Intrinsic magnetic phenomena in chiral $p$-wave superconductors

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Failing to fetch me at first keep encouraged,
Missing me one place search another,
I stop somewhere waiting for you.

— Walt Whitman, Leaves of Grass
The layered perovskite Sr$_2$RuO$_4$ has attracted widespread attention ever since its identification as an unconventional superconductor in 1994. Experimental evidence points to an odd parity spin-triplet state with a two-component order parameter and broken time-reversal symmetry. This makes the material an ideal candidate for chiral $p$-wave pairing. However, proposed edge currents have not been detected despite huge efforts and interpretations regarding domain walls remain conflicting. The abundance of intriguing properties as well as the open issues together with constant new discoveries keep the field active.

In this thesis we explore magnetic phenomena intrinsic to chiral $p$-wave superconductors. Inspired by observations, model systems are constructed and subsequently analyzed using the phenomenological Ginzburg Landau approach. Our focus lies on the formulation and minimization of the free energy functional, using both analytical and numerical tools. Results are interpreted with regard to experiments and also taking previous theoretical work into account. After a general introduction, we highlight developments made concerning the methodology, before we discuss the following three phenomena in detail.

**Spontaneous surface flux pattern**

The first phenomenon we study is the flux pattern appearing spontaneously at the surface. Such magnetic effects have been proposed theoretically, but have not been detected experimentally. Here we compute the detailed shape of the flux pattern including self-screening for a disk-shaped sample, taking into account band structure effects through the gradient term coefficients of the Ginzburg Landau functional, and systematically scanning the surface parameters. We find that both the magnitude and shape of the flux pattern, its direction, and also the resulting total flux, are highly sensitive to all the considered parameters. We conclude that these magnetic effects are not a universal feature of chiral $p$-wave superconductors. Additionally, we discuss the flux at impurities and contrast it with the flux at the surface.

**Topologically frustrated Josephson junction**

The second phenomenon we study are the different limiting mechanisms of the critical current in cylindrically-shaped Josephson junctions between a conventional $s$-wave and a chiral $p$-wave superconductor. Such systems appear naturally in eutectic Sr$_2$RuO$_4$-Ru, and this project is motivated by the observation of an anomalous temperature dependence of the critical current in Pb-Ru-Sr$_2$RuO$_4$ devices. Depending on the phase winding of the chiral $p$-wave superconductor, the junction is in a topologically trivial or frustrated state. In the latter, a line-shaped flux pattern appears spontaneously and we show that only an
inhomogeneous coupling leads to a finite critical current. We conclude that the unconven-
tional limiting mechanism corresponds to the underlying pinning-depinning transition. 
Additionally, we present a phase diagram describing the evolution of the different states 
of the junction.

**Half-quantum vortices on c-axis domain wall**

The third phenomenon we study are the non-trivial features of c-axis domain walls. First, 
we show that such domain walls are decoupled in isotropic systems but acquire a finite cou-
pling in anisotropic systems. The phase difference across the domain wall then depends on 
the sign of the anisotropy of the electronic structure and can only take discrete values with 
a periodicity of $\pi$, therefore supporting half-quantum vortices. We find that the charac-
teristic length of these vortices along the domain wall critically depends on the magnitude 
of the anisotropy. In the isotropic limit, the vortex explodes, while for small anisotropies 
it can be described by a standard sine-Gordon model. In the strongly anisotropic limit, 
on the other hand, the vortex becomes smaller than the relevant screening length and 
non-local effects have to be considered.

In summary, we exemplify how versatile the phenomenological Ginzburg Landau approach 
is by exploring such divers situations as surfaces, interfaces, junctions, impurities, and 
domain walls. We further demonstrate that even intricate details of in the electronic 
structure can be taken into account qualitatively, and how external boundary conditions 
hardly accessible in a microscopic approach can be included naturally in this framework.
Kurzfassung


**Spontane Oberflächenströme**

Das erste Phänomen, das wir untersuchen, ist die Struktur von Magnetflüssen, die spontan an der Oberfläche auftreten. Dieser Effekt wurde theoretisch hervorgesagt, jedoch im Experiment nie bestätigt. Hier berechnen wir die genaue Form dieser Magnetflüsse unter Einbezug der Selbstabschirmung für scheibenförmige Proben, wobei Bandstrukturreffekte durch die Gradiententerme des Ginzburg Landau Funktionals berücksichtigt und die Oberflächenparameter systematisch variiert werden. Wir stellen fest, dass sowohl die Grösse als auch die Form, die Richtung, wie auch der resultierende totale Fluss höchst sensitiv gegenüber allen berücksichtigten Parametern sind. Daraus schliessen wir, dass diese magnetischen Effekte keine universelle Eigenschaft von chiralen \( p \)-Wellen Supraleitern sind. Ferner diskutieren wir den Magnetfluss an Einschlüssen und stellen diesen dem Fluss an der Oberfläche gegenüber.

**Topologisch frustrierte Josephson–Kontakte**

Das zweite Phänomen, das wir untersuchen, sind die verschiedenen Begrenzungsmechanismen des kritischen Stromes in zylinderförmigen Josephson–Kontakten zwischen einem konventionellen \( s \)-Wellen und einem chiral \( p \)-Wellen Supraleiter. Solche Systeme treten natürlicherweise in eutektischem Sr₂RuO₄–Ru auf, wobei dieses Projekt auf der Beobachtung einer anomalen Temperaturabhängigkeit des kritischen Stromes in Pb–Ru–Sr₂RuO₄...
Kurzfassung


Halbzahlig quantisierte Wirbel auf $c$–Achsen Domänenwänden


Zusammenfassend zeigen wir exemplarisch wie vielseitig die phänomenologische Ginzburg Landau Theorie ist, indem wir solch unterschiedliche Situationen wie Oberflächen, Grenzflächen, Kontakte, Einschlüsse und Domänenwände untersuchen. Ferner zeigen wir, dass komplexe Eigenschaften der zugrundeliegenden elektronischen Struktur qualitativ berücksichtigt, und dass externe Randbedingungen, die in einem mikroskopischen Ansatz kaum beschreibbar sind, hier ganz natürlich behandelt werden können.
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This thesis has two preliminary chapters. In the general introduction in chapter 1, the background and necessary concepts are successively established. The three magnetic phenomena are proposed and motivated by bringing them in context with experimental observations and previous work. This chapter is intended to set the scope of this thesis by giving an overview and defining the most important notions, with ample references on different levels for a diverse audience. In chapter 2, the focus is on the methodology of modeling a chiral $p$-wave superconductor using the Ginzburg Landau approach, bringing together the different concepts introduced before. Both the analytical and numerical implementation of minimizing the free energy functional are explained. This chapter contains details and connections beyond what is usually provided in the papers, and the general methodological developments made during the progress of this thesis are highlighted.

In the main part, there is one chapter for each of the three magnetic phenomena, based on the publications. The flux pattern appearing spontaneously at the surface of a disk-shaped sample is explored in chapter 3. Another spontaneous phenomenon, the line-shaped flux pattern appearing in a cylindrically-shaped topologically frustrated Josephson junction, is the basis for the discussion of the unconventional limiting mechanism in chapter 4. Finally, the $c$-axis domain wall supporting half-quantum vortices is examined in chapter 5.

A comprehensive summary and general conclusions are drawn in chapter 6, interpreting the results in a broader context and also relating to the overall methodology, while specific conclusions are presented for each of the three phenomena in the main part.

In the appendix, there is supplementary information for the thesis in general, while specific appendices for a particular phenomenon appear at the end of the corresponding chapter in the main part. The appendix A contains a collection of different representations of the free energy and some particular expressions derived by variation. Details concerning the computations are provided in appendix B, first for the implementation in general, and then for each project in particular.
Introduction

In this introduction, the background of the thesis is outlined and the relevant underlying concepts are established. The magnetic phenomena are motivated and brought into context. The methodology is then described in detail in chapter 2.

First, superconductivity is presented from a historical perspective and the basic phenomenological properties are introduced alongside a description of the Ginzburg Landau free energy functional for conventional superconductors. The Josephson effect is also discussed, focusing on the sine-Gordon model for long junctions. Next, the notion of chiral p-wave pairing is developed both from a theoretical point of view by successively discussing the different pairing states in tetragonal crystals, and additionally from a material point of view by describing the candidate Sr$_2$RuO$_4$. Finally, each of the three intrinsic magnetic phenomena studied in this thesis is proposed, the inspiring experimental observations are summarized, and previous theoretical work is reviewed.

A comprehensive introduction to all the necessary ingredients is beyond the scope of this chapter. Rather, a selective manner is adopted, increasingly zooming in on the core concepts, reminding professional readers and defining the most important notions carefully, while the interested reader is provided with ample references at each stage.
1.1 Brief review of superconductivity from a historical perspective

Superconductivity has enchanted physicists ever since its discovery over a century ago and is a prime example of an emerging macroscopic many-body quantum phenomenon [1]. In this chronological overview we follow the experimental, material and theory milestones from the first observation in mercury to present-day unconventional superconductors, closing with a note on applications.

For further reading, the entertaining “very short introduction” by Blundell [2], the standard textbooks by Tinkham [3] or by de Gennes [4], or the comprehensive book by Waldram [5] are recommended.

1.1.1 Conventional superconductors

Sticking to the chronology, we first establish superconductivity as a stable thermodynamic state and next as a macroscopic quantum phenomenon, and review the phenomenological Ginzburg Landau approach and the microscopic BCS theory. To complete this description of conventional superconductors we also mention vortices in type II superconductors. A more detailed description of the Ginzburg Landau approach is presented in Sec. 1.2.1.

Superconductivity as a thermodynamic state

Superconductivity was observed for the first time in 1911 in the laboratory of Kamerlingh Onnes in Leiden [6], when they found that the resistivity of pure mercury suddenly dropped to zero below a critical temperature $T_c \approx 4.2$ K. Soon after, they also observed vanishing resistivity in lead ($T_c \approx 6$ K) and tin ($T_c \approx 4$ K) [7]. This first characteristic of being a perfect conductor gave superconductors their name, translated from the original Dutch ‘suprageleider’ [2]. However, cooling a perfect conductor across its transition temperature in an applied field and subsequently switching off the field would result in a state with field trapped inside the material – a different thermodynamic state than the one reached when switching the field on and off only after the cooling.

In 1933, Meissner and Ochsenfeld discovered that magnetic field is actually expelled from the material in the superconducting state [8]. This second characteristic of being a perfect diamagnet completed the picture and established superconductivity as a proper thermodynamic state, reached through a phase transition at the critical temperature $T_c$. But this expulsion of field is limited. There is a maximum, so-called thermodynamic critical field $H_c$, at which the superconductor is destroyed, as was discovered by Kamerlingh Onnes already in 1914 [9]. This critical field depends on temperature, such that superconductivity can be described by a proper $B$-$T$ phase diagram.

A first phenomenological description of these basic electrodynamic properties was given by the London brothers in 1935 through the London theory [10]. In a compact form the supercurrent density $J_s$ and the vector potential $A$ are related through

$$J_s = \frac{-n_se^2}{m^*c} A,$$

where $n_s$ is the density of the superconducting electrons, $e^*$ is their charge, $m^*$ is their mass, and where the so-called London gauge is chosen with $\nabla \cdot A = 0$ and $A \to 0$ in the bulk of the sample. The two London equations are recovered by taking the time derivative.
\[ \partial_t \mathbf{A} \text{ and the curl } \nabla \times \text{ of the above expression. For the magnetic field we then find} \]

\[ \lambda^2 \nabla^2 \mathbf{B} = \mathbf{B}, \quad (1.2) \]

where the parameter \( \lambda_L^2 = m^* c^2 / (4 \pi n_s e^* c^2) \) is called the London penetration depth and describes the expulsion of magnetic field at the surface of the superconductor.

While Kamerlingh Onnes found that the transition temperature for the disappearance of resistivity does not depend on the purity of the sample (as discussed in Ref. [5] and see also Anderson’s theorem below), the expulsion of magnetic field on the other hand was observed to depend on it, being less efficient the higher the concentration of impurities. This was explained by Pippard in 1953 [11], extending the local description by London to a non-local theory. Most importantly, he introduced a characteristic size \( \xi_0 \) of the superconducting wave function. Disorder effects are then included in the electromagnetic coherence length \( \xi^{-1} = \xi_0^{-1} + l^{-1} \) through the mean free path \( l \), distinguishing the clean \( (l \gg \xi_0) \) and the dirty limit \( (l \ll \xi_0) \), and resulting in an effective penetration depth \( \lambda_{\text{eff}}^2 \approx \lambda_L^2 (\xi_0/l) \gg \lambda_L \) in the dirty limit.

**Superconductivity as a macroscopic quantum phenomenon**

Already in 1948, Fritz London identified superconductivity as “a quantum mechanism of macroscopic scale” [12] and discussed a wave function for the superconducting electrons. While he missed the fundamental microscopic explanation, he described flux quantization, an inherent quantum phenomenon. Applying Bohr-Sommerfeld quantization to superconductors, also the action of the canonical momentum should be quantized, meaning that magnetic flux can only pass through a hole in a superconductor in quantized units being an integer multiple of the flux quantum \( \Phi_0 \), derived in detail below in Sec. 1.2.1. This was first observed in 1961 by Deaver and Fairbank [13] and by Doll and Nähauer [14].

In Russia, Landau had developed his famous theory for continuous (second order) phase transitions in the 1930s, where the spontaneous symmetry breaking is described by an order parameter [15]. In 1950, together with Ginzburg, they introduced a complex wave function \( \psi = |\psi| e^{i \phi} \) as the superconducting order parameter [16], putting forth the phenomenological Ginzburg Landau (GL) theory, a “masterstroke of physical intuition” [3]. The amplitude of the order parameter \( |\psi|^2 \) describes the density of the superconducting charge carriers, as in the London theory introduced above. Contrastingly, the order parameter is in general a space and temperature dependent quantity \( \psi(r,T) \). While the London theory is recovered as a limiting case, the Ginzburg Landau theory is capable of describing intricate superconducting phenomena, such as at the core of this thesis. In addition, the quantum nature of the superconducting state is captured through the phase of the order parameter \( \phi \), which describes the spontaneous breaking of the global \( U(1) \)-gauge symmetry. For example, the single-valuedness of the phase leads directly to flux quantization. Their theory also contains two characteristic length scales, the penetration depth \( \lambda \) and the coherence length \( \xi \) over which the order parameter varies, with their ratio called the Ginzburg Landau parameter \( \kappa = \lambda / \xi \), details see below in Sec. 1.2.1. This coherence length, however, has a rather different meaning than Pippard’s length scales (for a nice review see Sec. 10.13 and Table 10.1 in Ref. [5]), and the penetration depth is an effective length scale. The microscopic quantities only enter as ‘starred’ versions, such that the charge \( e^* \) and the mass \( m^* \) of the superconducting carriers remain phenomenolog-
ical parameters to be determined, as in the London theory. This has the advantage that real materials and in particular dirty superconductors can be describes quite naturally. However, this also means that the fundamental explanation for how the superconducting state is formed, is not included in this theory either.

The full microscopic explanation was finally put forward by Bardeen, Cooper and Schrieffer in 1957 with their brilliant BCS theory [17]. Experimental results from measurements of the specific heat and electromagnetic absorption had suggested that there should be a minimum energy for the excitations of quasiparticles in superconductors. In the BCS theory, they explained how a weak attractive interaction leads to a phase coherent condensed state of electrons with opposite momentum and spin, $|k, \uparrow\rangle$ and $|-k, \downarrow\rangle$, bound in so-called Cooper pairs. They introduced a characteristic length scale $\xi_{\text{BCS}}$ measuring the extension of these bound pairs, again distinct from the above described coherence lengths. They also established the minimum energy to break up such a Cooper pair to be $E_g = 2\Delta(T)$, where $\Delta(T)$ is called the energy gap, opening up at the Fermi surface. This temperature-dependent gap increases from zero just at the superconducting transition to a value $2\Delta(0) = 3.528k_B T_c$ at zero temperature. The complete picture for conventional superconductors is that due to a phonon-mediated attractive interaction two electrons form a Cooper pair with spin singlet and $s$-wave symmetry. Then, all the Cooper pairs together form a phase coherent macroscopic quantum state. A nice analogy is that of ballroom dancing, where first two dancers form a pair, and second all the pairs dance in unison (i.e. coherently) to the music.

Eventually, in 1959, Gor’kov made an important connection [18]. He derived the phenomenological GL theory from the microscopic BCS theory, a fact which will become important again in Sec. 2.1.2, and showed that the superconducting order parameter $\psi$ is directly proportional to the gap $\Delta$. It therefore also follows from theory that for Cooper pairs $e^* = 2e$, $m^* = 2m$ and $|\psi|^2 = n_s = n_e/2$.

Two types of superconductors

When introducing the spatially dependent order parameter, Ginzburg and Landau also investigated the surface energy of a superconducting half-space with an applied magnetic field on the normal side. They found that this surface energy depends on the parameter $\kappa$, vanishing when $\kappa = 1/\sqrt{2}$. They did not investigate this effect further because “from the experimental data it follows that $\kappa \ll 1$” [16]. However, there actually did exist alloys with $\kappa > 1/\sqrt{2}$, and unknowingly Shubnikov had already examined the magnetic behavior in that regime [19]. The detailed theoretical investigation was then made by Abrikosov in 1957 [20]. He found that for so-called type II superconductors with $\kappa > 1/\sqrt{2}$, distinguished from type I superconductors with $\kappa < 1/\sqrt{2}$, the magnetic field can actually penetrate the superconductor in the form of quantized flux lines, so-called Abrikosov vortices, details see below in Sec. 1.2.1. This mixed or Shubnikov state appears for values of the field between the lower $H_{c1}$ and the upper $H_{c2}$ critical field. He also identified the type of some known alloys by comparing his theoretical results to measured quantities. Nowadays we know that actually, while almost all elemental superconductors are type I, all non-elemental superconductors exhibit type II [21].
1.1. Brief review of superconductivity from a historical perspective

1.1.2 High temperature and unconventional superconductors

While superconductivity seemed fully understood after the groundbreaking work of BCS, the observed transition temperatures were very low, and there was no good way to predict new superconductors – there actually still is not today. We now know, however, that superconductivity is not limited to those low temperatures, nor to the electron-phonon coupling mechanism, nor to isotropic s-wave spin singlet pairing. In this section we discuss two concepts, high temperature superconductors and unconventional superconductors. Transition temperatures above or below roughly 25 K distinguish low from high temperature superconductors [22]. While definitions vary, here we follow Ref. [23] and call superconductors unconventional if they are strongly affected by scattering off non-magnetic impurities. This is Anderson’s theorem [24], who explained in 1959 that non-magnetic impurities do not affect isotropic s-wave pairing states, but that any impurity is pair breaking for states with higher angular momentum.

Unconventional superconductivity was discussed already in 1967, and the first such material, the heavy fermion U$_2$PtC$_2$, was actually already discovered in 1969, but not identified as such [25]. The first high temperature superconductor was then discovered in 1986 by Bednorz and Müller [26] in the cuprate Ba-La-Cu-O system. We start with an overview of transition temperatures and then present a short review of different classes of unconventional superconductors, and for more details refer to Refs. [25, 27, 28].

Transition temperatures

For elemental superconductors, the highest critical temperature is found in niobium with $T_c = 9.25$ K [29]. Simple composite superconductors have higher critical temperatures, but the highest known in 1986 was $T_c = 23$ K in Nb$_3$Ge [25]. Coming as a big surprise, it was discovered in 2001 that MgB$_2$ has $T_c = 39$ K [30]. Today, the highest critical temperature not under pressure is $T_c = 133$ K for the cuprate Hg-Ba-Ca-Cu-O system, observed in the group of Ott [31] in 1993. Recently, in 2015, superconductivity under the extremely high pressure of 90 gigapascals was observed in the sulfur hydride system at $T_c = 203$ K [32]. Not only does this material even seem to be a conventional superconductor, but it is “the first time that a previously unknown material predicted to be a high-temperature superconductor has been experimentally confirmed to be one” [28].

Unconventional superconductors

While unconventional superconductors do not necessarily have a high transition temperature, they exhibit unconventional pairing mechanisms and higher angular momentum pairing states. These go together, because for strongly correlated electron systems with more localized and thus slower electrons, the electron-phonon pairing mechanism is not strong enough to overcome the on-site Coulomb repulsion [27]. For higher angular momentum pairings the wave function vanishes for two electrons in the same place, avoiding the Coulomb repulsion. However, other mechanisms then have to mediate the Cooper pairing. For example, spin fluctuations can support spin triplet pairing [25]. But still today, the pairing mechanism of many unconventional materials and in particular the cuprates is not fully resolved. Most of these unconventional superconductors are rather complicated materials with rich phase diagrams, and where the superconducting properties might depend
Introduction

There are different classes of unconventional superconductors. The field of heavy fermion superconductors opened in 1979, when Steglich et al. [33] discovered superconductivity in CeCu$_2$Si$_2$. Even though these superconductors generally have a low transition temperature, the ratio with the Fermi temperature $T_c/T_F$ resembles that of high temperature superconductors. Organic superconductors had already been proposed in 1964, and were discovered in 1980 [25]. As mentioned above, a whole new era started when superconductivity in the cuprates was discovered by Bednorz and Müller in 1986, and in particular when soon after also a material with a transition temperature above the boiling point of liquid nitrogen was found [25]. While a lot has been learned and is understood about the cuprates, as stressed in Ref. [34], many details, especially of the rich phase diagram, are still under debate, see for example the review [35]. However, these copper-based materials remained the only ones with transition temperatures above 40 K, until the discovery of superconductivity in iron pnictides in 2008, reaching transition temperatures of $T_c = 56$ K, see for example the review [36].

