Fermi wave vector of the $\gamma$-band is found to be,

$$k_{F,y} = \frac{1}{a} \arccos \frac{\epsilon_0 - \mu - 2t_\gamma}{2t_\gamma + 4t'_\gamma}.$$  \hspace{1cm} (6.115)

Note that we can relate the nearest neighbor hopping to the effective mass through,

$$t_\gamma = \frac{\hbar^2}{2m^*a^2}.$$ \hspace{1cm} (6.116)

In the paper we use the following scaling factors,

$$
\begin{align*}
k_0 &= \frac{1}{a} \\
J_0 &= \frac{2et_\gamma}{h\kappa d} \\
B_0 &= \frac{4\pi}{c} J_0 a \\
A_0 &= \frac{1}{\gamma a}
\end{align*}
$$

with $\gamma = \frac{\pi}{\Phi_0} = \frac{e}{hc}$. Following [104] and [105] we define the coherence length and the London penetration depth at $T = 0$ and along the $x$-direction as

$$
\begin{align*}
\frac{1}{\lambda^2_L} &= \frac{4\pi e^2}{c^2 \hbar^2 \Omega N_x N_y} \sum_k \left[ 2 \left( \frac{\partial \epsilon(k)}{\partial k_x} \right)^2 \frac{\partial f(E(k))}{\partial E(k)} + \frac{\partial^2 \epsilon(k)}{\partial k_x^2} \right]_{T=0} \\
\xi_0^2 &= \frac{\sum_k |\nabla_{k_x} (\Delta_0(k)/E(k))|^2}{\sum_k |\Delta_0(k)/E(k)|^2},
\end{align*}
$$

where $\Omega = a^2 d$ is the volume of a unit cell of the material ($d$ is the lattice spacing along the $z$-direction). Note that the first term of the first equation vanishes due to the specific shape of the gap function. Note that we have $\xi_0 = \frac{2\sqrt{2}}{\pi} \xi_0^{\text{BCS}} \approx 0.9\xi_0^{\text{BCS}}$. In an isotropic system the BCS coherence length is simply given by $\xi_0^{\text{BCS}} = \frac{\hbar v_F}{\pi \Delta(0)}$.

The dimensionless expressions are then given through

$$
\begin{align*}
\frac{1}{F_1} &= \frac{1}{N_x N_y} \sum_k \frac{\partial^2 \epsilon(k)}{\partial k_x^2} \left( 1 - \frac{\xi(k)}{E(k)} \right) \\
F_2 &= \frac{\sum_k |\nabla_{k_x} (\Delta_0(k)/E(k))|^2}{\sum_k |\Delta_0(k)/E(k)|^2},
\end{align*}
$$

with

$$
\frac{1}{F_1} = \frac{1}{\lambda^2_L} \frac{c^2 \hbar^2 d}{4\pi e^2 t_\gamma}, \\
F_2 = \frac{\xi_0^2}{a^2}.
$$

Defining

$$l = \sqrt{\frac{F_1}{F_2}}$$ \hspace{1cm} (6.117)

we then have

$$\kappa = \frac{\lambda_L}{\xi_0} = l \left( \frac{c^2 \hbar^2 d}{4\pi e^2 t_\gamma a^2} \right)^{1/2} \approx 217 \ l,$$ \hspace{1cm} (6.118)

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where we have substituted the constants
\[
\begin{align*}
a &= 0.39 \text{ nm} \\
d &= 1.27 \text{ nm} \\
t_\gamma &= 0.4 \text{ eV}. \\
\end{align*}
\] (6.119)

From the we can rewrite the Maxwell’s equation as
\[
\begin{align*}
b_z(x_i) &= -\sum_{j=1}^i j_y(x_j) + C_0 \\
a_y(x_i) &= 2\frac{l^2}{\kappa^2} \sum_{j=1}^i b_z(x_j) + C_0'. \\
\end{align*}
\] (6.120) (6.121)

since we have
\[
\frac{B_{0a}}{A_0} = 2\frac{a^2}{\lambda_2^2} F_1 = 2\frac{\xi_0^2}{\lambda_2^2} F_1 = 2\frac{l^2}{\kappa^2}.
\] (6.122)

### 6.E Zero-energy edge states of the truncated bulk Hamiltonian

In the following we refer to the method developed in Ref. [108] in order to predict the existence of zero-energy edge states.