Besides these classes we especially mention the layered perovskite Sr$_2$RuO$_4$, a candidate material for chiral $p$-wave pairing studied in this thesis, and experimental results of which have inspired some of the magnetic phenomena. This material is introduced in depth in Sec. 1.3.2. For completeness, we also mention the more theoretical concepts of topological superconductors, which have received a lot of attention lately, see for example the review [37], and non-centrosymmetric superconductors, see for example the lecture notes [38].

1.1.3 Applications and the Josephson effect

Because of the low operating temperatures, there are no household applications using superconductors. On the other hand, for research or specific commercial applications, the transition temperature is usually not as important, but the limiting factors are rather the critical current density and other material properties. Below we mention some applications based on high magnetic fields and introduce the basic concept of Josephson junctions, which is then discussed in detail in Sec. 1.2.2.

High magnetic fields

Because a current, once induced, will essentially flow ‘forever’ in a superconductor, high magnetic fields can be sustained at low power consumption, while the superconductors of course need constant cooling. Research applications include the large hadron collider (LHC) at the CERN facility$^1$. The record for the highest field reached with an all-superconducting magnet is 27 Tesla at the National High Magnetic Field Laboratory$^2$. As for commercial applications, the main example is magnetic resonance imaging (MRI) in hospitals, while future applications now in construction include magnetic levitation railway systems, where the SCMaglev train in Japan has reached a speed$^3$ of 603 km/h on a test line.

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$^1$ http://cds.cern.ch/record/1997395 (checked 30/07/2017).
1.2. Phenomenology of superconductivity

Josephson junctions

The tunneling of Cooper pairs was investigated by Josephson in 1962 [39]. Before, it had been believed that only normal electrons can tunnel, and some even remained skeptical of the possibility of pair tunneling, see the story in Ref. [40], until it was demonstrated by Anderson and Rowell in 1963 [41]. Such pair tunneling happens when two superconductors are weakly connected, for example through a constriction, a normal metallic or an insulating region, the direct interface between two very different superconductors, or even by a planar crystal defect inside a single superconductor. Besides the flux quantization, the Josephson effect is another demonstration of the fundamental quantum nature of superconductivity. Very simply put, while the order parameters of two identical superconductors will have the same amplitude, they may in general differ in their phase, as described by the Ginzburg Landau theory. When connecting two superconductors, the physics of the junction will be governed by this phase difference of the two order parameters. Most intriguingly, when an external current is applied, a supercurrent can flow between the two superconductors without dissipation, up to a critical applied current.

Superconducting quantum interference devices (SQUIDs) combine the concepts of the Josephson effect and of flux quantization. With these devices, variations in magnetic flux even much below the flux quantum can be measured, which is used in research applications such as scanning-SQUID devices for imaging, but also has commercial applications for example in medicine [42].

1.2. Phenomenology of superconductivity

After this brief general introduction to superconductivity from a largely historical perspective, we now present a more detailed introduction to the Ginzburg Landau theory, which is the framework used throughout this thesis. We formally derive the phenomenological properties of superconductors and describe the important length scales, focussing on magnetic phenomena as relevant for this thesis. First, we consider the standard Ginzburg Landau free energy functional. Next, we add a coupling term to discuss Josephson junctions and derive the sine-Gordon equation.

Again, the books by Tinkham [3] and Waldram [5] are suggested for further details, where especially the latter illuminates many subtle issues. For more details on the second part about Josephson junctions we refer to the most instructive book by Orlando and Delin [43], as well as the book by Schmidt [44], and the well-known application-focussed book by Barone and Paternò [45].

1.2.1 The Ginzburg Landau free energy functional

Ginzburg and Landau [16] postulated a complex space- and temperature-dependent order parameter $\psi(r, T)$ to describe the superconducting phase transition. The free energy has to be scalar, real, and gauge-invariant, leading to the expansion of the free energy density

$$f = f_s - f_n = a_T |\psi|^2 + \frac{b}{2} |\psi|^4 + \frac{1}{2m^*} \left| \left( \frac{\hbar}{i} \nabla - \frac{e}{c} A \right) \psi \right|^2 + \frac{(\nabla \times A)^2}{8\pi},$$

(1.3)
where $A$ is the vector potential\textsuperscript{4}, and where the charge $e^*$ and mass $m^*$ of the superconducting charge carriers are a-priori unknown. Indeed, as reviewed above, this theory was postulated before Cooper pairs were known. This functional is the minimal expansion with which the phase transition and the phenomenological properties can be described, but this simple expression already contains information on the superconducting phase transition, the characteristic length scales of the superconductor, and can be extended to describe vortices or Josephson junctions through appropriate boundary conditions or by adding additional coupling or surface terms. We now treat these different concepts in turn.

**Phase transition, order parameter bulk value and critical field**

In a homogeneous system with no applied field, the free energy density reduces to

$$f = a_T|\psi|^2 + \frac{b}{2}|\psi|^4. \quad \text{(1.4)}$$

These two terms are already sufficient to describe the phase transition. When both $a_T$ and $b$ are positive, the free energy has a single minimum at $|\psi|^2 = 0$, as illustrated by the green line in the inset of panel [a] in Fig. 1.1. When $a_T < 0$, on the other hand, there is a minimum of the free energy at a finite value $|\psi|^2 = -a_T/b$ (blue line). The global phase $\varphi$ of the complex order parameter $\psi \in \mathbb{C}$, however, is not fixed by this minimization, as indicated by the dashed blue circle. It is the spontaneous breaking of the global $U(1)$-gauge symmetry, which picks a value for this global phase, while the local gauge symmetry is maintained.

Since the sign of $a_T$ alone determines the phase, we can expand this coefficient around the transition as $a_T = a(T - T_c)$, such that the full bulk solution of the order parameter amplitude is

$$|\psi_b(T)|^2 = \begin{cases} 0 & T > T_c \\ \frac{-a(T - T_c)}{b} & T \leq T_c \end{cases} \quad \text{(1.5)}$$

as illustrated in the main plot of panel [a] in Fig. 1.1. The free energy density is then

$$f = -\frac{a_T^2}{2b} = -\frac{H_c^2}{8\pi}, \quad \text{(1.6)}$$

which gives the thermodynamic critical field $H_c$.

**The coherence length**

The main strength of the Ginzburg Landau approach is the straightforward way to deal with spatial variations of the order parameter. We first discuss a change in the amplitude. We still consider a situation with no applied field, such that we can neglect the vector potential and use the ansatz $\psi(\mathbf{r}) = |\psi_b|u(\mathbf{r})e^{i\varphi}$ with a real $u(\mathbf{r})$, normalized by the bulk solution found above, and with a constant phase. Let us consider a system with boundary conditions\textsuperscript{5} $u(\mathbf{r}) = 0$ at $x = x_0$ and $u(\mathbf{r}) = 1$ in the bulk $x \to \infty$. Including the gradient

\textsuperscript{4} Throughout this thesis we will use Gaussian units where for example $\nabla \times \mathbf{H} = 4\pi/c \mathbf{J} + \partial_t \mathbf{D}/c$.

\textsuperscript{5} As discussed in Sec. 2.1.3, such a boundary condition can be formally introduced by adding a surface energy term $f_{\text{surf}} = g |\psi|^2 \delta(x - x_0)$ with $g \to \infty$. 

1.2. Phenomenology of superconductivity

Figure 1.1: Ginzburg–Landau phenomenology of conventional superconductors. [a] shows the temperature dependence of the bulk value of the order parameter amplitude and the free energy above (green) and below (blue) the phase transition, where the dashed circle describes the spontaneous breaking of the $U(1)$-gauge symmetry fixing the global phase; [b] and [c] introduce the characteristic length scales, the coherence length $\xi$ and the screening length $\lambda$, respectively, describing the distance over which the order parameter amplitude varies, and over which the magnetic field penetrates; [d] depicts an Abrikosov vortex for a type II superconductor with $\kappa = 4$, where the flux is quantized in a single flux quantum $\Phi_0$, and where both characteristic length scales are exemplified again.

Term and performing the variation with respect to the order parameter (see Sec. 2.2.1), we find the equation

$$u(x) - u(x)^3 - \frac{\hbar^2}{2am^*} \partial_x^2 u(x) = 0,$$

which has the solution

$$u(x) = \tanh \left(\frac{x - x_0}{\xi \sqrt{2}}\right),$$

where we have introduced the coherence length

$$\xi(T)^2 = \frac{\hbar^2}{-2m^*a_T} = \frac{K}{-a(T - T_c)},$$
and where we have used the general gradient term expansion parameter $K = \hbar^2/(2m^*)$, see below. This is the characteristic length for changes in the amplitude of the order parameter as illustrated in panel [b] in Fig. 1.1.

**The screening length**

The London equations are directly recovered for a completely rigid order parameter with a constant phase. Here we consider a system with boundary conditions $B = B_0 \hat{z}$ at $x = x_0$ and $B = 0$ in the bulk $x \to \infty$. Including the magnetic term, performing the variation with respect to the vector potential, and taking the curl, we recover Eq. (1.2)

$$\frac{\lvert \psi_b \rvert^2 e^{*2}}{2m^* c^2} B = \frac{\Delta B}{8\pi},$$

which has the solution

$$B(x) = B_0 e^{-\lambda x} \hat{z}$$

with the penetration depth

$$\lambda(T)^2 = \frac{m^* c^2}{4\pi e^{*2} \lvert \psi_b(T) \rvert^2} = \frac{1}{8\pi\gamma^2 K \lvert \psi_b(T) \rvert^2},$$

where we have used the parameter $\gamma = e^*/(hc)$, see below. The penetration of the magnetic field is illustrated in panel [c] in Fig. 1.1. This characteristic length determines in general the scale on which the magnetic field is screened inside a superconductor, not limited to penetration at the surface, and we will refer to it as the ‘screening length’ in the following.

**Flux quantization**

We now discuss a change in the phase of the order parameter, while keeping its amplitude rigid, $\psi(r) = \lvert \psi_b \rvert e^{i\phi(r)}$. From a variation with respect to the vector potential we find the equation for the supercurrent density

$$J_s(r) = \frac{e^* \hbar \lvert \psi_b \rvert^2}{m^*} \left( \nabla \phi - \frac{e^*}{hc} A \right) = 2c\gamma K \lvert \psi_b \rvert^2 (\nabla \phi - \gamma A) = 2c\gamma K \lvert \psi_b \rvert^2 (\nabla \phi - \gamma A),$$

which is gauge-invariant, and where we have again used $\gamma$. For a constant phase of the order parameter, the London equation (1.1) is recovered, which was only correct in the particular London gauge. Let us now consider a superconductor with a hole, threaded by magnetic flux. For a path $S$ around this hole and deep inside the bulk such that the supercurrent vanishes, we find

$$0 = \oint_S ds \cdot J_s(r) = \oint_S ds \cdot \left( \nabla \phi - \frac{e^*}{hc} A \right) = 2\pi n - \frac{e^*}{hc} \Phi,$$

\[6\] This can be formally derived by extending the magnetic term to $f_{\text{mag}} = (B - H)^2/(8\pi)$ for an applied field $H$, leading to the general boundary condition $n \times (B - H)_{\text{surf}} = 0.$
where we have used the single-valuedness of the phase and where $\Phi$ is the flux through the hole. Rearranging leads to

$$\Phi = \frac{2\pi \hbar c}{e^* n} = \frac{\hbar c}{e^* n} = \frac{2\pi}{\gamma} n \equiv \Phi_0 n,$$

(1.15)

defining the flux quantum $\Phi_0$ and resulting in a simple expression for the parameter $\gamma = 2\pi/\Phi_0$. The flux is therefore quantized, as already mentioned above, and can only take values which are integer multiples of the flux quantum. This is true for any flux threading superconductors and thus in particular also applies to vortices. The phase of the order parameter immediately reveals the quantum nature of superconductivity, as discussed above. For accuracy we note that in general, when the supercurrent cannot be taken to vanish, it is the so-called fluxoid $\Phi' = \Phi + (4\pi/c)\lambda(T)^2 \oint J_s$ which is quantized, see for example Sec. 4.5 of Ref. [3].

**Ginzburg Landau parameter**

For a self-consistent treatment of a general magnetic phenomenon both these characteristic length scales have to be considered. Their ratio is conveniently described by the temperature-independent Ginzburg Landau parameter

$$\kappa = \frac{\lambda(T)}{\xi(T)} = \sqrt{\frac{b}{8\pi\gamma^2 K^2}}.$$  

(1.16)

As already discussed above, it is also this parameter $\kappa$ which distinguishes the type I ($\kappa < 1/\sqrt{2}$) and type II ($\kappa > 1/\sqrt{2}$) superconductors. In the latter, Abrikosov vortices appear in the mixed phase between $H_{c1}$ and $H_{c2}$. While we have to refer to the standard references listed above for the further discussion, we use this most important magnetic phenomenon to illustrate again the meaning of the two characteristic length scales and the flux quantum. An Abrikosov vortex is illustrated in panel [d] in Fig. 1.1. The field of the vortex is quantized to be one flux quantum $\Phi_0$. It decays on the screening length $\lambda$. The order parameter is fully suppressed in the normal core of the vortex, on the length scale $\xi$. The interplay between these length scales will pop up again throughout this thesis when discussing the magnetic phenomena. Without derivation, see for example Ref. [3], we state the values of the lower critical field, and of the upper critical field for orbital depairing,

$$H_{c1} \approx \Phi_0 \frac{4\pi \lambda(T)^2}{\log \kappa \sqrt{2\kappa}} H_c \quad (\kappa \gg 1),$$

$$H_{c2} = \Phi_0 \frac{2\pi \xi(T)^2}{\log \kappa \sqrt{2\kappa}} = \sqrt{2\kappa} H_c.$$  

(1.17)

**Full free energy functional**

With the parameters introduced above, we can write a direct expansion form of the Ginzburg Landau functional

$$f = a(T - T_c)|\psi|^2 + \frac{b}{2} |\psi|^4 + K |(\nabla - i\gamma A) \psi|^2 + \frac{(\nabla \times A)^2}{8\pi},$$

(1.18)
which can be brought into the convenient dimensionless form

\[ \tilde{f} = -|u|^2 + \frac{|u|^4}{2} + \left| \left( \tilde{\nabla} - i\tilde{A} \right) u \right|^2 + \kappa^2 \left( \tilde{\nabla} \times \tilde{A} \right)^2, \]

(1.19)

by setting \( \psi = |\psi_b(T)|u \) and \( \gamma A = \tilde{A}/\xi(T) \), and by taking lengths in units of \( \xi(T) \) such that \( \tilde{\nabla} = \tilde{\nabla}/\xi(T) \), which leads to \( f = H_c(T)^2/(4\pi)\tilde{f} \). The only experimental input remaining is the Ginzburg Landau parameter \( \kappa \). The situation for chiral \( p \)-wave superconductors as introduced in below in Sec. 1.3 and discussed throughout this thesis is more complicated, however, because we consider an anisotropic material with different in-plane and out-of-plane parameters, and where the two-component order parameter introduced below leads to coupled terms, whose ratio also has to be considered. How to formulate the free energy in this case is discussed in detail in Sec. 2.1.

For a general situation, both, the amplitude and the phase of the order parameter, as well as the vector potential are space-dependent. For a self-consistent solution, we have to minimize the full free energy, which after variation corresponds to solving two coupled non-linear partial differential equations. Usually, this is only possible numerically, with a method such as described in Sec. 2.2.2. For the magnetic phenomena explored in this thesis, we always perform a full numerical analysis. However, often a lot of insight can already be gained from studying some limiting cases analytically. For conventional superconductors such examples include the domain wall energy, critical current of a thin film, vortices for \( \kappa \gg 1 \) etc., all described in the standard references. For each situation, the main effect is extracted and all other quantities are taken constant or approximated by some reasonable ansatz. In this thesis we also try to provide such analytical arguments for each phenomenon to accompany, support and explain our numerical results.

### 1.2.2 The sine-Gordon model for Josephson junctions

When two superconductors are weakly connected, they form a Josephson junction, as introduced above in Sec. 1.1.3. The physics of such systems are determined by the phase difference across the junction, and the applied field, current or voltage. For an introduction along the lines of the original work by Josephson [39] and for a detailed description of the various resulting phenomena, we refer to any of the standard references listed above. Here, we adopt a rather specific approach focusing on the results relevant for this thesis, which we derive by describing the coupling between the two superconductors through an additional term in Ginzburg Landau free energy functional, following Ref. [46]. We then discuss in detail the sine-Gordon model.

**Coupling term and phase difference**

For two identical superconductors 1 and 2 with a rigid order parameter amplitude but with different phases \( \psi_1 = |\psi_b|e^{i\phi_1} \), the lowest order coupling term is simply given by [46]

\[ f_{\text{coup}} = K_c|\psi_1 - \psi_2|^2 = 2K_c|\psi_b|^2(1 - \cos \phi), \]

(1.20)

where \( \phi = \phi_1 - \phi_2 \) is the phase difference between the two superconductors across the junction. The stable values for the phase difference minimizing the free energy are therefore \( \phi = 2\pi n \) for integer values \( n \). For a full gauge-invariant treatment, the gauge-invariant
1.2. Phenomenology of superconductivity

Phase difference has to be considered, such that integrating over the junction we find

\[ \varphi = \phi - \gamma \int_1^2 ds \cdot A. \]  

(1.21)

**Voltage-phase and current-phase relation**

When a voltage \( V \) is applied to the junction, the energy difference for a tunneling Cooper pair is \( e^*V = E_2 - E_1 \), with \( E_i \) the ground state energies on either side. In this situation, the Schrödinger equation for the Cooper pair wave functions has to be considered and their phase becomes time dependent, a nice description of which can be found in Ch. 4 of Ref. [44]. This directly leads to

\[ V = \frac{\hbar}{e^*} \frac{\Phi_0}{2\pi c} \frac{\partial_t \varphi}{\partial_t \varphi}. \]  

(1.22)

For a proper treatment of all the subtleties in deriving this result we refer to Refs. [5, 43]. For the free energy \( F = f f \) we can then write

\[ dF = IV dt = \frac{\Phi_0}{2\pi c} I d\varphi, \]  

(1.23)

such that the current \( I \) and the phase difference \( \varphi \) are the conjugate variables [46]. The Josephson supercurrent density is then simply given by the derivative of the free energy with respect to the phase

\[ J = \frac{2\pi c}{\Phi_0} \frac{\partial_f f}{\partial_f f} = \frac{2\pi c}{\Phi_0} 2K_c |\psi_b|^2 \sin \varphi = J_c \sin \varphi J, \]  

(1.24)

where we have introduced the critical current density

\[ J_c = \frac{4\pi c K_c |\psi_b|^2}{\Phi_0}. \]  

(1.25)

For an applied current up to this critical current, there is only tunneling of Cooper pairs. For a higher applied current, the junction becomes resistive, and also normal electrons tunnel. This is illustrated in panel [a] of Fig. 1.2 by the red line. The blue line, on the other hand, indicates the fundamental limit for an applied voltage, which is \( 2\Delta/e \), which we find for normal electron tunneling. The resistance \( I = V/R_n \) for the normal state of the junction was derived by Ambegaokar and Baratoff [47], and at \( T = 0 \) is given by \( I_c R_n = \pi \Delta(0)/(2e) \).

The study of Josephson junctions with an applied current \( I \leq I_c \) and no applied voltage is referred to as the study of basic Josephson junctions, as opposed to studying generalized Josephson junctions. In this thesis, we only consider basic Josephson junctions. For a review of the illustrative RCSJ-model and other effects in generalized junctions we refer to Orlando and Delin [43].

Basic Josephson junctions are further distinguished between lumped and extended junctions. In the former, both the phase difference and the magnetic quantities are considered uniform over the whole junction. We directly discuss extended junctions here, where both the phase and the field can vary along the junction.
Figure 1.2: Phenomenology of Josephson junctions. [a] shows the fundamental limits in the $I-V$ diagram for Cooper pair tunneling i.e. a Josephson supercurrent (red) and normal electron tunneling (blue); [b] shows a long Josephson junction between two superconductors (grey) which are weakly connected (white), and with an applied current $J$ (green). The screening length of the superconductors is $\lambda$, and the effective width of the junction $d$. The current can penetrate over a distance $\lambda J$, the Josephson penetration depth, into the junction.

Field-phase relation

Considering a field or current applied to the junction and integrating the gauge-invariant phase difference along a closed path crossing the junction, we find the field-phase relation

$$B = \frac{\Phi_0}{2\pi d} (\hat{n} \times \nabla \varphi),$$

with the junction normal $\hat{n}$ and with $d = \lambda_1 + \lambda_2 + d_0$ the effective width of the junction with the two screening lengths $\lambda_i$ and the actual width of the interface $d_0$. A detailed derivation of this result can be found for example in Ref. [43].

One important concept can easily be derived. We found above that the stable states of the junction are for phase differences $\varphi = 2\pi n$ with integer $n$. Let us consider a situation where, due to some boundary conditions for example because of an applied field or current, the phase increases by $2\pi$ between two stable states, over a distance $w$ along the junction.

Using the geometry shown in panel [b] of Fig. 1.2, the magnetic flux through that part of the junction is then given by

$$\Phi = \int_{y}^{y+w} dy \int_{x-d/2}^{x+d/2} dx \ B \cdot \hat{z}$$

$$= \frac{\Phi_0}{2\pi d} \int_{y}^{y+w} dy \int_{x-d/2}^{x+d/2} dx \ (\hat{x} \times \nabla \varphi) \cdot \hat{z} = \frac{\Phi_0}{2\pi} \int_{y}^{y+w} dy \ \partial_y \varphi = \Phi_0.$$
will be derived below. Such junctions are referred to as long. On the other hand, if the
junction is much smaller than this length scale, the self-fields can be neglected, which is
referred to as a short junction.

There is one caveat related to the field-phase relation (1.26). The fundamental limit for
changes in the magnetic field in superconductors is the screening length \( \lambda \). Usually,
the characteristic length of the Josephson junction (\( \lambda_J \) for long and the proper length \( l \) for
short junctions) is much longer than this screening length. In certain cases the screening
length can be much larger. Then, a non-local version of the phase-field relation has to be
considered, see for example the review [48]. We will encounter such a situation in Ch. 5,
and refer to Sec. 5.2 for details.

**Sine-Gordon equation for long junctions**

In general, both the applied field and the self-fields have to be taken into account such that
the field-phase relation (1.26) has to be combined with Ampère’s law. For a junction with
normal \( \hat{x} \) and an applied field \( \mathbf{B} = B_0 \hat{z} \) at the junction surface \( y = y_0 \), the field-phase
relation becomes \( B_z(y) \propto \partial_y \varphi \) such that the current is \( J_x \propto \partial_y^2 \varphi \). Combining this in turn
with the current-phase relation (1.24), we find

\[
\partial_y^2 \varphi = \frac{8 \pi^2 d}{c \Phi_0} J_c \sin \varphi = \frac{\sin \varphi}{\lambda_J^2},
\]

where we have introduced the Josephson penetration depth \( \lambda_J \). Substituting the expression
for the critical current from Eq. (1.25), it is given by

\[
\lambda_J^2 = \frac{c \Phi_0^2}{4(2\pi)^3 c d K_\psi |\psi_b|^2}.
\]

Alternatively, we could have taken the coupling term and the magnetic term of the free
energy, together with the field-phase relation, and performed a variation with respect to
\( \varphi \), to arrive at the same result. This characteristic length scale is illustrated in panel [b]
of Fig. 1.2. Its meaning is further demonstrated by considering the particular solution to
the partial differential equation (1.29),

\[
\varphi(y) = 4 \arctan \left( e^{y/\lambda_J} \right).
\]

The Josephson penetration depth therefore measures the width of one phase slip from
\( \varphi = 0 \) to \( \varphi = 2\pi \) which corresponds to one Josephson vortex carrying one flux quantum
\( \Phi_0 \), as introduced above. This will be discussed again and in more detail in Sec. 4.2.1.

We note that equation (1.29) was first derived by Ferrell and Prange [49], and is some-
times referred to as the Ferrell-Prange equation. However, for the generalized situation
with additional time-dependent terms, we find the so-called sine-Gordon equation, see for
example Ref. [43], named by M. Kruskal in analogy to the klein-Gordon equation [50].
Introduction

1.3 Chiral $p$-wave pairing

After this short review of the most relevant phenomenological concepts of conventional superconductors and Josephson junctions, we now discuss in detail unconventional superconductors with chiral $p$-wave pairing, as studied throughout this thesis. This is one of the most intriguing states for which to apply the Ginzburg Landau approach, because the order parameter has two complex components, leading to an intricate functional with several coupling terms. In addition, because defects can affect the two order parameter components differently, fascinating behavior emerges from studying additional terms arising in these situations. Chiral $p$-wave superconductors are, however, not only interesting on a conceptual level. Most of the projects studied in this thesis are ultimately inspired and motivated by experimental observations in connection with the material Sr$_2$RuO$_4$, which is a candidate for chiral $p$-wave pairing.

This section has two parts. First, the chiral $p$-wave state is introduced formally by identifying it as one of the superconducting states in tetragonal crystals. We present the generalized Ginzburg Landau functional for two-dimensional representations and discuss the stable phases of the homogeneous part, while further details of formulating the functional for chiral $p$-wave pairing are given in Sec. 2.1. Second, we describe the material Sr$_2$RuO$_4$ and provide both experimental evidence and theoretical arguments in favor and against the realization of this particular pairing state.

1.3.1 Odd parity states in tetragonal crystals

In order to formally arrive at chiral $p$-wave pairing, we introduce the convenient $d$-vector formalism, discuss the influence of the lattice structure, and present the generalized Ginzburg Landau functional. While we mention the underlying concepts, the focus is always on the application to tetragonal crystals.

For details beyond this short overview we recommend the pedagogical lecture notes by Sigrist [27], the technical work by Sigrist and Ueda for the group-theoretical aspects concerning the generalized Ginzburg Landau framework [51], the book by Mineev and Samokhin [52], and the review by Mackenzie and Maeno for an in-depth discussion of tetragonal crystals with triplet pairing [53].

The $d$-vector formalism for triplet pairing

For unconventional superconductors, the spin part of the Cooper pair wave function can also have odd parity. In general, the gap function is therefore a complex $2 \times 2$ matrix in spin space. In the elegant $d$-vector formalism introduced by Balian and Werthamer [54] (nicely summarized in Sec. IV.A of Ref. [53] with examples in Appendix D), the gap for odd-parity spin triplet pairing is represented as

$$\hat{\Delta}_k = \begin{pmatrix} \Delta_{k,\uparrow\uparrow} & \Delta_{k,\uparrow\downarrow} \\ \Delta_{k,\downarrow\uparrow} & \Delta_{k,\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} -d_x(k) + id_y(k) & d_z(k) \\ d_z(k) & d_x(k) + id_y(k) \end{pmatrix} = i(d(k) \cdot \hat{\sigma})\hat{\sigma}_y, \quad (1.32)$$

where $\hat{\sigma}_i$ are the Pauli matrices, and for comparison for even-parity spin singlet pairing as

$$\hat{\Delta}_k = \begin{pmatrix} \Delta_{k,\uparrow\uparrow} & \Delta_{k,\uparrow\downarrow} \\ \Delta_{k,\downarrow\uparrow} & \Delta_{k,\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} 0 & \psi(k) \\ -\psi^*(k) & 0 \end{pmatrix} = i\psi(k)\hat{\sigma}_y. \quad (1.33)$$
1.3. Chiral $p$-wave pairing

This $d$-vector transforms like a vector under spin rotations. In a single compact form it contains information on both the orbital and the spin part of the wave function, and on the gap structure through $\hat{\Delta}_k \hat{\Delta}_k^\dagger = |d(k)|^2 \hat{\sigma}_0 + i (d \times d^*) \hat{\sigma}$. For non-unitary states, defined by $|d \times d^*| \neq 0$, there are two distinct energy gaps for the two different spin orientations. Such spin-polarized states, however, have in general a reduced condensation energy and are less favorable except for biased systems as for example the A1-phase of superfluid $^3$He. In the following, we only consider unitary states, defined by $|d \times d^*| = 0$. In these states, all electrons are paired, the direction of the $d$-vector is perpendicular to the plane of equal-spin pairing, and the gap is directly accessible through $d \cdot d^* = |\Delta_k|^2$.

Influence of the crystal structure

In addition to the more involved pairing state, the crystal structure also plays an important role for unconventional superconductors. In general, any physical quantity has to respect the symmetries of surrounding material and can accordingly be decomposed in its irreducible representations. In a crystal, the orbital rotations are therefore no longer free in space under $SO(3)$, but are reduced to the point group of the crystal, and are therefore restricted to the irreducible representations of that point group. In the Landau theory of phase transitions, each irreducible representation leads to a state with a different transition temperature. The corresponding order parameter can then be decomposed in the independent basis functions of that irreducible representation [55].

Here, we focus on tetragonal crystals and their most symmetric point group $D_{4h}$, also called ‘full tetragonal symmetry’ [56], following the example given in [27]. The cuprate superconductors, as well as the material Sr$_2$RuO$_4$ discussed in Sec. 1.3.2, have such a tetragonal crystal structure. The point group $D_{4h}$ has five even and five odd irreducible representations $\Gamma_{\pm}$, where $\Gamma_\pm^z$ is two-dimensional, while $\Gamma_{\pm}^{\pm\mp}$ are one-dimensional. We assume spin-orbit coupling to be strong enough that the spin can be considered ‘locked’ to the lattice and rotates together with the orbital rotations\(^7\). Here, we focus on triplet pairing and the odd parity states only, anticipating the discussion of Sr$_2$RuO$_4$, while the even parity states are important for the cuprate superconductors with $d$-wave pairing.

The four one-dimensional odd parity representations $\Gamma_{\pm}^{\mp\mp}$ can be described by a single order parameter each. The corresponding $d$-vectors are $d_{\Gamma_{\pm}^{\mp\mp}} = \hat{x}k_x + \hat{y}k_y$, $d_{\Gamma_{\pm}^{\pm\mp}} = \hat{x}k_y - \hat{y}k_x$, $d_{\Gamma_{\pm}^{\pm\pm}} = \hat{x}k_x - \hat{y}k_y$, and $d_{\Gamma_{\pm}^{-\mp\mp}} = \hat{x}k_y + \hat{y}k_x$. These states are called helical and can be understood as states where the two spin directions have opposite chirality (see below), but where the overall state has no net chirality [58]. They have no symmetry-imposed nodes, do not break time reversal symmetry, but are topological. The $\Gamma_{\mp}^{-}$ state is an analogue of the B-phase (Balian-Werthamer phase) of superfluid $^3$He. The corresponding Ginzburg Landau functional for all these states has the same form as for conventional superconductors given in Eq. 1.3.

The two-dimensional odd parity representation has the two independent basis functions $\{k_x \hat{x}, k_y \hat{y}\}$. Introducing an order parameter with two complex components,

$$\eta = (\eta_x, \eta_y) \in \mathbb{C}^2,$$

(1.34)

\(^7\) Without spin-orbit coupling, all the triplet states discussed below would be degenerate, originating from the $\Gamma_5^z$ representation [57].
the full \( d \)-vector for this representation is given by
\[
d(k) = \hat{z} (\eta_x k_x + \eta_y k_y).
\] (1.35)

It points along the out-of-plane \( z \)-direction and describes in-plane equal-spin pairing. The generalized Ginzburg Landau functional for this state is the topic of the next section.

Finally, we note one caveat. While we have used the basis functions \( k_x \) and \( k_y \) throughout the above discussion, on the crystal lattice the functions \( \sin k_x \) and \( \sin k_y \) (for nearest-neighbor hopping only) are more appropriate, see also footnote 33 in Ref. [53]. This does not influence the basic form of the Ginzburg Landau functional but can become important when determining the expansion coefficients, see the discussion in Sec. 2.1.2, and for more details see Ref. [59].

Generalized Ginzburg Landau functional

Even for multi-component order parameters in a crystal, the Ginzburg Landau functional still has to be real, scalar, and gauge-invariant, but now in addition invariant under all symmetry operations of the given point group. For higher-dimensional order parameters there are in general more, and also coupled terms. For the two-dimensional irreducible representations\(^8\) of the point group \( D_{4h} \), the homogeneous part of the generalized Ginzburg Landau functional is given by [51]
\[
F[\eta_x, \eta_y] = \int d^3 r \left[ a (T - T_c) |\eta|^2 + b_1 |\eta|^4 + \frac{b_2}{2} \left( \eta_x^2 \eta_y^2 + \eta_x^2 \eta_y^2 \right) + b_3 |\eta_x|^2 |\eta_y|^2 \right].
\] (1.36)

There is now a set of expansion coefficients \( \{b_i\} \) for the fourth order terms\(^9\). As in the conventional case, these coefficients are in general material dependent. However, only the whole set can directly be related to physical quantities, while the ratios within the set have to be derived from the microscopic theory. More details on choosing these expansion coefficients are given in Sec. 2.1.2.

Here, we focus on simple stability considerations, leading to a phase diagram for the different possible uniform bulk phases. Following Ref. [27], we use the convenient ansatz \( \eta = \eta_b(T)(\cos \alpha, e^{i\gamma}\sin \alpha) \), which leads to the free energy
\[
F[\eta_x, \eta_y] = \int d^3 r \left[ a (T - T_c) \eta_b^2 + \left( b_1 + \frac{1}{4} \sin^2(2\alpha)(\cos(2\gamma)b_2 + b_3) \right) \eta_b^4 \right].
\] (1.37)

The free energy has to be bounded below for all \( \alpha \) and \( \gamma \), which is only possible if the term in the curly brackets is positive. This leads to the restriction
\[
4b_1 \pm b_2 + b_3 > 0.
\] (1.38)

\(^8\) While we focus on odd parity, the two-dimensional even-parity representation \( \Gamma_5^2 \) with the basis functions \( \{k_x, k_y, k_z\} \) has the same expression for the generalized Ginzburg Landau functional as given in Eq. 1.36, and the phase diagram of the stable phases also applies, see Ref. [27].

\(^9\) There is a second convention, see for example Ref. [51], using coefficients \( \beta_i \) for the fourth order term,
\[
f_{\text{fourth}} = \beta_1 (|\eta_x|^2 + |\eta_y|^2)^2 + \beta_2 (\eta_x^2 \eta_y - \eta_x \eta_y^*)^2 + \beta_3 |\eta_x|^2 |\eta_y|^2
\]
with the relations \( \beta_1 = b_1, \beta_2 = b_2/2, \) and \( \beta_3 = b_2 + b_3 \). We always use \( b_i \) throughout this thesis.
1.3. Chiral $p$-wave pairing

In addition, there are three combinations of $\alpha$ and $\gamma$ for which there is a range of $\bar{b}_i = b_i/b_1$ minimizing the free energy. The sign of $(\cos(2\gamma)\bar{b}_2 + \bar{b}_3)$ determines the stable angle $\alpha$. Then, for $\alpha = \pm \pi/4$, the sign of $\bar{b}_2$ determines the stable angle $\gamma$. The resulting bounds, together with the overall restriction from Eq. 1.38, lead to the three phases A, B and C listed below in Table 1.1 and illustrated in Fig. 1.3.

Table 1.1: The three stable phases of the two-dimensional irreducible representations $\Gamma^\pm_5$ of the full tetragonal point group $D_{4h}$ as illustrated in Fig. 1.3.

<table>
<thead>
<tr>
<th>phase</th>
<th>$\alpha$</th>
<th>$\gamma$</th>
<th>bounds</th>
<th>state</th>
<th>broken symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>$\pm \pi/4$</td>
<td>$\pm \pi/2$</td>
<td>$</td>
<td>b_2</td>
<td>&gt; b_3$, $b_2 &gt; 0$</td>
</tr>
<tr>
<td>B</td>
<td>$\pm \pi/4$</td>
<td>0, $\pi$</td>
<td>$</td>
<td>b_2</td>
<td>&gt; b_3$, $b_2 &lt; 0$</td>
</tr>
<tr>
<td>C</td>
<td>0, $\pi/2$</td>
<td>any</td>
<td>$</td>
<td>b_2</td>
<td>&lt; b_3$</td>
</tr>
</tbody>
</table>

Each phase is still two-fold degenerate and associated with a broken symmetry connecting the two degenerate states. The B and the C phases break rotation symmetry, reducing $D_{4h}$ with $a = b \neq c$ to the orthorhombic $D_{2h}$ with $a \neq b \neq c$, yielding small lattice deformations [27]. Both these phases have line nodes, which reduce the gain from condensation energy.
The A phase, on the other hand, has only point nodes and is energetically favorable. Here, time reversal symmetry $K$ is broken, and the $d$-vector is given by

$$d(k) = \hat{z} (k_x \pm ik_y),$$  \hspace{1cm} (1.39)

with the order parameter for the uniform bulk phase given by

$$\eta = \eta_b(T)(1, \pm i).$$  \hspace{1cm} (1.40)

This is the so-called chiral $p$-wave state, an analogue of the A-phase (Anderson-Brinkman-Morel phase) of superfluid $^3$He. The name ‘chiral’ refers to the phase winding by $\pm 2\pi$ as $k$ follows a closed path in the $k_x$-$k_y$-plane on the Fermi surface around the $k_z$-axis [58]. This is therefore a topological state, where the topological invariant is this integer winding number, the Chern number of this system.

**Summary: The unitary nodeless odd-parity pairing states**

To summarize, starting from the full tetragonal symmetry $D_{4h}$, we find several possible states with diverse properties. First, we distinguish even-parity singlet and odd-parity triplet states. We focus on the latter. A comprehensive overview of all possible triplet states in $D_{4h}$ can be found in Table IV of Ref. [53]. The next distinction is between unitary and non-unitary states. We discarded the latter as energetically less favorable in the absence of spin bias. From the unitary states, only keeping the nodeless states, which have a higher gain in condensation energy, we are left with the one-dimensional helical states for $\Gamma_{1-4}$ and the two-dimensional chiral state, all with the same gap amplitude $|\Delta(k)|^2 \propto k_x^2 + k_y^2$. While both states are topological, they are distinguished by the broken time reversal symmetry and chirality of the latter.

**1.3.2 Candidate material Sr$_2$RuO$_4$**

Ever since its discovery as an unconventional superconductor, the material Sr$_2$RuO$_4$ has kept both experimentalists and theorists busy. The debate about its pairing symmetry is ongoing, which sparks increasingly carefully conducted experiments, pushes efforts in crystal growth and sample preparation, requires an ever more thorough interpretation of the observed results, and also provokes questioning the adopted theoretical descriptions. The ultimate goal lies beyond solving the “puzzle” of this particular material alone but also comprises a deeper understanding of unconventional superconductivity in general [60].

As an example, many previous works applying the phenomenological Ginzburg Landau approach to chiral $p$-wave systems used the expansion coefficients calculated for a rotationally symmetric cylindrical Fermi surface, which is indeed reasonable at first sight. At the heart of this thesis, however, is the study of phenomena emerging for a choice of coefficients beyond this isotropic symmetry, as discussed in detail in Sec. 2.1.2. These theoretical advances were ultimately inspired by observations (or the lack thereof) in Sr$_2$RuO$_4$, while their implications are not limited to this material.

In this section we first describe the material properties of Sr$_2$RuO$_4$ and present the early experiments and theoretical arguments leading to the proposal of chiral $p$-wave pairing, focusing on triplet pairing and broken time reversal symmetry. We then outline the key
arguments for and against this claim. Those aspects highly relevant for this thesis are discussed in detail later, in Sec. 1.4, where we motivate the three magnetic phenomena and also introduce the eutectic material realization Sr$_2$RuO$_4$-Ru and its 3-Kelvin phase.

For an in-depth discussion we refer to the early reviews by Mackenzie and Maeno from 2003 [53] and by Bergemann et al. from 2003 [61], the material-based review by Maeno et al. from 2012 [62], the theory-based review by Kallin from 2012 [63], and the very recent review highlighting modern developments by Mackenzie et al. from 2017 [60].

**Layered perovskite without copper**

The material Sr$_2$RuO$_4$ has the $n = 1$ Ruddlesden-Popper layered perovskite structure A$_2$BO$_4$ as shown in Fig. 1.4 [64, 65]. The single (n=1) ABO$_3$ perovskite layers are spaced by double AO rock salt layers, but with the next perovskite layer offset by (1/2, 1/2). The measured in-plane lattice parameter is $a = 0.3862$ nm, and the out-of-plane parameter is $c = 1.2722$ nm, corresponding to $c \approx a(2 + \sqrt{2})$ [53]. This body-centered full tetragonal symmetry is described by the point group $D_{4h}$, discussed in detail above in Sec. 1.3.1.