#### 6.E.1 Bulk loops

We have seen in section 6.3 that the edge Hamiltonian can be interpreted as a sum of one-dimensional Hamiltonians parametrized by \( k_y \). Writing the bulk Hamiltonian as \( h_{k_y}(k_x) \) and \( m_{k_y}(k_x) \), there is a one to one correspondence from \( h_{k_y}(k_x) \) to \( m_{k_y}(k_x) \) for all \( k_x \in (-\pi/a, \pi/a) \cong S^1 \). Hence we can parametrize a loop in \( \mathbb{R}^3 \) for a fixed \( k_y \) as \( l : k_x \in S^1 \mapsto m_{k_y}(k_x) \in \mathbb{R}^3 \). The loop for \( k_y \) is then given by \( \cup_{k_x \in S^1} m_{k_y}(k_x) \). We write the corresponding one-dimensional bulk Hamiltonian as \( \mathcal{H}_{k_y}^{\text{bulk}}[l] \). In the following we call \( l^* \) a loop that lies on a two-dimensional plane of \( \mathbb{R}^3 \) such that it surrounds the origin \( \mathcal{O} \).

From there we can construct an effective edge Hamiltonian by performing the inverse Fourier transform (in the \( x \)-direction) and imposing the truncation : \( h_{ij,k_y} = 0 \) for \( i, j \notin [1, \ldots, N] \). We write the effective edge Hamiltonian obtained in this way as \( \mathcal{H}_{k_y}^{\text{edge}}[l, e] \) (\( e \)' refers to the kind of edges obtained through the truncation).

In the case of a charge-conjugation symmetric bulk Hamiltonian—in the sense of section 6.3.1—, and under the conditions that (i) the bulk Hamiltonian of the system has \( m_x = \xi_0 = 0 \), i.e. the vectors (the loop) \( m_{k_y}(k_x) \) lie in the \( m_x, m_y \)-plane, and (ii) the loop surrounds the origin \( \mathcal{O} \), it is easy to shown that the corresponding effective edge Hamiltonian, \( \mathcal{H}_{k_y}^{\text{edge}}[l^*], e \) = \( a_k^\dagger_k a_{k_y}^\dagger a_{k_y} \), satisfies the chiral symmetry—in the sens of section 6.3.2—, that is \( \hat{\Gamma} \mathcal{H}_{k_y} \hat{\Gamma}^\dagger = -\mathcal{H}_{k_y} \) with \( \hat{\Gamma} = \hat{\sigma}_z \otimes 1 \) [108].

As a consequence, if the effective edge Hamiltonian has one edge state, say on side \( L \), with the non-zero energy \( E \), i.e. \( |l^*, E, L\rangle \), then it must have an other edge state with the energy \(-E\), i.e. \( |l^*, -E, L\rangle \) (since the operator \( \hat{\Gamma} \) is local, \( |\psi\rangle \) and \( \hat{\Gamma}|\psi\rangle \) are localized at the same edge). This chiral symmetry will play an essential role in the following.

We consider now the one dimensional bulk Hamiltonian given by the vector, \( m(k_x) = (\cos k_x, -\sin k_x, 0) \). It corresponds to the unit circle in the \( m_x, m_y \)-plane centered on the origin \( \mathcal{O} \), we call this loop \( l_c \). It is easy to show that the effective edge Hamiltonian corresponding to this loop has two exact zero-energy edge states, one at \( i = 1 \) and one at \( i = N \), see [108].

We can now state the main argument that lies on the fact that if we transform adiabatically the loop \( l_c \) into another loop \( l^* \) (belonging to a two-dimensional plane and surrounding the origin) without crossing the origin—i.e. the bulk gap is not closed—and such that chiral symmetry is conserved, then the zero-energy edge states are conserved. Indeed, when performing the transformation from \( l_c \) to \( l^* \), the chiral symmetry guarantees that if one of the zero-energy edge states, say \( |l_c, 0, L\rangle \), goes away from the zero energy, then an other edge state should appear at the same edge with the opposite energy. But if
the transformation is done adiabatically without closing the bulk gap, new edge states can only appear by pair! So, since the number of edge states localized on the same edge is odd, at least one edge state will remain at zero-energy, i.e. it is protected by the chiral symmetry.