Superconductivity in crystals with such structures was first observed in the cuprates mentioned in Sec. 1.1.2, which ignited the experimental efforts to examine similar materials. The superconductivity in Sr$_2$RuO$_4$ was discovered in 1994 by Maeno et al. [66], being the first layered perovskite material not containing copper found to be a superconductor. The critical temperature, however, is much lower than in the cuprates and strongly depends on the sample purity, indicating unconventional superconducting behavior. The extrapolated limit for pure samples is $T_c \approx 1.5$ K [23].

The electronic structure is quasi two-dimensional and determined by the RuO$_2$ planes. In the perovskite layers, the O$^{2-}$ ions form corner-sharing octahedra with the Ru$^{4+}$ ion in the center [61, 67]. The 4d-orbital of ruthenium is then further split by the oxygen crystal field into the three-dimensional $t_{2g}$ and the two-dimensional $e_g$ subspaces. The former has
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a lower energy because the lobes of the \{xy, xz, yz\}-orbitals lie between the oxygen ions. The in-plane \(d_{xy}\)-orbitals form the two-dimensional \(\gamma\)-band of the Fermi surface, while the \(d_{xz}\) and \(d_{yz}\)-orbitals hybridize into the two one-dimensional \(\alpha\) and \(\beta\) bands. The dispersion along the out-of-plane direction is weak, such that the system is considered quasi two-dimensional. A nice visualization of the full Fermi surface is shown in Fig. 28 of Ref. [61]. While multiband superconductivity is discussed for \(\text{Sr}_2\text{RuO}_4\) [60, 68, 69], in this thesis we use the common picture of a dominant \(\gamma\)-band [70].

A further description of all the properties of \(\text{Sr}_2\text{RuO}_4\) is beyond this short introduction and we refer to the reviews cited above. The only quantity actually entering our numerical analysis is the Ginzburg Landau parameter \(\kappa_{ab} = 2.6\) [62] which sets the relative scale of the coherence length and the penetration depth, and the superconducting anisotropy \(\gamma_s\) introduced in Sec. 2.1.2. To get a feeling of magnitude, we note that the in-plane coherence length at zero temperature is \(\xi_{ab}(T = 0) = 66\ \text{nm}\) and the out-of-plane value is \(\xi_{ab}(T = 0) = 3.3\ \text{nm}\), with \(\gamma_s = 20\) [62], but see the discussion below.

What is the superconducting state of this material? Because of the sensitivity to impurities it is unconventional. Further, because the normal state Fermi liquid parameters are very similar to those of superfluid \(^3\text{He}\), Rice and Sigrist suggested that \(\text{Sr}_2\text{RuO}_4\) might also have spin-triplet pairing [57]. As discussed above in Sec. 1.3.1, the remaining distinction then depends on time-reversal symmetry, which seems to be broken. These two aspects are discussed below, closing with a short summary of other arguments for and against this claim. Because an in-depth and exhaustive discussion is beyond the scope of this section, we refer to the standard reviews mentioned above for more details and references to further experiments.

Spin triplet pairing

First evidence for spin triplet pairing comes from measuring the spin susceptibility, which is accessible through the Knight shift measured in NMR experiments. While the susceptibility of spin singlet pairing is affected by magnetic fields, it is not affected for spin-triplet pairing when the field is applied in the plane of equal-spin pairing, that is, perpendicular to the \(d\)-vector, as explained in Ref. [60]. While it was first confirmed experimentally by Ishida \textit{et al.} in 1998 [71] that there is indeed no change in the susceptibility across the superconducting transition for fields perpendicular to the \(d\)-vector, the same result was found also for fields parallel to the \(d\)-vector. While these results are therefore somewhat inconclusive, they are even less compatible with spin singlet pairing.

Additional evidence for an odd parity pairing state comes from phase sensitive measurements involving Josephson junctions, for example reviewed by Liu [64]. As discussed in Sec. 2.1.3, for the two-component order parameter in \(p\)-wave superconductors, only the component parallel to the \(s\)-wave superconductor can couple, and according to a coupling term \(f_{\text{coup}} = K_c \left\{ \psi_n^* \mathbf{d}(\mathbf{k}) \cdot (\hat{n} \times \hat{k}) + \text{c.c.} \right\} [72]\). On the one hand, tunneling is therefore only expected parallel to the layers, but not perpendicular to them, called the ‘selection rule’ and first confirmed by Jin \textit{et al.} in 2000 [73]. On the other hand, for a SQUID as described by Geshkenbein \textit{et al.}, odd parity superconductors have a minimum for zero applied flux (while even parity superconductors have a maximum) [74]. This was confirmed by Nelson \textit{et al.} in 2004 [75].
1.3. Chiral $p$-wave pairing

Broken time reversal symmetry
Evidence for broken time reversal symmetry comes from $\mu$SR experiments which are a probe for intrinsic magnetism, appearing for example at impurities such as discussed in Sec. 3.4.2, or other defects. This was first observed by Luke et al. in 1998 [76]. In particular, it was established that the additional $\mu$SR signal always occurs at $T_c$, even if the transition temperature is lowered by adding impurities to the sample, as reviewed in Ref. [63].

Additional evidence comes from the polar Kerr effect, combining the Faraday effect and a time-reversal operation such as a mirror, as reviewed in Ref. [77]. The resulting Kerr angle can be measured in an interferometer, and was first observed by Xia et al. in 2006 [78], and again later by Kapitulnik et al. with an unprecedented precision [77]. The measured effects are also consistent with the expected formation or absence of domains influenced by in-field or zero-field cooling. The detailed interpretation of the source of these results is still under discussion, as reviewed in Ref. [63].

Discrepancies surrounding chiral $p$-wave pairing
While the evidence compiled above seems very clear and even provoked the early claim by M. Rice in 1998 that “we now have a complete description of the unconventional superconductivity of Sr$_2$RuO$_4$” [79], the most recent review by Mackenzie et al. from just this July 2017 is titled “Even odder after twenty-three years” [60]. What has happened?

A first challenge came from the charge edge currents, which had been proposed theoretically, but have not been detected so far. This is discussed in detail below in Sec. 1.4.1. However, it is now accepted and further supported by the work shown in Ch. 3, that the charge edge currents themselves are not a universal feature. On the other hand, the expected presence of (quasiparticle) edge states has been firmly reported by several groups [80–82]. Furthermore, some of the results from different experiments lead to very different requirements on the size and structure, or even absence, of domain walls. But the formation of domain walls obviously depends on many external and internal factors, see Sec. 1.4.3 below. Still, there remain unresolved issues, in particular in connection with the upper critical field limiting. $H_{c2}\|c$ behaves as expected. $H_{c2}\|ab$ on the other hand seems to be limited by other effects than the expected orbital depairing, and in a discontinuous first order transition, while Pauli paramagnetic limiting is not compatible with the unaffected spin susceptibility discussed above, see Sec. VII.B in Ref. [53] and the section “Apparently contradictory results” of Ref. [60]. Recent theoretical work by Ramires and Sigrist suggested that interorbital effects might explain these features [83]. Another inconsistency arises because different approaches for determining the superconducting anisotropy $\gamma_s$ lead to rather different values for this quantity [53]. Then again, further support for triplet pairing was found rather recently, when an alternative probe for such pairing, the long range penetration into a ferromagnetic material as described in Ref. [84], was measured for the first time in Au/SrRuO$_3$/Sr$_2$RuO$_4$ junctions by Anwar et al. in 2016 [85].

In summary, although there is no direct evidence against the chiral $p$-wave pairing, several results are not consistent with such a simple picture.
1.4 Intrinsic magnetic phenomena

A particularly fascinating feature of chiral $p$-wave superconductors are the intrinsic magnetic phenomena emerging because of their broken time reversal symmetry and chirality. In this thesis we present theoretical research on idealized model systems assuming a pure chiral $p$-wave state on the dominant $\gamma$-band. We propose three phenomena, explored in one chapter each in the main part of this thesis:

- Spontaneous surface flux patterns (Ch. 3),
- Topologically frustrated Josephson junctions (Ch. 4), and
- Half-quantum vortices on $c$-axis domain walls (Ch. 5).

We refer to these phenomena as ‘intrinsic’, in contrast to ‘engineered’ phenomena, while they may be either ‘spontaneous’ (no external applied field) or ‘induced’. The flux pattern at the surface appears spontaneously without any applied field. Cylindrical Josephson junctions are formed naturally in a eutectic material, and the flux line in the topologically frustrated state appears spontaneously without any applied current. Domain walls come naturally to any system with degenerate ground states, and the half-quantum nature of the vortex is an intrinsic feature.

In this section, we introduce and motivate these phenomena. Observations in Sr$_2$RuO$_4$ inspiring the model systems are presented, and relevant previous work is reviewed, both experimental and theoretical. In particular, while the material Sr$_2$RuO$_4$ was only introduced briefly above, those properties relevant for the different projects are explained in detail here. Finally, the essential features of each phenomenon are outlined.

1.4.1 Spontaneous surface flux pattern

In the first project we revisit the notorious issue of the charge edge current and magnetic flux pattern predicted to appear spontaneously at the surface of chiral $p$-wave superconductors, but never detected experimentally.

Experimental inspiration

In chiral $p$-wave superconductors, topology-induced chiral edge states give rise to quasiparticle currents along the surface, transporting both energy and charge [86]. While these two are obviously related and emerge from the same underlying physics, their features are very different. The topologically protected quasiparticle (energy) current, connected to the charge neutral Majorana zero mode, is described straightforwardly [58] and would be experimentally accessible, for example, through the quantized thermal Hall conductivity [87, 88]. The charge edge current and the resulting spontaneous magnetic flux pattern...
1.4. Intrinsic magnetic phenomena

near the surface, on the other hand, is a more obscure feature both quantitively and qualitatively, as charge is not a conserved property of the Bogolyubov quasiparticles [89]. Thus, the direction and magnitude of supercurrents at the edge subtly depend on microscopic details of the bulk electronic states and scattering properties of the surface.

Precisely this supercurrent plays a central role in the debate around the pairing symmetry of Sr$_2$RuO$_4$ (see Sec. 1.3.2). While multiple theoretical works (reviewed below) have predicted a detectable magnetic flux at the surface, not a single trace of it has been discovered in the extensive experimental search using both Hall bar [90] and SQUID [91, 92] scanning techniques, as well as cantilever magnetometry [93]. A review of possible experimental approaches with quantitative estimates was given by Kwon et al. [94].

**Previous theoretical work**

On the theoretical side, after the original proposal and because of the experimental null results, there have been various suggestions related to the spontaneous edge current, based on both microscopic and phenomenological arguments. However, the situation still remains inconclusive. Importantly, any explanation for the absence of magnetic flux at the surface has to be reconciled with the magnetic signatures observed in the µSR experiments [76]. In the ‘reference scenario’ Matsumoto and Sigrist assumed specular scattering at a planar surface and a cylindrical Fermi surface [95]. Ashby and Kallin considered rough and pair breaking surfaces [96], while Lederer et al. considered a metallic surface layer [97]. They both also analyzed the impact of changing some of the Ginzburg Landau coefficients. Huang and Yip studied a very small-size disk geometry for both specular and diffusive surfaces, and in addition in an external magnetic field [98]. Sauls discussed the influence of retroreflection [99]. Fernández Becerra et al. considered an anisotropy of the Fermi surface [100], again also in an applied field. Other approaches include multi-band theories [69], higher Chern numbers [101], or higher angular momentum triplet pairing [102, 103].

Recently, Bouhon and Sigrist studied a tight-binding model for the $\gamma$-band on a square-lattice [104]. They found a non-trivial dependence of the direction of the edge current on the surface orientation in combination with band structure effects beyond a cylindrical Fermi surface, and for specular scattering at the surface. In particular, they showed that for high band fillings the current flows in the opposite direction when comparing straight and zigzag edges, that is, orientations along the crystal axes or diagonal to them in the basal plane. Based on this they proposed a ‘current reversal’ for an octagonally shaped sample combining these two surface orientations, as illustrated in Fig. 1.5.

**Phenomenological model**

In Ch. 3 we revisit the spontaneous surface flux pattern combining the previous efforts and adding new aspects. First, we incorporate the recent results for the band structure and geometry aspects by Bouhon and Sigrist in a phenomenological model by considering a disk-shaped sample and qualitatively including the band structure effects. We further extend this model by taking into account a variety of surface conditions beyond the idealized specular scattering. We include previously studied limits such as diffuse scattering and full pair breaking, as well as surface types with finite extrapolation lengths for both order parameter components, reminiscent of a metallic surface layer. In addition, we continu-
Introduction

![Figure 1.5: Sketch of the direction of the charge edge current in an octagonally shaped sample combining the straight and zigzag surface orientations in the basal plane. At low filling the isotropic limit is recovered and the current flows in a single direction around the disk. At high filling, on the other hand, expected for Sr$_2$RuO$_4$ assuming chiral $p$-wave pairing and using the standard parameters [61], there is current reversal around the sample. [Adapted from Ref. [104]].](image)

ously interpolate between these limits. The Ginzburg Landau formalism provides an ideal framework for this. The flux at the curved surface in a proper circular geometry can be analyzed in real space straightforwardly, and the different material and surface properties can be covered by varying only a small number of parameters in the free energy functional, which are scanned systematically for a comprehensive overview. The detailed shape of the flux pattern is computed including self-screening and selected analytical arguments are derived to support our discussion.

Furthermore, such a spontaneous flux pattern not only appears at the surface, but at any boundary or defect. We additionally discuss the situation at internal impurities, to contrast it with the surface whose properties depend on external factors.

1.4.2 Topologically frustrated Josephson junction

In the second project we study cylindrical Josephson junctions between a conventional $s$-wave and a chiral $p$-wave superconductor appearing naturally in eutectic Sr$_2$RuO$_4$-Ru.

Material inspiration

In eutectic Sr$_2$RuO$_4$-Ru materials, excess Ru segregates from the bulk material to form $\mu$m-size Ru-metal inclusions in the Sr$_2$RuO$_4$ crystal. In this environment superconductivity appears as an inhomogeneous phase, the so-called 3-Kelvin phase, already at an onset temperature of $T_{3K} \approx 3$ K, twice as high as the bulk superconducting transition temperature $T_c \approx 1.5$ K [105]. It has been proposed that filamentary superconductivity nucleates at the interfaces between Ru and Sr$_2$RuO$_4$ [106, 107], likely due to local internal strain [108]. Assuming that the bulk superconducting phase has chiral $p$-wave symmetry, one finds that the structure of the 3-Kelvin phase is different and thus an additional transition beyond mere percolation has to occur on the way to full coherence throughout the system.
1.4. Intrinsic magnetic phenomena

1.4.1. Intrinsic magnetic phenomena

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Figure 1.6: Different possible phases of the filamentary $p$-wave superconductivity around the Ru inclusions in the 3-Kelvin phase, depending on the winding number $N$ and whether time reversal symmetry is broken (TRSB) or not (TRS). Only the B-phase is compatible with a chiral bulk state.

This additional transition involves both time reversal symmetry breaking and the change of overall topology. Several experiments give hints of such an additional transition within the 3-Kelvin phase between $T_{3K}$ and $T_c$ [109–111].

The different possible phases of this filamentary superconductivity in the 3-Kelvin phase as identified by Kaneyasu et al. [112] are illustrated in Fig. 1.6. In the A-phase, only the order parameter component parallel to the interface nucleates. This phase is time-reversal symmetric (TRS) and has no phase winding $N = 0$. In the A’-phase, also the perpendicular order parameter component nucleates. In this phase, time reversal symmetry is broken (TRSB), but it has still no phase winding. Finally, in the B-phase, there is a finite phase winding. From this state, the homogeneous bulk phase can be reached by percolation.

**Experimental inspiration**

Depositing a lead film on the top surface of eutectic samples, Nakamura et al. have realized Pb/Ru/Sr$_2$RuO$_4$ devices [113] as sketched in Fig. 1.7. First, they analyzed an extended contact [113], but later even proceeded to study particular junction configurations produced with a focused ion beam [114]. In these devices, the superconductivity of Pb penetrates into the Ru inclusion by proximity between the two conventional $s$-wave superconductors with $T_{c,Pb} \approx 7.2$ K [114] and $T_{c,Ru} \approx 0.5$ K [113]. On the other hand, there is little direct penetration of this superconductivity into Sr$_2$RuO$_4$ due to its electronic structure with a very weak dispersion along the c-axis [53] and because the coupling between an $s$-wave state and the chiral $p$-wave state along the c-axis is rather weak for symmetry reasons [115], see also the ‘selection rule’ discussed above. Therefore, mediated by the proximity-induced superconducting Ru-inclusions, the Pb film can be treated as indirectly coupled to the superconductor Sr$_2$RuO$_4$, yielding an extended Josephson contact through the interface between Ru and Sr$_2$RuO$_4$.

In these Pb/Ru/Sr$_2$RuO$_4$ Josephson junctions, Nakamura et al. observed an anomalous
Figure 1.7: Schematic of the Pb/Ru/Sr$_2$RuO$_4$ device. External current is applied to the eutectic Sr$_2$RuO$_4$-Ru material through a Pb film, which is indirectly coupled to the Sr$_2$RuO$_4$ bulk mediated by the proximity-induced superconductivity in the Ru inclusions.

temperature dependence of the critical current [113], shown in Fig. 1.8 (left). There are two unconventional features. First, the Josephson current already appears at a temperature $T_{3K}$, above the $T_c$ of bulk Sr$_2$RuO$_4$, most likely indicating a coupling to the 3-Kelvin phase. Upon lowering the temperature, the critical current $I_c$ first increases as expected. Second, however, at around the bulk critical temperature $T_c$ the critical current drops rather suddenly. It then recovers quickly and increases further at lower temperatures.

This unusual behavior of the critical current described above can be dissected by introducing two curves increasing monotonically with decreasing temperature as sketched in Fig. 1.8 (right). Proposing that each curve originates from a distinct mechanism limiting the critical current associated with a different topological state of the junction such as introduced above in Fig. 1.6, this raises two questions. What are the different limiting mechanisms? What is the phase diagram of the evolution of the states at the interface?

Previous theoretical work
Kaneyasu and Sigrist have analyzed the Josephson coupling between the inclusion supporting $s$-wave superconductivity and the surrounding chiral $p$-wave bulk and introduced the concept of topological frustration [116]. While the trivial states (A- and A'-phase), including the state that first nucleates at $T_{3K}$, are optimally coupled to the $s$-wave inclusion, the finite phase winding of the topological states (B-phase and chiral bulk) leads to a phase frustration. While the trivial situation is limited through the standard mechanism, the phase mismatch results in the formation of a spontaneous line-shaped flux pattern to release the frustration. This can be at the expense of interface energy, leading to the appearance of a Josephson-like vortex on the interface, or at the expense of line energy, leading to an Abrikosov-like vortex in the center of the inclusion. They showed that the latter is only favorable at very high coupling strengths and may emerge from the former in a spontaneous depinning transition from the interface to the center of the inclusion at low temperatures.
In other work by Kaneyasu et al., they have studied the phase transitions in eutectic Sr$_2$RuO$_4$-Ru on the way from the 3-Kelvin phase to the chiral $p$-wave bulk state [112]. The Ru inclusion itself is treated to be in the normal state, that is, any coupling to the proximity-induced $s$-wave superconductivity is neglected. They found that indeed the order parameter component parallel to the interface first nucleates in the time-reversal symmetric and topologically trivial A-phase. However, subsequently there is a first order transition from the A-phase directly to the time-reversal symmetry breaking and topologically non-trivial B-phase, at a temperature considerably above the bulk transitions temperature. The A$'$-phase is never realized. Finally, the homogeneous bulk phase is then reached by percolation.

**Phenomenological model**

Based on these previous results, we refine the two questions stated above. What is the mechanism limiting the critical current in the topologically frustrated state of the junction, based on the presence of the spontaneously appearing line-shaped magnetic flux pattern? What is the evolution of the different states of the junction when the Josephson coupling is not neglected, and may the onset of the phase compatible with the bulk topology essentially be reduced to the bulk critical temperature? In this project we address both questions. We obtain a simple and illustrative model of the Pb/Ru/Sr$_2$RuO$_4$ devices by considering a single Ru inclusion embedded in the Sr$_2$RuO$_4$ bulk, and by approximating the Pb contact by an externally applied current.

In the first and main part, we examine in detail the unconventional limiting mechanism of the extended Josephson junction. The Ru inclusion is modeled as a cylindrical $s$-wave...
superconductor embedded in a chiral \( p \)-wave bulk. Using a sine-Gordon framework, the phase winding is introduced in the Josephson phase difference and the externally applied current is included through appropriate boundary conditions. This model allows us to analyze and compare both the topologically trivial and frustrated situation, at both zero and finite applied current, and in addition in both the short and the long junction limit, that is, in different coupling limits. The full model is solved numerically, while the different limits are additionally analyzed analytically.

In the second part, we describe how the presence of superconductivity in the Ru inclusion, induced by proximity from the Pb contact, influences the nature of the state at the interface during the evolution from the filamentary nucleation in the 3-Kelvin phase to the chiral \( p \)-wave bulk. We formulate a Ginzburg Landau model containing the essential features of the system. The 3-Kelvin phase is modeled as a space-dependent critical temperature and the coupling to the \( s \)-wave order parameter enters through appropriate boundary conditions. We compute numerically which configuration minimizes the free energy functional, depending on the strength of the \( s \)-wave order parameter, and combine the results in a phase diagram.

1.4.3 \( c \)-axis domain wall

In the third project we study non-trivial features of \( c \)-axis domain walls depending on the anisotropy of the electronic structure.

Motivation

The chiral \( p \)-wave state \( d(k) = \Delta_p (k_x \pm ik_y) \hat{z} \) is doubly degenerate between the two chiralities \( \pm \) connected by time-reversal symmetry. Therefore, depending on the quality of the sample and the history of cooling, domains of opposite chirality can form. For a layered superconductor with a considerable superconducting anisotropy \( \gamma_s \) and a quasi-two-dimensional electronic structure, there are two types of domain walls. The in-plane domain walls separate regions of opposite chirality within the layers, while \( c \)-axis domain walls separate layers of opposite chirality and span the whole \( ab \)-plane.

The in-plane domain walls have been studied extensively from a theoretical point of view. Previous work considered their magnetic properties (spontaneous flux patterns as introduced above in Sec. 1.4.1 and discussed in Ch. 3 also appear at domain walls) [95, 117, 118], the stable configuration within the basal plane and near the surface [119, 120], and their influence on the Josephson effect [59, 120]. They have been drawn upon to explain various experimental observations in \( \text{Sr}_2\text{RuO}_4 \), such as the internal magnetic fields observed in \( \mu \text{SR} \) experiments [76], unusual Josephson interference patterns [121], anomalous switching between different critical current states in \( \text{Nb/Ru/Sr}_2\text{RuO}_4 \) junctions [122], or strong flux pinning [123]. The requirements on their size varies across the different experiments (see Table 1 of Ref. [124] for a review), and other experiments indicate the absence of domain walls [125]. The situation is further complicated by the dependence of domain wall size and formation on various external and internal factors such as impurities, defects, cooling history, magnetic fields etc. Ultimately, so far there is no direct evidence for their existence [90–92, 126].

The \( c \)-axis domain walls, while mentioned in the discussion of the scanning probe results
[91], have – to our knowledge – never been thoroughly studied from a theoretical point of view. However, they are energetically more favorable than the in-plane domain walls, because of the weak interlayer coupling.

**Phenomenological model**

We explore the structure and magnetic properties of c-axis domain walls taking into account the anisotropy of the electronic structure $\nu$ introduced in Eq. (2.22) and illustrated in Fig. 2.2. While for an isotropic system the two domains are decoupled, we show that there is a finite coupling for anisotropic systems. To determine the behavior of the order parameter across the domain wall, we analyze the relevant terms in the Ginzburg Landau free energy functional where the anisotropy $\nu$ enters through the coefficients as described in Sec. 2.1.2. Using the variational ansatz introduced by Sigrist and Agterberg in Ref. [119], we compute the shape of the order parameter. These analytic results are in agreement with those obtained from numerically minimizing the free energy. Furthermore, they are supported by a semiclassical Bogoliubov-deGennes calculation for different chiral $p$-wave pairings on a square lattice performed by my collaborator Wen Huang. We find that the energetically favorable phase difference across the c-axis domain wall depends on the sign of the anisotropy and has a periodicity of $\pi$, while the detailed shape of the order parameter amplitude across the domain wall depends on the magnitude of the anisotropy. Because the phase difference has a non-trivial $\pi$-periodicity, the smallest vortices supported by the domain wall carry only half a flux quantum. We analyze the structure of these vortices and show that their characteristic length along the domain wall critically depends on the magnitude of the anisotropy. We explain the limiting behavior analytically, and numerically compute the detailed structure of these vortices over the full range of anisotropies $\nu$. In the isotropic limit the domains are essentially decoupled and the vortex explodes along the domain wall. On the other hand, with increasing anisotropy $\nu$, the vortex shrinks below the relevant screening length, which is rather large because of the strong anisotropy of the superconductor $\gamma_s$. In this limit, we observe a crossover to an Abrikosov vortex with the Josephson character only retained in the core, which we describe through a non-local sine-Gordon model.
This chapter addresses the methodology of the formulation and the minimization of the Ginzburg Landau functional used throughout this thesis. First, we introduce the different ingredients available to describe a specific system and its particular properties: the representation of the order parameter, an appropriate coordinate system, the choice of the expansion coefficients, and additional boundary terms such as surface or coupling terms. While the focus here is on chiral $p$-wave pairing which has one of the more intricate free energy functionals, these considerations can be applied to any pairing symmetry.

Once constructed, the next step is the minimization of the free energy functional. The variational procedure leads to a set of coupled non-linear partial differential equations, which can usually only be solved for very restricted limiting cases, while the whole range of results is accessible numerically. Still, the analytical results often provide a deeper understanding of the underlying behavior, and serve as a verification of the numerical results. We review the one-step Newton-Jacobi method used throughout this thesis for the numerical minimization and discuss it in light of other methods available.
2.1 Formulating the Ginzburg Landau functional

Chiral $p$-wave superconductors are described by the two-dimensional odd parity $\Gamma_{-5}$ representation of $D_4h$ as introduced in Sec. 1.3.1. The order parameter has two complex space-dependent components, $\eta(r) = (\eta_x(r), \eta_y(r))$. The uniform bulk state is given by $\eta = \eta_0(1, \pm i)$ with a relative phase difference of $\pi/2$, which is two-fold degenerate with the two chiralities $\pm 1$, connected by the broken time reversal symmetry. The full generalized Ginzburg Landau functional, including the gradient and magnetic terms, is given by [51]

$$\mathcal{F}[\eta_x, \eta_y, A] = \int d^3r \left[ a(T - T_c)|\eta|^2 + b_1|\eta|^4 + \frac{b_2}{2} \left( \eta_x^2 \eta_y^2 + \eta_x^2 \eta_y^2 \right) + b_3|\eta_x|^2|\eta_y|^2 \right.\right.$$  
$$+ K_1 \left( |D_x \eta_x|^2 + |D_y \eta_y|^2 \right) + K_2 \left( |D_x \eta_y|^2 + |D_y \eta_x|^2 \right) \right.$$  
$$+ \left\{ K_3(D_x \eta_x)^*(D_y \eta_y) + K_4(D_x \eta_y)^*(D_y \eta_x) + \text{c.c.} \right\}$$  
$$+ K_5 \left( |D_x \eta_x|^2 + |D_y \eta_y|^2 \right) + \frac{(\nabla \times A)^2}{8\pi},$$

with the critical temperature $T_c$, the sets of expansion coefficients $a$, $\{b_i\}$, and $\{K_i\}$, the gauge-invariant derivative $D = \nabla - i\gamma A$, where $\gamma = 2e/(\hbar c) = 2\pi/\Phi_0$ with the flux quantum $\Phi_0$, and the vector potential $A$.

2.1.1 Representation of the order parameter and coordinate system

Depending on the sample geometry and the effect under consideration, the Ginzburg Landau functional can get heavily simplified by choosing a suitable representation of the two-component order parameter and an appropriate coordinate system. Below we highlight the most common examples, while the specific versions chosen for each of the studied phenomena are introduced in the corresponding chapters.

The full expression of the Ginzburg Landau functional for a different representation of the order parameter and a different coordinate system while keeping all the expansion coefficients undetermined is in general lengthy, in particular the gradient terms. In most problems, however, there are enough initial assumptions that the free energy is indeed simplified. Different expressions of the free energy are collected in Appendix A.

The two opposite chiralities

For the $\pm$-representation of the order parameter, the two opposite chiralities of the two-fold degenerate bulk state are accessed directly. The $d$-vector is rewritten as

$$d = \hat{z} (\eta_+(k_x + ik_y) + \eta_-(k_x - ik_y)), \quad \text{(2.2)}$$

where the order parameter components $\eta_\pm$ are given by

$$\left( \eta_+, \eta_- \right) = \frac{1}{2} \left( \eta_x - i\eta_y, \eta_x + i\eta_y \right), \quad \text{(2.3)}$$

and with the inverse relation given by

$$\left( \eta_x, \eta_y \right) = (\eta_+ + \eta_-, i(\eta_+ - \eta_-)). \quad \text{(2.4)}$$
Please note that the absolute value of this state is $|\eta|^2 = |\eta_x|^2 + |\eta_y|^2 = 2(|\eta_+|^2 + |\eta_-|^2)$. In another commonly used convention the prefactor is chosen to be $1/\sqrt{2}$ to circumvent this issue, which comes at the expense of the nice expression for the $d$-vector.

The interpretation is straightforward. In the uniform bulk phase, only one of these two components is finite. This representation is particularly useful when the two chiralities do not get mixed, because then all the coupling terms disappear in the Ginzburg Landau functional. Such simple situations are considered below when deriving the phenomenological parameters. Also, this representation is highly convenient when describing domain walls such as in Ch. 5.

Because this representation is not tied to any coordinate system, both cartesian and polar coordinates may be used, such as more appropriate for a given model system. In a cartesian coordinate system the gauge-invariant derivative can also be represented as

$$D_\pm = D_x \pm iD_y,$$

simplifying some of the expressions, see for example Eq. (A.8).

**Boundary conditions at general defects**

Away from the uniform bulk phase, while the two components $(\eta_x, \eta_y)$ of the order parameter are always coupled, they are often affected differently by boundaries or defects such as impurities, surfaces, interfaces or domain walls, where the translational invariance of the system is broken. The distinction then is between the components of the order parameter perpendicular and parallel to the boundary or defect, such that a convenient representation is

$$\eta = (\eta_\perp, \eta_\parallel) = (n \cdot \eta, (n \times \eta) \cdot \hat{z}),$$

with the normal vector $n$ of the boundary.

There are two limiting cases where this representation is particularly useful. One, for straight defects in the basal plane not parallel to the crystal axis, using a rotated cartesian coordinate system, and where $n = \text{const}$ along this line. Or two, for circular boundaries or defects with $n = r$, using polar coordinates, such as the disk-shaped sample in Ch. 3 or the cylindrical Josephson junction in Ch. 4. The coordinate system obviously has to respect the structure of the boundary or defect. Therefore, in the former rotated cartesian coordinates are appropriate, while in the latter polar coordinates have to be used.

**Phase winding**

The real-space phase winding of the chiral state [58] is accessible through the phase of the order parameter component parallel to a closed path $s_n$ with a normal vector $n$ in the basal plane. For $\varphi(n) = \arg[\eta_\parallel]$ we define the winding number [127]

$$N = \oint ds_n \cdot \nabla \varphi(n).$$

This winding number $N$ characterizes the topology of our state. For the bulk chiral $p$-wave state $N = \pm 1$, while the trivial state with $N = 0$ for example nucleates in the 3-Kelvin phase in eutectic Sr$_2$RuO$_4$, see Fig. 1.6 and Ch. 4, in particular Sec. 4.4.
Modeling a chiral \( p \)-wave superconductor

For a rotationally symmetric sample, it is particularly useful to explicitly introduce this winding number. In the isotropic limit, i.e. also a rotationally symmetric electronic structure, the phase winding then contains all the angular dependence, see Sec. 3.2.1. Using polar coordinates, in this limit the order parameter can therefore be separated and parametrized according to

\[
\eta_\pm(r, \theta) = \tilde{\eta}_\pm(r)e^{i(N\pm 1)\theta},
\]

and for \((\eta_\perp, \eta_\parallel) = (\eta_r, \eta_\theta)\)

\[
(\eta_r(r, \theta), \eta_\theta(r, \theta)) = (\tilde{\eta}_r(r), \tilde{\eta}_\theta(r))e^{iN\theta}.
\]

2.1.2 Expansion coefficients

Comparing the free energy functional for chiral \( p \)-wave given in Eq. (2.1) to the expansion form of the functional for conventional \( s \)-wave given in Eq. (1.18), the basic expansion structure is the same. Because of the two-component order parameter there are intricate coupled terms \((b_{2-3} \text{ and } K_{2-4})\), and because of the layered crystal structure there are additional terms \((K_5)\). Therefore, the expansion coefficients\(^1\) \( b \) and \( K \) here become sets of coefficients \( \{b_i\} \) and \( \{K_i\} \). All the real expansion coefficients \( a, \{b_i\} \) and \( \{K_i\} \) depend on material properties, but not all are directly accessible from experiments. Therefore, determining the ratios between these sets of coefficients \( a, \{b_i\} \), and \( \{K_i\} \) follows the same principle as before in Sec. 1.2.1, relating them to the phenomenological parameters accessible in experiments. On the other hand, finding the ratios within the sets \( \{b_i\} \) and \( \{K_i\} \) is more involved. The stability considerations derived in Sec. 1.3.1 and summarized in Table 1.1 lead to some restrictions for the \( \{b_i\} \), but actual values can only be determined from microscopic models. We want to stress that the basic form of the free energy functional is purely phenomenological and was only later connected to the microscopic theory by Gor'kov [18], as discussed in Sec. 1.1.1.

Concerning the layered crystal structure, here we consider a continuous anisotropic system such as described by Kogan in Ref. [129] or by Blatter \textit{et al}. in Ref. [130]. We do not take into account any Lawrence-Doniach\(^2\) kind of coupling between the layers. This means, we assume \( \xi_c \gg s \), where \( s \) is the interlayer distance. This is reasonable considering the material parameters of \( \text{Sr}_2\text{RuO}_4 \), see Sec. 1.3.2, but see for example the discussion regarding observations made in experiments on vortex crossings in the group of Hasselbach [132]. This anisotropy means that for each phenomenological parameter there is now an in-plane and an out-of-plane version, while in addition there are in principle different in-plane versions because of the two-component order parameter and the broken in-plane rotational symmetry.

In this section we first derive the ratios between the sets, relating them to the phenomenological parameters, and provide a dimensionless form of the free energy functional. Next,

\(^1\) The second-order homogeneous term is always diagonal in the basis functions of the irreducible representation, and in a continuous bulk system only has a single expansion coefficient \( a \). An effective component-specific critical temperature emerges when the perpendicular and parallel component get affected differently, as discussed below, which happens at boundaries, defects, or for example when the system is under strain [128].

\(^2\) A nice review of the different theoretical approaches is given by Chapman \textit{et al}. in Ref. [131].
2.1. Formulating the Ginzburg Landau functional

we review how to set the ratios within the sets, based on models ranging from a simple Fermi sphere model to more involved lattice models.

Phenomenological parameters

For the purpose of deriving the underlying parameters, we consider only the most simple situations to lowest order, where there is no mixing between the two degenerate ground states. It is therefore convenient to use the ±-representation, because the corresponding expression of the free energy does not contain any coupled terms if only a single ground state is considered. Combining Eq. (A.2) and Eq. (A.6), and setting $\eta_- = 0$, we find

$$
\mathcal{F}_+ = \int d^3 r \left[ 2a(T - T_c)|\eta_+|^2 + (4b_1 - b_2 + b_3)|\eta_+|^4 
+ (K_1 + K_2) \left( |D_x \eta_+|^2 + |D_y \eta_+|^2 \right) 
+ i(K_3 - K_4) ((D_x \eta_+)^*(D_y \eta_+) - c.c) 
+ 2K_5 |D_z \eta_+|^2 + \left( \nabla \times A \right)^2 ight],
$$

where the third line will drop out in all situations considered below, and also does so in the weak-coupling approximation.

The bulk order parameter amplitude is obtained from minimizing the homogeneous functional as for Eq. (1.5), and is given by

$$
|\eta_b(T)|^2 = \frac{-a(T - T_c)}{4b_1 - b_2 + b_3},
$$

which is positive because for the chiral $p$-wave sector (the A-phase in the stability discussion of Sec. 1.3.1) the fourth order coefficients $4b_1 - b_2 + b_3 > 0$.

The in-plane and the out-of-plane coherence lengths are derived as for Eq. (1.9), and are

$$
\xi_{ab}(T)^2 = \frac{K_1 + K_2}{-2a(T - T_c)},
$$

$$
\xi_c(T)^2 = \frac{K_5}{-a(T - T_c)}.
$$

The terms in-plane and out-of-plane have a straightforward meaning here, with $\xi_{ab}$ describing the characteristic length for changes in the order parameter amplitude within the layers, while $\xi_c$ is the characteristic length for changes in the order parameter amplitude across the layers, as illustrated in the top row of Fig. 2.1. Their ratio is called the superconducting anisotropy parameter [53]

$$
\gamma_s = \frac{\xi_{ab}}{\xi_c} = \sqrt{\frac{K_1 + K_2}{2K_5}}.
$$

Strictly speaking, following the derivation as for Eq. (1.9) implies a boundary condition $|\eta_+|_{\text{surf}} = 0$, which we also adapted for the illustration in Fig. 2.1. However, we already mentioned that at boundaries or defects the parallel and perpendicular components get affected differently, such that the actual changes of the order parameter are described
by a component-specific and situation-specific characteristic length. For example, let us consider a surface with \( \hat{n} = \hat{x} \) at \( x = 0 \) and with specular scattering such that the perpendicular component is fully suppressed, \( |\eta_x(x = 0)| = 0 \), while to lowest order the parallel component is not affected, \( |\eta_y| = \text{const} \). Following Ref. [51], we use the ansatz \( (\eta_x, \eta_y) = |\eta_b(T)| \left( \tanh(x/(\sqrt{2} \xi(T))), \pm i \right) \) and find

\[
\xi_{\perp}(T)^2 = \frac{K_1}{2b_1 |\eta_b|^2}. \tag{2.14}
\]

The parallel component would change on a length scale

\[
\xi_{\parallel}(T)^2 = \frac{K_2}{2b_1 |\eta_b|^2}, \tag{2.15}
\]

see also the discussion of the extrapolation lengths in Sec. 3.2.1 or the top plot in Fig. 3.4. Therefore, the ‘coherence length’ \( \xi_{ab} \) defined in Eq. (2.12a) can be understood as a general or average length scale. We use this length scale for the dimensionless expression of the free energy given in Eq. (2.20). It is particularly useful, because it does not change across different situations, nor for the choices of the ratios of the gradient term coefficients \( \{K_i\} \) considered in this thesis, see discussion below, such that different results are always comparable, for example in Ch. 3.

The situation for the screening length is a bit more involved, but fundamentally as for Eq. (1.12). Here, even though many authors use the words in-plane and out-of-plane, we have to be very carefully what we refer to. As illustrated in the middle row in Fig. 2.1, the relevant direction is that of the screening currents, and not that of the applied field. This makes sense, but may lead to some confusion, as there are two situations leading to in-plane screening lengths \( \lambda_{ab} \). Assuming a rigid order parameter, both an applied field \( B_0 \hat{z} \) applied to the side of the layered sample and leading to a vector potential \( A_y(x) \), as well as an applied field \( -B_0 \hat{x} \) applied to the top of the sample and leading to a vector potential \( A_y(z) \) result in screening currents in the \( y \)-direction. Only an applied field \( B_0 \hat{y} \) applied to the side of the sample leads to a vector potential \( A_z(x) \) and results in out-of-plane screening currents. The resulting screening lengths are given by

\[
\lambda_{ab}(T)^{-2} = 8\pi \gamma^2 (K_1 + K_2)|\eta_b(T)|^2 \tag{2.16a}
\]

\[
\lambda_{c}(T)^{-2} = 16\pi \gamma^2 K_5 |\eta_b(T)|^2. \tag{2.16b}
\]

These are related through the superconducting anisotropy parameter as

\[
\frac{\lambda_{ab}}{\lambda_{c}} = \sqrt{\frac{2K_5}{K_1 + K_2}} = \frac{1}{\gamma_s}. \tag{2.17}
\]

For a two-component order parameter, there can in general also be different in-plane versions for the screening length, for example for the B- and C-phase as introduced in the stability discussion of Sec. 1.3.1, and see discussion of the London equation on p. 207f of Ref. [27].

For the Ginzburg Landau parameter we adopt the standard approach for anisotropic
2.1. Formulating the Ginzburg Landau functional

<table>
<thead>
<tr>
<th>Coherence length</th>
<th>in-plane</th>
<th>out-of-plane</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\xi_{ab}$</td>
<td>$</td>
<td>\eta_0</td>
</tr>
<tr>
<td></td>
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<table>
<thead>
<tr>
<th>Screening length</th>
<th>$\lambda_{ab}$</th>
<th>$\lambda_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$-B_0 \hat{z}$</td>
<td>$B_0 \hat{y}$</td>
</tr>
</tbody>
</table>

| Upper critical field | $H_{c2||c}$ | $H_{c2||ab}$ |
|----------------------|------------|-------------|
| Top view             |            |             |

Figure 2.1: The phenomenological parameters for continuous anisotropic layered superconductors. There is an in-plane and an out-of-plane coherence length, referring to the direction over which the order parameter varies; and an in-plane and an out-of-plane screening length, referring to the direction of the screening currents (green). Also, there are two different upper critical fields, for an external field (red) applied perpendicular or parallel to the layers.