It was been shown in Ref. [109] that the bulk Chern number of the system can be interpreted as the degree of covering of the origin by the mapping \((k_x, k_y) \mapsto m(k_x, k_y)\), as we go through the Brillouin zone, i.e. through the torus \((k_x, k_y) \in (-\pi/a, \pi/a) \times (-\pi/a, \pi/a) \cong T^2\). Hence a non-zero bulk Chern number guaranties the existence of at least one such a loop \(l^*\).

6.E.2 Chiral \(p\)-wave state

In this section we apply the previous argument to the edge Hamiltonian obtained through the truncation of the bulk Hamiltonian with the chiral \(p\)-wave state. We will see that we need a generalization of the surfaces that contain the loops \(l^*\) discussed above, from two-dimensional flat planes to curved surfaces.

- In the case of the (100)-edges the good quantum number is \(k_y\). The corresponding bulk Hamiltonian is written in the unrotated axes as (the following parametrization of the gap function is defined in the next section),

\[
\begin{align*}
\mathbf{m}_{k_y}(k_x) &= \begin{pmatrix}
\phi_x(k) \text{Re} \Delta_x \text{(bulk)} + \phi_y(k) \text{Re} \Delta_y \text{(bulk)}, -\phi_x(k) \text{Im} \Delta_x \text{(bulk)} - \phi_y(k) \text{Im} \Delta_y \text{(bulk)}, \xi(k)
\end{pmatrix}, \\
&= \Delta_0 (\sin ak_x \cos \alpha/2 - \sin ak_y \sin \alpha/2, -\sin ak_x \sin \alpha/2 + \sin ak_y \cos \alpha/2, \\
e_0 - 2t_s (\cos ak_x + \cos ak_y) - 4t'_s \cos ak_x \cos ak_y).
\end{align*}
\]  

(6.123)

We show in Fig. 6.16.A the envelope obtained by the loops \(\cup_{k_x \in S^1} \mathbf{m}_{k_y}(k_x)\) as we vary \(k_y\) from 0 to \(-2\pi\). As mentioned above the non-zero bulk Chern number is related to the fact that this envelope traps the origin. We clearly see that the loop for \(k_y = 0, \cup_{k_x \in S^1} \mathbf{m}_0(k_x)\), defines a plane that contains the origin,
moreover it is the only one. We note that this property is not changed when we vary the parameters $\xi_0, t_x, t'_y$, and $\alpha$.

It is easy to show that the effective edge Hamiltonian (obtained through the inverse Fourier transform of the bulk Hamiltonian and truncation) respects the charge-conjugation symmetry at $k_y = 0$. This leads to the existence of two zero-energy edge states, one on each edge, say $|l_{c}, E = 0, L \rangle$ and $|l_{c}, E = 0, R \rangle$. We have shown in section 6.3.1 that the full edge Hamiltonian, Eq. (6.35), is particle-hole symmetric at $k_y = 0$ as a consequence of the charge-conjugation symmetry of the system and the special value $k_y = -k_y = 0$. Then, as we have argued in the previous section, since this symmetry is conserved at the point $k_y = 0$ and we have an odd number of edge states on each side, at least one zero-energy edge state on each side is conserved at $k_y = 0$, i.e. the zero-energy edge state is protected by the charge-conjugation symmetry. We find those zero-energy edge states in the numerical self-consistent solution presented below.
• In the case of the (\bar{1}10)-edges the good quantum number is $k_{\parallel}$. The corresponding bulk Hamiltonian is written in the rotated axes as, $(k_\perp, k_{\parallel}) = (k_x, k_y)$,

$$m_{k_y}(k_x) = \sqrt{2}\Delta_0 \left( \sin \tilde{k}_x \cos \tilde{k}_y \cos \alpha/2 - \sin \tilde{k}_y \cos \tilde{k}_x \sin \alpha/2,\right.$$  