Superconductors [129] and define

$$\kappa_{ab} = \frac{\lambda_{ab}}{\xi_{ab}} = \frac{\sqrt{4b_1 - b_2 + b_3}}{\sqrt{4\pi \gamma (K_1 + K_2)}}$$  \hspace{1cm} (2.18a)$$

$$\kappa_c = \frac{\lambda_{ab} \lambda_c}{\xi_{ab} \xi_c} = \gamma_s \kappa_{ab}.$$  \hspace{1cm} (2.18b)

The former is as in Eq. (1.16), while the latter is not $\lambda_c/\xi_c$, which can be understood from considering the sketches of bulk vortices in the bottom row of Fig. 2.1.
Finally, as in Eq. (1.17), the upper critical field is given by

\[
H_{c2||e} = \frac{\Phi_0}{2\pi \xi_{ab}(T)^2} \quad \text{and} \quad H_{c2||ab} = \frac{\Phi_0}{2\pi \xi_{ab}(T) \xi_c(T)} = \gamma_s H_{c2||e},
\]

where we follow the notations in Ref. [53]. Please note that these cannot uniquely be called in-plane and out-of-plane, as illustrated in the bottom row of Fig. 2.1. These definitions assume orbital depairing to limit the upper critical field in both directions, which actually does not seem to be the correct picture, see discussion in Sec. 1.3.2.

In the following, unless of special importance such as in Ch. 5, we drop the index \(ab\) such that the plain versions \(\xi, \lambda\) and \(\kappa\) always denote the in-plane parameters, while \(H_{c2}\) denotes the one parallel to the c-axis.

**Dimensionless free energy functional**

With these definitions at hand, we can introduce dimensionless quantities useful for the numerical treatment. The temperature is measured in units of \(T_c\), and we define \(t = T/T_c\).

The unit length is \(\xi_0 = \xi_{ab}(0)\), the unit for the order parameter is \(\eta_0 = \eta_0(0)\), and the vector potential is in units of \(1/(\gamma \xi_0)\) such that the magnetic field is in units of \(1/(\gamma \xi_0^2)\). Concerning the sets of expansion coefficients \(\{h_{1-3}\}\) and \(\{K_{1-4}\}\), we are left with one independent coefficient less than the size of the set such that only the ratios matter in the end, while the ‘unit’ of the set is given through the phenomenological parameters. Here we take the expansion coefficients \(K_i\) in units of \(K = K_1 + K_2\) and the \(b_i\) in units of \(b = 4b_1 - b_2 + b_3\), in accordance with the definition of \(\eta_0\) and \(\xi_0\). The free energy is then in units of \(\eta_0^2 \xi_0^3 aT_c\) and given by

\[
\mathcal{F}[\eta_x, \eta_y, A] = \int_{V_p} d^3r \left[ (t - 1)\eta^2 + \left( b_1 |\eta|^4 + b_2 \left( \eta_x^2 \eta_y^2 + \eta_x^2 \eta_y^2 \right) + b_3 |\eta_x|^2 |\eta_y|^2 \right) \right.
\]

\[
+ 2 \left[ K_1 \left( |D_x \eta_x|^2 + |D_y \eta_y|^2 \right) + K_2 \left( |D_x \eta_x|^2 + |D_y \eta_y|^2 \right) \right]
\]

\[
+ \left( K_3 (D_x \eta_x)^*(D_y \eta_y) + K_4 (D_x \eta_x)^*(D_y \eta_x) + c.c. \right] \]

\[
\left. + \frac{1}{\gamma_s^2} \left( |D_2 \eta_x|^2 + |D_2 \eta_y|^2 \right) + 2\kappa^2 (\nabla \times A)^2 \right] ,
\]

where all quantities now have the units described above but without any special notation. What remains to be fixed is the Ginzburg Landau parameter \(\kappa = \kappa_{ab}\) and the superconducting anisotropy \(\gamma_s\), which we usually take to be 2.6 and 20 [62], respectively, but see the overview and discussion in Sec. B.2. In this dimensionless form of the free energy we have kept the temperature term \((t - 1)\) explicitly, as opposed to Eq. (1.19), where on the other hand the temperature dependent quantities were used as units. This allows us to introduce component-specific and space-dependent effective critical temperatures useful in some situations such as the disk-shaped sample discussed in Ch. 3 or the 3-Kelvin phase discussed in Sec. 4.4, and to compare results across temperatures.
2.1. Formulating the Ginzburg Landau functional

Ratios within the sets \{b_i\} and \{K_i\}

We have already mentioned that a first restriction for the \(b_i\) comes from the stability considerations discussed in Sec. 1.3.1, leading to bounds on the \(b_i\) for the chiral \(p\)-wave state in the A-phase. In addition, defining the phenomenological parameters as described above already reduces the independent coefficients by one, fixing a ‘unit’ for each set. To determine the remaining ratios, however, we have to rely on detailed calculations based on microscopic theories. In this section we do not derive any of the results, but present a comprehensive overview. For detailed calculations the reader is referred to the thesis by Adrien Bouhon [59]. We note that while the Ginzburg Landau approach provides a straightforward way to consider strong-coupling parameters, in this thesis we always assume weak-coupling.

We first discuss the expansion coefficients of the fourth order homogeneous term. With \(\{\phi_x(k), \phi_y(k)\}\) the basis functions of the irreducible representation \(\Gamma_5^-\) of the full tetragonal point group \(D_{4h}\) we write the superconducting gap \(d(r, k) = \hat{z} (\eta_x(r)\phi_x(k) + \eta_y(r)\phi_y(k))\). In any weak-coupling approach for the chiral \(p\)-wave state on the \(\gamma\)-band, the coefficients \(b_i\) are then related to the band and gap structure as

\[
\begin{align*}
    b_1 &\sim \langle \phi_x^4 \rangle_{FS} \\
    b_2 &\sim 2\langle \phi_x^2 \phi_y^2 \rangle_{FS} \\
    b_3 &= 2(b_2 - b_1),
\end{align*}
\]

where \(\langle \cdot \rangle_{FS}\) is an average over the Fermi surface. Both \(b_1 > 0\) and \(b_2 > 0\), and also \(2b_1 > b_2\), such that all bounds of the A-phase are respected (as expected by construction). The ‘unit’ \(b = 4b_1 - b_2 + b_3\), introduced above because of \(\eta_0\), now becomes \(b = 2b_1 + b_2\). With the additional constraint given by Eq. (2.21c), there is only one independent coefficient left, reducing the weak-coupling coefficients to the thick red line in the phase diagram in Fig. 1.3. The single remaining degree of freedom can conveniently be parametrized by defining an anisotropy parameter \(\nu\), introduced by Agterberg [133], and given by

\[
\nu = \frac{\langle \phi_x^4 \rangle_{FS} - 3\langle \phi_x^2 \phi_y^2 \rangle_{FS}}{\langle \phi_x^4 \rangle_{FS} + \langle \phi_x^2 \phi_y^2 \rangle_{FS}} = \frac{2b_1 - 3b_2}{b},
\]

with \(\nu \in [-1, 1]\). This simplifies the fourth order homogeneous term of the free energy functional, in particular for the \(\pm\)-representation, see Eq. (A.3). In summary, the three a-priori independent expansion coefficients \(b_i\) reduce to only two independent quantities \(\nu\) and \(b\) for any weak-coupling approach, such that

\[
\begin{align*}
    b_1 &= \frac{3 + \nu}{8} b \tag{2.23a} \\
    b_2 &= \frac{1 - \nu}{4} b \tag{2.23b} \\
    b_3 &= \frac{-1 - 3\nu}{4} b. \tag{2.23c}
\end{align*}
\]

Physically, \(\nu\) measures the deviation of the system from full rotational symmetry, as illustrated in Fig. 2.2. It describes the anisotropy of the full electronic structure, including
Modeling a chiral $p$-wave superconductor

Figure 2.2: The anisotropy $\nu$ of the electronic structure for chiral $p$-wave pairing on the $\gamma$-band in a tetragonal crystal for a weak-coupling approach, plotted against $b_3/b_1$ such as to give the values of $\nu$ along the thick red line in Fig. 1.3.

both the anisotropy of the Fermi surface and the anisotropy of the gap function$^3$, for more details see the discussion in Ch. 6 of Ref. [59].

For a completely rotationally symmetric system with $\phi_x(k) = k_x$ and $\phi_y(k) = k_y$, corresponding to the isotropic limit, the anisotropy vanishes, $\nu = 0$, while for a full (rotated) square, $|\nu| = 1$. We note that for Sr$_2$RuO$_4$ the anisotropy is usually estimated to be around $\nu \approx -0.6$ for $\sin k_x \pm i \sin k_y$ pairing on the $\gamma$-band, see also Table 5.1 on p. 88 of Ref. [59]. However, for other models of Sr$_2$RuO$_4$, very different values may result [89, 101]. In this thesis we always use the expansion coefficients of the isotropic limit for the $\{b_i\}$ unless stated otherwise. In particular, the anisotropy $\nu$ plays a central role in Ch. 5. Ratios beyond this weak-coupling approach have for example been considered by Ashby and Kallin in a discussion of the spontaneous flux pattern [96]. For completeness we also note that the $b_i$ for the isotropic limit have been derived much earlier, see Ref. [52].

Next, we discuss the gradient term coefficients. Setting $K = K_1 + K_2$ because of $\xi_0$, there are three independent coefficients left. For these ratios, however, the situation is a bit more involved, because both the basis functions and the derivatives enter. In any weak-coupling approach they are related to the band and gap structure as

$$K_1 \sim \langle \phi_x^2 v_x^2 \rangle_{FS}$$  \hspace{1cm} (2.24a)

$$K_2 \sim \langle \phi_y^2 v_y^2 \rangle_{FS}$$  \hspace{1cm} (2.24b)

$$K_3 = K_4 = \langle \phi_x \phi_y v_x v_y \rangle_{FS}. \hspace{1cm} (2.24c)$$

First of all, from Eq. (2.24c) we find that for any weak-coupling approach $K_3 = K_4$, leaving us with two independent coefficients. In a quasiclassical approach the basis functions are

---

$^3$ Quoting from the introduction to Ch. 6 of Ref. [59], “the lattice version of the Bogoliubov-de Gennes equations for the $\gamma$-band of Sr$_2$RuO$_4$ assuming the chiral $p$-wave state [...] 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)”. 

---
2.1. Formulating the Ginzburg Landau functional

\( \phi_i = v_i \), the components of the Fermi velocity, which corresponds to “identifying the anisotropy of the gap function with the anisotropy of the Fermi surface” [59]. This leads to the further restriction \( K_2 = K_3 = K_4 \), leaving one independent coefficient, for which we can use the anisotropy \( \nu \) introduced above. Therefore, for the quasiclassical approach the four a-priori independent expansion coefficients \( K_i \) are reduced to two independent quantities \( \nu \) and \( K \), such that

\[
K_1 = \frac{3 + \nu}{4} K
\]

\[
K_2 = K_3 = K_4 = \frac{1 - \nu}{4} K.
\] (2.25b)

However, these considerations do not apply to a weak-coupling approach on a lattice. There, \( K_1 + K_2 \) is not even constant when the band filling is varied. Because Eq. (2.24c) holds for any weak-coupling approach, there are therefore three independent coefficients. For more details we refer to Ref. [59]. In this thesis, unless stated otherwise, we use the coefficients for the isotropic limit (\( \nu = 0 \)). The coefficients from the quasiclassical approach defined with the anisotropy \( \nu \) are used in Ch. 5, while we will come back to the issue of the ratios on the lattice in detail in Sec. 3.1.2, where we discuss how the ratio \( K_1/K_2 \) changes significantly with the band filling, leading to interesting current-reversal effects. Finally, for completeness we note that the derivation of the ratios in the isotropic limit for a simple Fermi sphere model by Machida et al. can be found in the appendix of Ref. [134].

2.1.3 Boundary and coupling terms

So far we have only considered the bulk part of the free energy. However, for any boundary or defect, there are additional terms, which we now discuss in this section. In general, each such term will come with its own additional coefficients, which again have to be determined. Here we first discuss the surface term (used in Ch. 3), and then describe the coupling term to an s-wave superconductor (used in Ch. 4), while some other additional terms will be introduced when necessary, such as the impurity term in Sec. 3.4.2 or the effective terms describing the 3-Kelvin phase in Sec. 4.4. Finally, we also comment on how most effects can easily be incorporated by considering a component-specific and space-dependent effective critical temperature.

The straightforward treatment of the divers effects at boundaries and defects described in this section is one of the greatest assets of the Ginzburg Landau approach. While in the microscopic approaches for example surface effects can also be included, their treatment away from some limiting cases such as specular scattering is tedious, and has to be done case-by-case. In the Ginzburg Landau approach, on the other hand, the coefficients of the additional terms can be scanned systematically over their full range, such as done in this thesis. The limitation here is to connect a given value of these coefficients to an actual physical situation. For example, while some of the surface types \( s \) considered in Ch. 3 have a clear meaning, such as the full specular scattering or the full pair-breaking surface type, for others it is not as obvious which kind of surface they correspond to.
Surface free energy and the effective critical temperature

The most general description of a surface is through an additional effective surface free energy respecting all the terms allowed in the lower symmetry. For the chiral $p$-wave state this is given by [51]

$$F_{\text{surf}}[\eta_x, \eta_y] = \int_{A_p} d^2r \left[ (g_1 (n_x^2 + n_y^2) + g_2 n_z^2) |\eta|^2 
+ g_3 (n_x^2 - n_y^2) (|\eta_x|^2 - |\eta_y|^2) 
+ g_4 n_x n_y \left( \eta_x^* \eta_y + \eta_y^* \eta_x \right) \right]$$

(2.26)

with $A_p$ the surface of the superconductor with the outward normal $n$, and where the coefficients $\{g_i\}$ contain all the properties of the surface. They can in principle also be derived microscopically and constitute an effective boundary condition, see Sec. 11.1 in Ref. [5]. In general, these coefficients may be spatially dependent. In this thesis, however, we always assume translational invariance along the surface.

The full boundary conditions are then obtained from a variation of the full free energy with respect to the order parameter components, see Sec. 2.2.1. As an example, let us consider a planar surface at $x = x_0$ with $n = \hat{x}$ such that $\eta = \eta(x)$ and $A = A_y(x)\hat{y}$, that is, using the London gauge, and assuming weak-coupling with $K_3 = K_4$, for which we find

$$[K_1 \partial_x \eta_x - i \gamma A_y K_3 \eta_y + (g_1 + g_3) \eta_x]_{x_0} = 0$$

(2.27a)

$$[K_2 \partial_x \eta_y - i \gamma A_y K_3 \eta_x + (g_1 - g_3) \eta_y]_{x_0} = 0.$$  

(2.27b)

For one-component order parameters, the extrapolation length $b$ is defined as [4]

$$\left| \frac{D_n \eta}{|\eta|} \right|_{\text{surf}} = \frac{1}{b},$$

(2.28)

which measures the penetration of the order parameter into the adjacent material (proximity effect) and is gauge-invariant. Here this can only be used as an a-priori boundary condition if the vector potential is ignored completely, that is, if self-screening is neglected, such that there is no mixing between the two components in the boundary conditions Eq. (2.27). For the surface at $x = x_0$ we then find the extrapolation length of each component

$$b_x = \frac{K_1}{(g_1 + g_3)},$$

(2.29a)

$$b_y = \frac{K_2}{(g_1 - g_3)},$$

(2.29b)

for $K_i > 0$ and $g_1 \geq g_3 \geq 0$, see Sec. 3.1.3. For the self-consistent case where self-screening is not neglect, we note that the extrapolation length can always be extracted a-posteriori from the result, as done in Sec. 3.2.1 and see Fig. 3.5. In general, however, it is space dependent, even if the $\{g_i\}$ are not.

We prefer to use a convenient intermediate approximation$^4$, where a component-specific
2.1. Formulating the Ginzburg Landau functional

and space-dependent effective critical temperature is introduced. For the example of the surface at \( x = x_0 \) and regrouping the surface term we find

\[
\mathcal{F}_{\text{surf}}[\eta_x, \eta_y] = \int dy dz \left[ (g_1 + g_3) |\eta_x|^2 + (g_1 - g_3) |\eta_y|^2 \right]_{x=x_0}.
\]

This can be combined with the second order homogeneous term by defining

\[
T_{\text{eff}}^{c,i}(x) = T_c - T_{c,i}(x)
\]

with the component-specific surface critical temperatures

\[
T_{c,x}(x) = \frac{g_1 + g_3}{a} \delta(x - x_0) \quad \text{and} \quad T_{c,y}(x) = \frac{g_1 - g_3}{a} \delta(x - x_0).
\]

This is particularly useful and straightforward to implement numerically, and preferable over direct boundary conditions such as given in Eq. (2.27), see the discussion below in Sec. 2.2.2. In addition, it is easily adapted for general surface orientations, see Sec. 3.1.3, while the full direct boundary conditions for a curved surface in polar coordinates as given in Eq. (A.11) look rather daunting. In a similar fashion we can also formulate more complicated effective critical temperatures at boundaries such as in the 3-Kelvin phase, see Sec. 4.4.

**Coupling terms**

The Josephson coupling between a conventional \( s \)-wave superconductor with order parameter \( \psi_s \) and a chiral \( p \)-wave superconductor with order parameter \( \eta \) relies on the effect of spin-orbit coupling in order to provide lowest order pair tunneling \([115]\), leading to a coupling term \([72]\)

\[
f_{\text{coup}} = K_c [\psi_s^* (\hat{z} \cdot (\hat{n} \times \hat{\eta})) + \text{c.c.}],
\]

where \( K_c \) is a real coupling constant and \( \hat{n} = \hat{r} \) the normal of the interface in the direction from the \( s \)-wave to the chiral \( p \)-wave superconductor, see also Sec. 3.2.2 in Ref. [59]. On the one hand, there is no tunneling along the \( c \)-direction, but only for in-plane junctions. On the other hand, only the order parameter component parallel to the junction couples. Such a coupling term is used to describe the cylindrical Josephson junction in Ch. 4, see also Sec. 4.1.2, and we remind the discussion of the phase sensitive measurements from Sec. 1.3.2. Finally, we note that the structure for the coupling term to other superconducting states is summarized in Table XI in Ref. [51].

**Applied magnetic field**

For completeness we also mention the full magnetic term in an applied field \( H \), given by

\[
f_{\text{mag}} = \frac{(B - H)^2}{8\pi},
\]

which can be understood as a Legendre transformation to the now appropriate Gibbs free energy. Variation with respect to the vector potential then leads to the boundary condition

\[
B \times n|_{\text{surf}} = H \times n|_{\text{surf}}.
\]

Based on this, for example the boundary condition for the gradient of the phase difference across the cylindrical Josephson junction in an external field is derived in Sec. 4.1.4.
2.1.4 Summary

To summarize, the procedure for formulating the Ginzburg Landau free energy functional is as follows. For a given situation, the most appropriate coordinate system and representation of the order parameters is chosen, the ratios for the expansion coefficients in the sets \( \{ b_i \} \) and \( \{ K_i \} \) are selected, and any additional terms are identified. Generally, all parameters which are not expected to play an essential role are chosen as simple as possible. For example, the expansion coefficients take the isotropic values unless the effect under study relies on certain features of the electronic structure. Or, the geometry is taken as symmetric as possible. This process is described in detail for each phenomenon at the beginning of the corresponding chapters. In the final chapter 6 we recapitulate the choices for these ‘ingredients’ of the free energy functional used for the three intrinsic magnetic phenomena explored in this thesis.

While the hope is that the resulting functional is heavily simplified, in some situations it is only feasible to do the transformations using a computer algebra system supporting complex variables and capable of advanced symbolic computation and simplifications such as Mathematica [135]. This is done for example to prepare the free energy for the disk-shaped sample in Ch. 3.

Finally, we note that this approach can be applied in a similar fashion to any pairing symmetry, and we refer to the tables in Ref. [51] for the corresponding bulk, boundary and coupling terms.

2.2 Analyzing the Ginzburg Landau functional

After formulating the Ginzburg Landau free energy functional, we proceed to analyze it. The full shape of the order parameter and the vector potential can only be found by minimizing the whole functional self-consistently. However, some insight can already be gained by closely studying the resulting convenient and hopefully simplified expression of the functional or by deriving the proper boundary conditions.

In this section we first comment on this analytical approach and formally introduce the calculus of variation, even though we have applied it many times before. Next, we discuss in detail how to numerically minimize the full free energy functional self-consistently. Again, this section, while targeted at the example of chiral \( p \)-wave superconductivity, can easily be adapted to any pairing symmetry.

2.2.1 Analytical arguments

As mentioned above, the first step always has to be a close look at the resulting expression of the free energy functional. Some common forms are compiled in Sec. A.1. For example, in Sec. 5.1 the effective domain wall coupling term is identified in the free energy functional without having to take any further steps beyond its proper formulation.