$$-\sin \tilde{k}_x \cos \tilde{k}_y \sin \alpha/2 + \sin \tilde{k}_y \cos \tilde{k}_x \cos \alpha/2,\right.$$  

$$\epsilon_0 - 4t_\gamma \cos k_x \cos k_y - 2t'_\gamma (\cos 2\tilde{k}_x + \cos 2\tilde{k}_y) \right) . \tag{6.124}$$

with $\tilde{k}_i = ak_i/\sqrt{2}$. We show in Fig. 6.16.B the envelope given by the loops $\cup_{k_x \in S} \{m_{k_y}(k_x)\}$ as we vary $k_y \in (-\pi/\sqrt{2} a, \pi/\sqrt{2} a]$. The origin is trapped by this envelope, as we expect from the non-zero bulk Chern number. We again find the loop at $k_y = 0$ that surrounds the origin, see Fig. 6.17 (a). However, we also find two other loops at $k_y = \pm 0.732\pi/\sqrt{2} a$, which each defines a surface that contains the origin: we show one of them in Fig. 6.17 (b). We see that the surfaces defined by these loops are now curved ! Also we need here to generalize the loop-surfaces from flat planes (considered in [108]) to curved surfaces (note that they have to be flat at least in one direction, here the $m_{x}$-direction). We illustrate the crossing of the origin by the loop-surface in Fig. 6.17 (c-d) which shows one loop for three different values of $k_y$ (looking at them in the $m_{x}$-direction). We clearly see that as we vary $k_y$ from 0.6\pi/\sqrt{2} a to 0.85\pi/\sqrt{2} a, the surface defined by the loop crosses the origin. We call $k_{y,0}$ the point at which the crossing happens. This corresponds precisely to the point $k_{y,0}$ defined in section 6.3.2, i.e. this is the crossing point of the Fermi surface with the small square of Fig. 6.2 (b).

We show on Fig. 6.18 the spectrum of the truncated Hamiltonian with rotated edges for $\epsilon_0 = -0.3$. It has the same structure as the full model studied in this chapter.

To summarize : in the case of rotated edges, we expect to find a zero-energy edge state at $k_y = 0$ and at $k_y \approx \pm k_{y,0}$, on both edges. This is precisely what we find in the numerical self-consistent solution. We finish this section by noting that the zero-energy bound states are not necessary exact, i.e. $\min |E_0| \gtrless 0$, due to finite size effect (for instance for $N$ even, there is no state at $k_y = 0$). Taking the limit $N \to \infty$ they would become exact as $\min |E_0| \sim 1/N \to 0$. 

Figure 6.18: Truncated Hamiltonian spectrum with rotated edges for $\epsilon = -0.3$. 

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure6.18.png}
\caption{Truncated Hamiltonian spectrum with rotated edges for $\epsilon = -0.3$.}
\end{figure}
Chapter 7

Prospects

7.1 Josephson effect at a Ru inclusion: domain wall and Josephson vortex interplay

Based on the results of chapter 2 concerning the structure of a domain wall as a function of its orientation with respect to the main crystal axes, we give a simple model that accounts for the effect of domain walls on the critical Josephson current at a Ru inclusion in Sr$_2$RuO$_4$. We first show that the presence of domain walls leads to the creation of an additional Josephson vortex at the interface. Assuming the possible motion of the Josephson vortex and the domain walls through external perturbations we give an interpretation of the Josephson experiment on Nb/Ru/Sr$_2$RuO$_4$ junctions reported by the group of Maeno in Ref. [69].

Let us start by showing on Fig. 7.2 the measurements of the $I$-$V$-curve of Nb/Ru/Sr$_2$RuO$_4$ Josephson junctions reported in Ref. [69]. We see a strong switching behavior of the junction between zero and non-zero voltage regime. This corresponds to a switching between different values of the Josephson critical current of the junction. This phenomenon is only observed for temperature below the critical temperature of Sr$_2$RuO$_4$, $T_{c,SRO} = 1.5$ K, whereas the critical temperature of Nb lie higher $T_{c,Nb} = 9.5$ K and the Ru inclusion becomes superconducting through the proximity effect. This is the evidence that the origin of the switching is an intrinsic feature of Sr$_2$RuO$_4$. This lead the authors of the experimental study to make the assumption of the presence domain walls in Sr$_2$RuO$_4$ reaching the inclusion interface.

We give here detailed discussion based on our results on the stable domain walls’ structure. This allows us to derive a simple model for the critical current. We will see that it is natural for this physical setup to assume the interplay at the interface between domain walls and a Josephson vortex. The phenomenon observed can than be well explained through the moving of the Josephson vortex and possibly also of the domain walls under external perturbations.

We assume that two domain wall reach a Ru inclusion (a cylinder defect) in Sr$_2$RuO$_4$ with the angles $\theta_1$ and $\theta_2$, respectively (in the following we write $\theta_1 \equiv \theta_i$). We take the crystal axis as the reference frame and we work in the polar coordinates. We assume that the phase with the winding number $N = +1$ lies in the range $\theta \in (\theta_1, \theta_2)$ and the phase $N = -1$ lies in $\theta \in (\theta_2, 2\pi + \theta_1)$ (we assume sharp domain walls for simplicity). Only the azimuthal component of the order parameter plays a role in the Josephson effect for this geometry, $\varphi_\theta = \phi_\theta - \phi_s$. It is given in the two domains by

\[
\begin{align*}
\phi_\theta(\theta) &= \phi_0 - \theta_1 + \theta, & \text{for } \theta \in (\theta_1, \theta_2), \\
\phi_\theta(\theta) &= \phi_0 + 2\theta_2 - \theta_1 + \alpha_2 - \theta, & \text{for } \theta \in (\theta_2, 2\pi + \theta_1).
\end{align*}
\]

(7.1)

We have chosen the convention to take the sign $+$ for positive trigonometric angles (anti-clock wise winding). Across the first domain wall we have $\phi_\theta(\theta^-_1) = \phi_\theta(\theta^+_1) - \alpha_1 = \phi_0 - \alpha_1$. The condition of single-valuedness of the order parameter requires that,

\[e^{i\phi_\theta(\theta^-_1)} = e^{i\phi_\theta(2\pi + \theta^-_1)},\]

that is $2(\theta_2 - \theta_1) + \alpha_2 + \alpha_1 - 2\pi = 0$, or in general,

\[2(\theta_2 - \theta_1) + \alpha_2 + \alpha_1 \mod 2\pi = 0.\]

(7.2)
We will now use the following result presented in chapter 2: the domain wall energy and the global phase shift as a function of the domain wall orientation, given in Fig. 2.7 and Fig. 2.8 respectively. We found that for the second domain wall of this geometry ($\theta_2$) there are two degenerate stable configurations at the domain wall's angles, $\theta_2 \mod \pi/2 = \pm 0.21\pi$, with the corresponding phase shifts $\alpha = \pm 0.32\text{rad}$ (for the first domain wall of this geometry, we have, $\theta_1 \mod \pi/2 = \pm 0.21\pi$, with the phase shifts, $\alpha = \mp 0.32\text{rad}$). Between two stable orientations, the domain wall is in a metastable state.

We find that the condition (7.2) is satisfied when the two domain walls lie along one of the main crystal axes, since then $\alpha_{1,2} = 0$ and $\theta_2 - \theta_1 = \pi$. However this corresponds to the metastable configuration of the domain walls the highest in energy (i.e. the less favorable), as we can see in Fig. 2.7. The main consequence of our study of the domain wall's structure is that in general the physical constrain (7.2) cannot be satisfied without any other contributions to the phase winding, and especially so when the two domain walls lie in their most stable configurations. This can be circumvented by the system through the creation of a Josephson vortex at the interface. Indeed, it is energetically more favorable to create a vortex which energy scales as a length (one dimensional defect) than to move the domain walls with an energy cost that scales as a surface (two dimensional defect). The condition of single-valuedness can then be recovered with a Josephson vortex contributing to the phase winding by,

$$\Delta \phi_V = 2\pi - \alpha_1 - \alpha_2 - 2(\theta_2 - \theta_1).$$

(7.3)