Ultimately, however, the standard way to minimize a functional is the calculus of variation [136]. For the Ginzburg Landau functional of a one-component superconductor, in principle we have to vary with respect to the real and imaginary part of the complex order parameter. However, it can be shown straightforwardly that this corresponds to varying
with respect to the order parameter and its complex conjugate, treating them as independent variables, see for example Sec. 4.3 in Ref. [5]. For completeness, and repeating the boundary conditions from above, variation results in [42]

\[ \frac{\partial f}{\partial \psi^*} + D \cdot \frac{\partial f}{\partial (D\psi)^*} = 0 \] 
with \( n \cdot (D\psi)_{surf} = \frac{\psi_{surf}}{b} \) \hspace{1cm} (2.36a)

\[ \frac{\partial f}{\partial A} + \nabla \times \frac{\partial f}{\nabla \times A} = 0 \] 
with \( n \times (B - H)_{surf} = 0 \) \hspace{1cm} (2.36b)

where \( b \) is the extrapolation length introduced in Eq. (2.28) and \( H \) is an applied field. The variation with respect to \( \psi^* \) leads to the first Ginzburg Landau equation, while the variation with respect to the vector potential leads to the second Ginzburg Landau equation. The expression for the supercurrent enters through

\[ \nabla \times \frac{\partial f}{\nabla \times A} \propto J. \] \hspace{1cm} (2.37)

This will lead to an important check on the numerical solution, see the discussion below.

However, for a two-component order parameter and more involved additional terms, the safest approach is to do partial integrations until there are no more derivatives left of the quantity with respect to which the variation is performed. This is how the boundary conditions written above in Eq. (2.36) are derived, but such a simple expression does not hold for a more complicated free energy functional. All the terms resulting from the partial integrations make up the proper boundary conditions. These can be analyzed, even without deriving the full Ginzburg Landau equations. This is done for example in Sec. 3.2 where we use selected boundary conditions to support the numerical results.

Furthermore, it can be helpful to do the variation using symbolic computation. This is especially necessary if the expression for the free energy itself has only been found this way in the first place, as discussed above. Because the computer algebra system will treat the order parameter as a proper complex variable (or the functional could not have been formulated this way), it now also has to be tricked by relabelling \( \psi \equiv p_1 \) and \( \psi^* \equiv p_2 \) as two independent variables to proceed. This was done to derive the underlying full boundary conditions for the disk-shaped sample stated in Sec. A.2.

On the other hand, almost always there is some limiting case where the resulting coupled non-linear partial differential equations can be solved, maybe by decoupling them, by linearizing, or by neglecting the vector potential. Also, there are many common solutions to recurring equations, such as the sine-Gordon equation discussed in Sec. 4.1.4 and Sec. 5.1, which can be found in the literature. Even if only a very restricted limiting case can be solved, this can be highly useful as an initial guess in the iterative numerical minimization method described in the next section.

2.2.2 Numerical minimization

In this section we describe the computational method used throughout this thesis to numerically minimize the Ginzburg Landau free energy functional. The full general problem is to minimize a functional depending on 7 functions (the real and imaginary parts of the two order parameter components and the three components of the vector potential), each
Modeling a chiral \( p \)-wave superconductor, of which depends on 3 dimensions. For all the situations considered in this thesis, luckily there are at most two important dimensions, and we only discuss this case in the following. While it is probably not really feasible to solve a complicated fully three-dimensional problem using the method described here, it can in principle be extended to any number of dimensions straightforwardly.

In this section we only describe the underlying method, while details on the numerical parameters for each of the phenomena are listed in Appendix B, together with some specific notes on the implementation of the algorithm.

The computational approach for minimizing a functional has two parts, as described in Sec. 18.2.4 in the German book by Törnig [137], based on which M. Sigrist started using this kind of method. First, the continuous functions and the functional integral are approximated through discretization, resulting in a single high-dimensional functional. Second, this function is minimized. Both steps are discussed separately below.

### Discretization scheme

First, for a system in two dimensions \((x,y)\) on a domain \(x \in [x_{\text{min}}, x_{\text{max}}]\) and \(y \in [y_{\text{min}}, y_{\text{max}}]\), we define a mesh based on a regular grid with uniform step size in the following way. As illustrated in Fig. 2.3 on the left, there are \(n+1\) mesh points in the \(x\)-direction with an iterator \(i \in \{0, 1, \ldots, n\}\), and \(m+1\) mesh points in the \(y\)-direction with an iterator \(j \in \{0, 1, \ldots, m\}\), leading to the step sizes

\[
h = \frac{x_{\text{max}} - x_{\text{min}}}{n} \quad \text{and} \quad s = \frac{y_{\text{max}} - y_{\text{min}}}{m}. \tag{2.38}
\]

The site \((i,j)\) then corresponds to the coordinates \((x_i, y_j) = (x_{\text{min}} + ih, y_{\text{min}} + js)\). This is the most simple mesh possible. In the final section we then discuss the advantages and disadvantages, and comment on other discretization schemes for example based on a nonuniform mesh, an adaptive mesh, or using finite elements.

Next, using as an example a functional \( \mathcal{F} \) of a single function \( g(x,y) \), we first discretize this function on the mesh as \( g_{ij} = g(x_i, y_j) \). The derivatives of this function appearing in the functional are then approximated using a central differences scheme\(^5\), resulting in mean values and derivatives in the middle of each cell (labeled \((i,j)\) according to the lowest indices of its vertices), as illustrated on the top right in Fig. 2.3, given by

\[
m_{ij} = g(x_i + h/2, y_j + s/2) = \frac{g_{ij} + g_{i+1,j} + g_{i,j+1} + g_{i+1,j+1}}{4} \tag{2.39a}
\]

\[
dx_{ij} = \partial_x g(x_i + h/2, y_j + s/2) = \frac{-g_{ij} + g_{i+1,j} - g_{i,j+1} + g_{i+1,j+1}}{2h} \tag{2.39b}
\]

\[
dy_{ij} = \partial_y g(x_i + h/2, y_j + s/2) = \frac{-g_{ij} - g_{i+1,j} + g_{i,j+1} + g_{i+1,j+1}}{2s}, \tag{2.39c}
\]

where now the iterators only are \(i \in \{0, 1, \ldots, n-1\}\) and \(j \in \{0, 1, \ldots, m-1\}\). For a boundary term, additional values are defined. For example, let us consider a situation where the function \( g(x,y) \) is constant on all boundaries except for \( x = x_{\text{max}} \), and where the boundary term only depends on \( g(x,y) \) but not on its derivatives. We then define the

\(^5\) This has a smaller error than a forward or backward scheme, see Ch. 6 in Ref. [138].
2.2. Analyzing the Ginzburg Landau functional

Figure 2.3: The domain is discretized using a simple mesh based on a regular grid with uniform step size. The continuous functions, i.e. the real and the imaginary part of each order parameter component and each component of the vector potential, are discretized on the vertices (blue dots). The functional is approximated by a middle Riemann sum using the mean and difference values in the middle of each cell (red dots), while additional mean values in the middle of the boundary links are introduced for the boundary term (green dots).

mean values in the middle of each link on the right boundary, as illustrated on the bottom right in Fig. 2.3, with only one iterator $j \in \{0, 1, ..., m - 1\}$, resulting in

$$b_j = g(x_n, (j + 0.5)s) = \frac{g_{nj} + g_{n,j+1}}{2}. \quad (2.40)$$

Finally, the full functional integral given by

$$\mathcal{F}[g(x,y)] = \int_{x_{\min}}^{x_{\max}} \int_{y_{\min}}^{y_{\max}} \mathrm{d}x \mathrm{d}y \mathcal{F}[g, \partial_x g, \partial_y g] + \int_{y_{\min}}^{y_{\max}} \mathrm{d}y B[g(x_{\max}, y)] \quad (2.41)$$

is approximated by a middle Riemann sum

$$\mathcal{F}[g(x,y)] \approx hs \sum_{i=0}^{n-1} \sum_{j=0}^{m-1} \mathcal{F}[m_{ij}, dx_{ij}, dy_{ij}] + s \sum_{j=0}^{m-1} B[b_j] \equiv A(g_{ij}). \quad (2.42)$$

This is now a function in the high-dimensional space of $(n + 1) \times (m + 1)$ values $g_{ij}$

$$\mathbb{R}^{(n+1) \times (m+1)} \rightarrow \mathbb{R}$$

$$g \mapsto A(g), \quad (2.43)$$

and can be minimized by any standard method, one of which will be discussed in the next section. We note, however, that we are usually not primarily interested in the minimum value of this function, $A^*$, that is, the minimum value of the free energy, but rather its coordinates $g_{ij}^*$, that is, the shape of the order parameter and vector potential.
One-step relaxed Newton-Jacobi method

The second step is the minimization of the function $A(g)$, that is, solving $\partial A / \partial g_{ij} = 0$. In Sec. B.1 we work out the details of actually performing these derivatives, see Eq. (B.1), describe how they can be computed automatically, and comment on some implementation issues. Here, we describe the underlying algorithm. We only keep one index$^6$ for the vector $g = \{g_i\}$. The minimization then corresponds to solving the $(n + 1) \times (m + 1)$ coupled (but no longer partial differential) non-linear equations

$$a_i \equiv \frac{\partial A}{\partial g_i} = 0. \quad (2.44)$$

Throughout this thesis we use a one-step relaxed Newton-Jacobi method, which we describe here following Ch. 3.2 of the book by Gardan [139], but see also the book by Ortega and Rheinboldt [140] originally from 1970. The advantages and disadvantages of this method are discussed below.

First, we apply the iterative Newton method

$$g^{k+1}_i = g^k_i - J^{-1}a_j, \quad (2.45)$$

where the Jacobian $J_{ij}$ in our case is the symmetric Hessian

$$J_{ij} = H_{ij} = \left( \frac{\partial a_i}{\partial g_j} \right) = \left( \frac{\partial^2 A}{\partial g_i \partial g_j} \right) = H_{ji}, \quad (2.46)$$

which for the finite differences scheme as described above and in the case of only one input function is tridiagonal and strictly diagonally dominant [141]. This Hessian $H_{ij}$ is fully known and does not have to be approximated. In multiple dimensions, the Newton method is conveniently separated into

$$g^{k+1}_i = g^k_i + z_i, \quad (2.47a)$$

$$J_{ji}z_i = -a_j, \quad (2.47b)$$

such that we are left with finding the solutions $z_i$ of the latter, which is a linear problem.

Second, dropping all indices, we use an iterative Jacobi method$^7$ to solve Eq. (2.47b), splitting $J = D - C$ into the diagonal $D$ and the off-diagonal part $-C$, resulting in

$$Jz = (D - C)z = -a \Leftrightarrow z = D^{-1}Cz - D^{-1}a, \quad (2.48)$$

which is then iteratively solved in an $m$-step process according to

$$z = D^{-1}C(D^{-1}Cz - D^{-1}a) - D^{-1}a$$

$$\vdots$$

$$z = -\left[I + \cdots + [D^{-1}C]^{m-1}\right]D^{-1}a. \quad (2.49)$$

---

$^6$ This would be done in any implementation anyway, turning the two-dimensional arrays into one-dimensional arrays through $i + j \cdot (n + 1)$.

$^7$ Following the standard literature [141], because of the properties of our Hessian, this is an appropriate choice.
Finally, combining the primary (or outer) Newton method with the secondary (or inner) one-step Jacobi method, and including a relaxation parameter \( w \), we find

\[
g^{k+1}_i = g^k_i - w \frac{a_i}{\partial a_i/\partial g_i} = g^k_i - w \frac{\partial A}{\partial g_i},
\]

(2.50)

with \( A(g^k) \) depending on all the old values only. For the functional \( F \) given above in Eq. (2.41) and approximated by the Riemann sum given in Eq. (2.42), this corresponds to

\[
g_{ij}^{\text{new}} = \begin{cases} 
  g_{ij}^{\text{old}} - w \frac{\partial F}{\partial g_{ij}} & i < n \\
  g_{nj}^{\text{old}} - w \frac{\partial F}{\partial g_{nj}} + \frac{1}{\pi} \frac{\partial B}{\partial g_{nj}} & i = n.
\end{cases}
\]

(2.51)

The Newton iterations \( k \to (k+1) \) are continued until \( |a_i|^2 < \delta \) for a threshold value \( \delta \).

While this can of course simply be understood as approximating (or ‘preconditioning’) the Hessian by its diagonal in the first place, this detailed analysis demonstrates the actual steps taken. This allows to change the method to other types, and is the required basis to be able to discuss the convergence, stability, applicability etc.

Also, we note that this one-step Newton-Jacobi method is equivalent to the one-step Jacobi-Newton method, while for the \( m \)-step methods this equivalence does not hold [140].

**Discussion**

Above all, the enormous advantage of this discretization scheme and minimization method for our purposes is their extreme simplicity. For example, for the disk-shaped sample considered in Ch. 3, the free energy functional is so complicated it is only really feasible to formulate and prepare it for the numerical minimization using symbolic computation, as discussed in Sec. B.1. Any other considerations only come second to this criterium. In any case, for such a non-linear problem with coupled terms it is difficult to capture its “practical efficiency” through mathematical conditions, see Sec. 3.2.5. of Ref. [139].

The second advantage is the possibility to minimize the functional rather than solve the corresponding equations, in particular with respect to the boundary conditions. We stress that for the algorithm as shown in Eq. (2.51) we do not use direct boundary conditions such as Eq. (2.27) appearing during the variation process. Rather, the additional terms of the free energy are added at the boundary or defect as applicable. With this approach less mesh points are needed near the boundary. As an exception, when the actual value of either the order parameter or the vector potential is known on a mesh point, then this is used. As an example, we consider again the situation at a planar surface with \( n = x \) described above. For full specular scattering with \( g_1 = g_3 \), see Sec. 3.1.3, we find for the perpendicular component \( \eta_\perp|_{\text{surf}} = 0 \). This is implemented as a direct condition \( \eta_{\perp,n} = 0 \). The resulting boundary condition for the parallel component is \( \partial_x \eta_\parallel|_{\text{surf}} = 0 \) such that \( \eta_\parallel|_{\text{surf}} = \text{const} \). However, using this as a direct boundary condition would result in having to set \( \eta_\parallel,n = \eta_\parallel|_{n-1} \). This extends the boundary condition by half a step \( h/2 \) away from the actual boundary, requiring very small step sizes \( h \) for a proper result. On the other hand, if the surface energy \( (g_1 + g_3)|\eta_\parallel|^2 \) is added at the boundary, this condition
is included naturally, but only directly at the boundary, while in addition the full free energy is respected on every mesh point. This procedure is especially straightforward for a component-specific and space-dependent effective critical temperature, simply introducing different values $T_{c,i}$ on different mesh points.

On the other hand, an obvious disadvantage is that this method will only find local minima, but not necessarily the global minimum. In our implementation this is not controlled actively, but only through the starting point (initial guess). We usually implement an iterative scheme on top of the one-step relaxed Newton-Jacobi method, first computing the results for a limit where the results are known (at least approximately), and then slowly varying the essential parameters, taking the previous result as the next initial guess. This emphasizes the importance of closely analyzing the functional analytically first.

An important overall check is comparing the current derived directly from the vector potential $j \propto \nabla \times (\nabla \times A)$ to the current obtained through the variation of the free energy with respect to the vector potential $\partial f / \partial A$. The latter usually gives a more precise result, because it only contains first-order derivatives, but the two should coincide for a dense enough mesh. In addition, while the full analytical results are usually restricted to limiting cases only, even if simple symmetry arguments are found, such as described in Sec 3.2.3, these can be used to check the numerical results a-posteriori.

Another aspect not discussed so far is gauge-invariance. This is not controlled actively throughout the mesh in this method, but only through proper initial and boundary conditions. We usually adopt a ‘minimal gauge’, where the vector potential only contains the minimally necessary information and is fixed far away from the boundary or defect. However, there are actively gauge-controlling methods, see the review by Du [142] and references therein, or the manual-style paper by Milošević and Geurts [143] and references therein, the approach of which was used for example in Ref. [100].

Finally, we also comment on different discretization schemes. While a non-uniform mesh (different step sizes), an adaptive mesh (changing during the minimization), or even a finite-elements scheme would be highly desirable, these again make the whole algorithm more complicated, interfering with the automatic preparation described in Sec. B.1. As a reference, however, we mention the finite-elements scheme as applied in the group of Babaev to compute for example the results in Ref. [144], and we refer to other work of that group for details on their numerical approach. Their scheme would have been useful to compute the structure of the half-quantum vortex in Sec. 5.2, see also discussion in Sec. B.2.3, while for all other projects the uniform regular mesh described above was clearly sufficient.

To summarize, here we have described a simple yet powerful numerical method for the minimization of the Ginzburg Landau free energy functional, which is used throughout this thesis. It is straightforward to implement and running such a program is feasible on any advanced high-performance workstation, making the full parameter ranges of various phenomena accessible, such as those described in the following chapters.
Phenomena
Magnetic flux may appear spontaneously at the surface of chiral $p$-wave superconductors, but no experimental evidence has been found so far, as reviewed in Sec. 1.4.1. Here we study the detailed shape of the flux pattern at the surface of a disk-shaped sample, including self-screening, using the Ginzburg Landau formalism. Different surface types are analyzed by systematically scanning through a range of boundary conditions. Moreover, specific features of the electronic band structure are included, which affect the coefficients in the free energy functional.

In this chapter, we first describe the phenomenological model in detail. The disk-shaped sample geometry is introduced and the treatment of the band structure effects using phenomenological parameters is explained. The theoretical aspects of the boundary conditions are derived and we show how the relevant form of the surface term can be understood as a component-specific and space-dependent effective critical temperature. Special attention is paid to the practical aspects of setting the surface parameters, also relating the values considered here to the surface types described in previous work.

We then present a detailed analysis of the full results obtained from numerically minimizing the free energy and tuning all the parameters described above. Selected analytical results from a direct analysis of the free energy are also included. We find that the flux pattern is extremely sensitive to all the considered parameters and conclude that it is not a universal feature of chiral $p$-wave superconductivity. Finally, we comment on the temperature dependence of the flux pattern and on the flux at impurities in the appendix to this chapter.

This chapter is based on S. B. Etter, A. Bouhon, and M. Sigrist, in review for PRB [arXiv:1710.07998].
3.1 Phenomenological model

There are three essential aspects entering our revisit of the spontaneous surface flux pattern: the disk-shaped geometry, the treatment of band structure effects, and the description of surface properties. In this section we discuss each aspect in turn to formulate our phenomenological model, including references and reviews of related previous work as applicable. Finally, we comment on how to systematically analyze the Ginzburg Landau free energy functional for the identified parameters.

3.1.1 Disk-shaped sample

We consider the surface of a disk-shaped sample. In order to avoid the discussion of boundary effects at the top and bottom surfaces, the two-dimensional disk is extended to a cylinder infinite along the crystal c-axis, see Fig. 3.1 on the left, and assuming translational invariance along the c-axis. The radius is chosen such that \( R \gg \xi_0, \lambda \). Even in the case of a Fermi surface anisotropy we assume at least \( C_4 \) symmetry such that a quarter disk, as shown in Fig. 3.1 on the right, contains all information.

This circular geometry includes at once all possible surface orientations with a normal vector in the basal plane, and additionally allows us to study the effect of surface curvature. Furthermore, there is a correspondence of the result at a given angle in this disk-shaped sample to the result for a planar surface tangent to that angle. For the analytical results, we can directly consider the limit \( R \to \infty \), while for the numerical results the correspondence of course strongly depends on the considered radius. This basically gives us access to the result for any surface orientation.

It is natural to use polar coordinates \( r = (r, \theta, z) \) for this geometry, where \( r \in [0, R] \) and \( \theta \in [0, \pi/2) \). We define \( \theta = 0 \) and \( \theta = \pi/2 \) as the crystal a- and b-axis, respectively. With the translational invariance along the c-axis we ignore any z-dependence such that the order parameter is \( \eta(r) = \eta(r, \theta) \) and the vector potential is \( A(r) = (A_r(r, \theta), A_\theta(r, \theta), 0) \) with a partial gauge. The magnetic flux only has a z-component, \( B(r) = B_z(r, \theta) \hat{z} \), with the boundary condition \( B_z(R, \theta) = 0 \) in the absence of an external field as assumed here.
3.1. Phenomenological model

3.1.1 Continuum limit

The ratio $K_1/K_2$ for different band fillings in a square-lattice tight-binding model for the dominant $\gamma$-band [104]. At small filling, i.e. in the continuum limit, the isotropic limit $K_1/K_2 \to 3$ is recovered. Current reversal occurs below the threshold $K_1 = K_2$ (dashed). The filling of Sr$_2$RuO$_4$ for chiral $p$-wave pairing is indicated. [Based on code by A. Bouhon, parameters of Ref. [61]].