We can now write a simple model for the Josephson current at a Ru inclusion. We assume that a sharp Josephson vortex lies between the two domain wall at an angle, $\theta_V \in (\theta_1, \theta_2)$ (the case $\theta_V \in (\theta_2, 2\pi + \theta_1)$ is similar). The Josephson critical current at the interface is then given by,

$$\begin{align*}
I_c &= \max_{\phi_0} \left\{ \int_{\theta_1}^{\theta_0} \frac{d\theta}{2\pi} \sin (\phi_0 + \theta) + \int_{\theta_V}^{\theta_2} \frac{d\theta}{2\pi} \sin (\phi_0 + \Delta \phi_V + \theta) + \int_{\theta_2}^{2\pi + \theta_1} \frac{d\theta}{2\pi} \sin (\phi_0 + \Delta \phi_V + \alpha_2 + 2(\theta_2 - \theta)) \right\}. 
\end{align*}$$

(7.4)

[The energy of the interface reached its minimum at the maximum critical current.]

In the following we will assume that the first domain wall is locked in a stable configuration and allow the second domain wall to change its orientation. Then we assume the two following cases corresponding to the two stable configurations of the first domain wall,

(i) $\theta_1 \mod \pi/2 = 0.21\pi$, $\alpha_1 = -0.32\text{rad}$,

(ii) $\theta_1 \mod \pi/2 = -0.21\pi$, $\alpha_1 = 0.32\text{rad}$.

(7.5)

We show in Fig. 7.1 the computed critical current as a function of the relative position of the second domain wall, i.e. $\theta_2 - \theta_1$ ($\theta_1$ is kept fixed in one of the two stable positions). The case (i) is shown in Fig. (a) and the case (ii) in Fig. (b) (the phase shift profile of the second domain wall for each case is plotted on the side). The different lines (with different colors) correspond to different positions of the Josephson vortex on the interface, $\theta_V \in (\theta_1, \theta_2)$.

We clearly see that there is a competition between the energy of the interface and the energy of the domain walls. Indeed we find that the highest critical current is reached when the second domain wall lies at a position $1.1\pi < (\theta_2 - \theta_1) < 1.5\pi$ which doesn’t correspond to the most stable domain wall’s configuration. On top of that, the position of the highest critical current strongly depends on the position of the Josephson vortex. Therefore if the system is submitted to external perturbations (change of temperature, change of current driven through the interface) it is likely that we change the internal configuration of the domain walls and of the vortex, leading to a strong change of the critical current of the junction. The black lines show the range of values of the critical current that can be achieved simply through the moving of the Josephson vortex. The effect can even be stronger if one domain wall jumps from one stable configuration to another.

This gives a good basis for the explanation of the Josephson experiment on Nb/Ru/Sr$_2$RuO$_4$ reported in Ref. [69].
Figure 7.1: Maximum critical Josephson current, $I_c$, as a function of the relative position of the second domain wall ($\theta_2 - \theta_1$) for different Josephson vortex positions: along the arrow (black to red) we have $\theta_V/(\theta_2 - \theta_1) = 1, 0.875, 0.75, 0.625$, and 0.5. (a) The first domain wall ($\theta_1$) is located at a stable state with $\alpha_1 > 0$, case (i). (b) The first domain wall ($\theta_1$) is located at a stable state with $\alpha_1 < 0$, case (ii). We also show the corresponding phase shift profile of the second domain wall, $\alpha_2 = \alpha(\theta_2)$. The vertical full lines show the stable states of the second domain wall, and the vertical dashed lines show the crystal orientations for which we have a sign change of $\alpha_2$ (those correspond to the directions $\theta \mod \pi/4 = 0$).

Figure 7.2: $I$-$V$-curve of the Nb/Ru/Sr$_2$RuO$_4$ junctions taken from Ref. [69].
Bibliography


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List of publications

- **A. Bouhon** and M. Sigrist,
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  submitted

- **A. Bouhon** and M. Sigrist,
  "Geometry and band structure dependence of edge and domain wall states in a topological chiral p-wave superconductor",
  in preparation
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