Following Sec. 2.1.1, here it is convenient to use the representation of the order parameter accessing the components parallel and perpendicular to the surface. For the disk geometry this means

$$\eta = (\eta_\perp, \eta_\parallel) = (n \cdot \eta, (n \times \eta) \cdot \hat{z}) = (\eta_r, \eta_\theta) = (\eta_r \cos \theta + \eta_\phi \sin \theta, -\eta_r \sin \theta + \eta_\phi \cos \theta),$$

(3.1)

with the normal $n = \hat{r} = \cos \theta \hat{x} + \sin \theta \hat{y}$. Additionally, the phase winding number $N = \pm 1$ and the homogeneous bulk value $\eta_b$ are introduced explicitly as

$$\eta = (\eta_\perp, \eta_\parallel) = \eta_b(u, iv)e^{iN\theta},$$

(3.2)

with the still complex and fully space-dependent functions $u(r, \theta)$ and $v(r, \theta)$. The homogeneous bulk phase is then given by $(\eta_\perp, \eta_\parallel) = \eta_b(1, \pm i)e^{\pm i \theta}$.

3.1.2 Band structure effects

Any material properties, including the band structure effects, enter the Ginzburg Landau free energy functional through of the expansion coefficients, as discussed in Sec. 2.1.2. An instructive and for our purpose relevant example is the ratio $K_1/K_2$, which is crucial for the behavior of the order parameter near the surface and determines the direction of the edge current. Bouhon and Sigrist noticed that this ratio varies strongly with band filling [104] and is directly related to the proposed current reversal, as reviewed in Sec. 1.4.1. The ratio changes from $K_1/K_2 = 3$ for an isotropic (circularly cylindrical) Fermi surface to values $K_1/K_2 < 1$ for higher filling, as illustrated in Fig. 3.2. For chiral $p$-wave pairing, Sr$_2$RuO$_4$ would have a ratio $K_1/K_2 \approx 0.69$, based on parameters from Bergemann et al. [61], compatible with a similar ratio of 0.71 mentioned by Lederer et al. [97].

Here, we therefore focus on the coefficients $K_1$ and $K_2$. While varying the ratio $K_1/K_2$, we still fix $K_1 + K_2 = K = \text{const}$, such that, by choosing the coherence length $\xi_0^2 = $...
Spontaneous surface flux pattern

\((K_1 + K_2)/(2aT_c)\) as the unit length, the basic length scale of the order parameter remains constant, as discussed in Sec. 2.1.2. We note, however, that in a proper lattice model the parameter \(K = K_1 + K_2\) also varies with band filling. We keep the standard isotropic ratios for all other coefficients \((b_1 = 3/8, b_2 = -b_3 = b/4\) and \(K_3 = K_4 = K/4\)), for simplicity and to accentuate the main effects. In our systematic analysis we cover the range \(K_1/K_2 \in [1/3, 3]\), such that ultimately \(K_1 \leftrightarrow K_2\) are switched compared to the isotropic value.

However, as will become apparent from a close analysis of the free energy functional, see for example Eq. (3.13) or Fig. 3.13 and the surrounding discussion, the resulting magnetic flux scales more like \((K_1 - K_2)/K \in [-0.5, 0.5]\) rather than the ratio \(K_1/K_2\). While the latter is a more convenient and dimensionless short form, and will always be used as the label, for the numerical minimization we vary the former in equal steps, see also Sec. B.2.1 for the computational details and Fig. B.1.

3.1.3 Surface types

To go beyond specular scattering, the general situation at the surface can be described by the surface term introduced in Eq. (2.26). Different surface properties enter through the choice of the corresponding expansion coefficients \(g_i\). For the disk geometry we rewrite the surface term for the normal vector \(\mathbf{n} = (\cos \theta, \sin \theta)\) and using the representation of the order parameter introduced above, we find

\[
\mathcal{F}_{\text{surf}}[\eta_\perp, \eta_\parallel] = \int \mathcal{R} \mathcal{d} \theta \left[ g_1 |\eta_\perp|^2 + \left( g_3 \cos^2(2\theta) + \frac{g_4}{2} \sin^2(2\theta) \right) \left( |\eta_\perp|^2 - |\eta_\parallel|^2 \right) \right. \\
- \left( g_3 - \frac{g_4}{2} \right) \sin(2\theta) \cos(2\theta) \left( \eta_\perp \eta_\parallel^* + \eta_\perp^* \eta_\parallel \right) \right].
\]  

These angular dependences appear on top of the possible angular dependences of the \(g_i\) themselves, which we, however, neglect here, assuming translational invariance along the surface. For a straight surface with \(\theta = 0\) we recover Eq. (2.30). Inserting the relation \(g_3 = g_4/2\) leads to a simple form of the surface term, where all angular dependences disappear,

\[
\mathcal{F}_{\text{surf}}[\eta_\perp, \eta_\parallel] = \int \mathcal{R} \mathcal{d} \theta \left[ (g_1 + g_3) |\eta_\perp|^2 + (g_1 - g_3) |\eta_\parallel|^2 \right].
\]

While strictly valid only for isotropic symmetry, we will use this form for the boundary conditions in the following, in order to reduce the number of variable parameters in the model. This form can be understood as a component-specific and space-dependent effective critical temperature, see also Eqs. (2.31) and (2.32),

\[
T_{e_i}^{\text{eff}}(r) = T_c - T_{e_i} \delta (r - R),
\]

with the perpendicular and parallel surface critical temperatures

\[
T_{e_\perp} = \frac{g_1 + g_3}{a} \quad \text{and} \quad T_{e_\parallel} = \frac{g_1 - g_3}{a},
\]

and assuming vacuum for \(r > R\).
3.1. Phenomenological model

The extrapolation length at the surface for a suppressed but finite component of the order parameter can be extracted a-posteriori from the results by adapting Eq. (2.28) to our geometry, where now $i = (\perp, ||)$,

$$\frac{1}{b_i} = \left| \frac{\partial_i \eta_i}{\eta_i} \right|_{r=R}. \tag{3.7}$$

**Scanning the surface coefficients**

Here, we address the more practical aspects of how to choose the coefficients $g_1$ and $g_3$, or $T_{c\perp}$ and $T_{c||}$, respectively, and which surface properties they describe.

First, we note that $g_1$ describes the effect of the surface on the whole order parameter, while $g_3$ captures how the two components are affected differently. At the surface, $T_{c\perp}^{\text{eff}} \leq T_{c\parallel}^{\text{eff}} \leq T_c$, leading to $g_1 \geq |g_3|$. In addition, we only consider cases where the perpendicular effective critical temperature is lower, $T_{c\perp}^{\text{eff}} \leq T_{c\parallel}^{\text{eff}}$, corresponding to $g_3 \geq 0$. The case $g_1 = g_3 = 0$ corresponds to a ‘virtual boundary’ in the interior of the superconductor without any effect on the order parameter and is excluded. The range $G$ of considered surface coefficients $g_i$ is therefore given by

$$G = \{ g_i \mid (g_1 \geq g_3 \geq 0) \land (g_1 + g_3 > 0) \land (g_4 = 2g_3) \}. \tag{3.8}$$

In the following, we focus on the boundaries of this range. An overview is given in Fig. 3.3, with $G$ shaded gray, and introducing the three main boundary regions A, B, and C, with an additional one to circumvent the origin, D. Three representative cases of particular interest are highlighted and illustrated by insets.
Spontaneous surface flux pattern

**Region A** The identity $g_1 = g_3$ is the upper bound and describes specular scattering. Here $T_{c\parallel} = 0$ and $\eta_{\parallel}$ is little affected. As $T_{c\perp}$ increases, $\eta_{\perp}$ is being suppressed more and more at the surface. This in turn leads to a slight increase of $\eta_{\parallel}$. In the limit $g_{1,3} \to \infty$, $\eta_{\perp}$ is fully suppressed and we use the direct boundary condition $\eta_{\perp}|_{R = 0}$.

**Region B** Along this region $\eta_{\perp}|_{R = 0}$ remains fully suppressed, while now $\eta_{\parallel}$ is also being suppressed more and more. The limit $(g_1 \to \infty, g_3 = 0)$ describes full pair breaking. Both components are fully suppressed and we also use the direct boundary condition $\eta_{\parallel}|_{R = 0}$.

**Region C** The $g_1$-axis is the lower bound. With $g_3 = 0$, $T_{c\perp} = T_{c\parallel}$. Both order parameter components are suppressed, but not completely, leading to a finite extrapolation length for both. A fine-tuned case is highlighted, at which the radially integrated flux vanishes without obvious reasons from a mathematical or symmetric point of view, discussed in detail in Sec. 3.2.1 below.

Both boundaries B and C describe effects of surface roughness or diffuse scattering. The difference is the full suppression of $\eta_{\perp}$ on B, while it is finite on C.

**Region D** Introduced to connect back to region A and circumvent the origin.

To systematically scan the surface parameters, we numerically compute the results for 31 cases $s \in \{0, \ldots, 30\}$ along the boundary (black dots in Fig. 3.3), quantitative details for which are given in Table B.1 in Sec. B.2.1, where we also describe the cut-offs introduced for $g_i \to \infty$ at which we use the direct boundary conditions $\eta_i(R) = 0$.

**Review of other theoretical work**

Here we briefly comment on the previous theoretical discussion covering various surface types. The commonly investigated situations are planar surfaces with specular scattering. Assuming full rotational symmetry around the $c$-axis, a peak value for the surface flux of the order of 1 mT has been obtained by Matsumoto and Sigrist [95]. This is often used as a reference in experimental investigations in Sr$_2$RuO$_4$ [90–92]. This case corresponds to our results at $s = 8$ for $K_1 = 3K_2$, where $\eta_{\perp} = 0$ at the boundary.

While in our approach we also cover ranges with finite $\eta_{\perp}$ (regions A and C), most treatments such as Refs. [96, 98, 145] impose the condition of full suppression of the perpendicular component $\eta_{\perp}$, following the pioneering work by Ambegaokar, de Gennes and Rainer [146]. These studies are therefore located along the region B. Ashby and Kallin [96] considered the special case of ‘diffuse’ scattering with an extrapolation length $b_{\perp} = 0.54$ as derived by Ambegaokar et al. We can identify this limit from our results a-posteriori (see Fig. 3.5), and find that it is approximately $s = 11$. Their analysis also includes ‘full pair breaking’ at the surface, which is our case $s = 18$.

A further type of boundary conditions are normal metallic surface layers with finite extrapolation lengths for both order parameter components, as discussed previously by Lederer et al. [97]. They have commented on the case $K_1 = K_2$ for identical extrapolation lengths $b_{\perp} = b_{\parallel}$. This is equivalent to our discussion of $K_1 = K_2$ and $g_3 = 0$ in region C. Recently, Bakurskiy et al. [147] have extended the discussion to different surface layers of varying roughness and metallic behavior. These works support our consideration of region C where both order parameter components remain finite at the surface. While they treat the actual surface type in a more controlled way than here, they do not include self-screening.
3.2 Systematic analysis

While these considerations have all been for planar surfaces, very small-size disk-shaped
samples have been considered by Huang and Yip [98] and by Suzuki and Asano [103].

3.1.4 Summary

To summarize, the ratio $K_1/K_2$ of the gradient term coefficients incorporates the relevant
band structure effects, and the two surface coefficients $g_1$ and $g_3$ allow us to tune between
different surface types, which are scanned systematically for a comprehensive overview.

Using polar coordinates for the disk-shaped sample, the flux depending on all these aspects
can be written as

$$B_z(r, \theta, K_1/K_2, g_1, g_3).$$

(3.9)

The two surface coefficients are grouped into 31 surface types $s$ as described above, such
that $B_z(r, \theta, K_1/K_2, s)$.

The detailed shape of the flux pattern, including self-screening, is computed numerically
by minimizing the Ginzburg Landau functional using the method described in Sec. 2.2.2.
In Appendix B, specific information about the implementation is provided. In particular,
all parameters entering the numerical analysis are listed in Sec. B.2.1.

In addition to the computational results, while an analytical solution of the full model is not
feasible, we can already gain useful information from studying the boundary conditions for
the order parameters and the equation for the angular current, obtained from the variation
of the free energy as described in Sec. 2.2.1. The full expressions are stated in Sec. A.2.
The resulting forms for some specific cases are included directly in the discussion of the
results below and serve as a support for our numerical results.

3.2 Systematic analysis

In this section we present the computational results together with analytical arguments
to arrive at a comprehensive description of the different situations at the surface. First,
we consider only the isotropic limit without angular dependence beyond the phase wind-
ing and discuss the three representative cases highlighted in Fig. 3.3. This allows us to
disentangle the influence of the sample surface from the impact of band structure effects.

Second, the effect of tuning the ratio $K_1/K_2$ is analyzed in the specular scattering limit,
to illustrate the band structure effects for a fixed surface type. Finally, the discussion is
extended to the full range of all parameters. Scanning all surface types $s$ and all ratios
$K_1/K_2$ over the ranges described above, we analyze selected extracted quantities below,
while the detailed results $B_z(r, \theta)$ at each $(s, K_1/K_2)$ are presented in the appendix to this
chapter, Sec. 3.4.3.

3.2.1 The isotropic limit

We start with the isotropic limit $K_1/K_2 = 3$, where the magnetic flux has no angular
dependence, $B_z(r)$. First, we discuss the three representative surface types $s = \{8, 18, 23\}$,
as highlighted in the overview Fig. 3.3, and then analyze the extrapolation length extracted
a-posteriori for all surface types.
The three representative surface types

In Fig. 3.4 we show the results for the three representative surface types full specular scattering \((s = 8)\), full pair breaking \((s = 18)\) and the fine-tuned case \((s = 23)\), computed for a disk of radius \(R = 40\xi_0\), which is on the order of a few \(\mu m\) \([62]\).

The order parameter components \(\eta_\perp\) and \(\eta_\parallel\) are shown in the top plot of Fig. 3.4. In the isotropic limit, we can choose a gauge where \(A_r = 0\) everywhere and \(A_\theta(r)\) with no angular dependence, such that \((\eta_\perp,\eta_\parallel) = |\eta_\parallel|(u(r),iv(r))e^{iN\theta},\) where \(u(r)\) and \(v(r)\) are real and there is no global phase. There is no angular dependence except for the phase winding with \(\partial_\theta \eta_i = iN\eta_i\) for each component.

From the full form of the boundary conditions, Eq. (A.11), and plugging in all ratios for the isotropic limit, we then find

\[
\begin{align}
-4(g_1 + g_3)\eta_\perp &= 3K \partial_r \eta_\perp + K\frac{\eta_\perp}{R} - i \left(\gamma A_\theta - \frac{N}{R}\right) K\eta_\parallel \\
&= 0 \quad \text{at } r = R,
\end{align}
\]

\[
\begin{align}
-4(g_1 - g_3)\eta_\parallel &= K \partial_r \eta_\parallel - K\frac{\eta_\parallel}{R} - i \left(\gamma A_\theta - \frac{N}{R}\right) K\eta_\perp \\
&= 0 \quad \text{at } r = R.
\end{align}
\]

For the specular scattering surface type \(s = 8\) we set \(\eta_\perp(R) = 0\) explicitly. For a disk of finite radius \(R\), the parallel component \(\eta_\parallel\) then does not have a vanishing slope at the surface, but a positive one due to the curvature

\[
\partial_r \eta_\parallel \bigg|_R = \frac{\eta_\parallel(R)}{R} > 0.
\]

This is in agreement with Huang and Yip \([98]\) and Suzuki and Asano \([103]\) who considered very small disk-shaped samples. For the full pair breaking case \((s = 18)\) we set \(\eta_\perp|_R = \eta_\parallel|_R = 0\) explicitly and both components are suppressed to zero. In the fine-tuned case \((s = 23)\) both components are suppressed but still have a finite extrapolation length on the order of the coherence length.

The magnetic flux \(B_z(r)\) is shown in the middle plot of Fig. 3.4. In the specular scattering case there is a single positive flux peak with the shape and value in agreement with Matsumoto and Sigrist \([95]\) and Ashby and Kallin \([96]\). In the full pair breaking case the flux has a similar peak shape, but with the maximum value reduced and the onset of the peak pushed inside, away from the surface, in agreement with Ashby and Kallin. In the fine-tune case, however, the flux has a different shape. The flux points in the other direction at the surface and then crosses to a positive value, from which it vanishes in the bulk, with both extremal values reduced compared to the two previous cases. Most interestingly, however, is the radially integrated value. It vanishes almost completely in this fine-tuned case. It is positive and negative, respectively, in the two adjacent surface types \(s = 22\) and \(s = 24\), and by interpolation it would vanish exactly at a case \(s \approx 22.8\), while locally the flux remains finite.

In the bottom plot of Fig. 3.4 we show the surface current \(J_\theta(r)\). The radial current \(J_r\) vanishes everywhere in the isotropic limit. The total angular current can be split into an ‘edge’ or ‘source’ part and a ‘screening’ part, defined such that both vanish in the bulk, far away from the surface. From the full equation for the angular current, Eq. (A.14),
Figure 3.4: Results for the three representative surface types full specular scattering \((s = 8)\), full pair breaking \((s = 18)\) and the fine-tuned case \((s = 23)\) in the isotropic limit \(K_1/K_2 = 3\). Shown are the absolute value of the order parameter components \(\eta_{\perp}\) and \(\eta_{\parallel}\), the magnetic flux \(B_z\), and the total current at the surface \(J_\theta\), with the ‘edge’ and the ‘screening’ parts indicated as defined in Eq. (3.12).
Spontaneous surface flux pattern

which is not restricted to the surface, we find

\[ \frac{2}{c\gamma K} J_{\theta,\text{edge}}(r) = \Im \left[ \partial_r \eta_{\parallel} \eta_{\parallel}^* - \eta_{\perp} \partial_r \eta_{\parallel}^* \right] \]

\[ \frac{2}{c\gamma K} J_{\theta,\text{screen}}(r) = \frac{4}{r} \Im \left[ \eta_{\perp} \eta_{\parallel}^* \right] - \left( \gamma A_0 - \frac{N}{r} \right) \left( |\eta_{\perp}|^2 + 3 |\eta_{\parallel}|^2 \right) \]

(3.12a)

(3.12b)

again plugging in all ratios for the isotropic limit and using the minimal gauge described above. In the specular scattering case, \( J_{\text{edge}} \) has a positive maximum right at the surface and decreases into the disk, on the order of the coherence length. The screening current \( J_{\text{screen}} \) is negative at the surface and has a peak slightly inside the disk, away from the surface, and extends on the wider scale of the screening length (by a factor of \( \kappa = 2.6 \)). The behavior in the full pair breaking case is basically the same, but with the onset pushed inside the sample and both current parts vanishing at the surface. Plugging the direct boundary condition \( \eta_{\perp}(R) = \eta_{\parallel}(R) = 0 \) at the surface into the expression for the current above, we indeed find \( J_{\theta}(R) = 0 \) at the surface. As we will see below, this even holds for any ratio \( K_1/K_2 \). For the fine-tuned case, however, the behavior is quite different. The basic shape looks the same as before, just inverted, with the surface current negative and a positive peak further inside the sample. However, the screening part is small everywhere, especially near the surface, such that the total current and the edge part almost coincide.

**Extrapolation length for all surface types**

The extrapolation lengths \( b_i \) for the two order parameter components can be extracted a-posteriori from the numerical results using Eq. (3.7) above. The result for the the isotropic limit is shown in Fig. 3.5, now for all surface types \( s \). Here, the extrapolation length is the same all around the disk, while in general it may be angular dependent.

For the region A, describing specular scattering, \( b_{\parallel} \) diverges, while \( b_{\perp} \) decreases as \( \eta_{\perp} \) is suppressed at the surface, until \( b_{\perp} = 0 \) for the full specular scattering (\( s = 8 \)). The slope of \( b_{\perp} \) when approaching this limit supports our choice of the cut-off \( g_0 \), as introduced in Sec. B.2.1 and mentioned above, at which we explicitly set \( \eta_{\perp}|_R = 0 \). For the region B, \( b_{\parallel} \) also decreases as \( \eta_{\parallel} \) is suppressed, while \( b_{\perp} = 0 \) remains fully suppressed, until both \( b_{\perp} = b_{\parallel} = 0 \) in the full pair breaking limit (\( s = 18 \)). Again, the slope approaching this limit supports the choice of \( g_0 \). Along the region C, both extrapolation lengths increase again. The parallel \( b_{\parallel} \) is always smaller than \( b_{\perp} \) by about 1/3. This can be seen from the boundary condition Eq. (3.10) above with \( g_3 = 0 \) and up to corrections because of curvature and self-screening. Finally, closing the triangle along D, \( b_{\perp} \approx \text{const} \) because \( g_1 + g_3 = 2g_m = \text{const} \), while \( b_{\parallel} \) increases until divergence.

We have also indicated the specific extrapolation length \( b_{\text{diff}} = 0.54 \) called “diffuse reflection” by Ambegaokar et al. [146] and examined within a Ginzburg Landau framework by Ashby and Kallin [96]. Our surface type \( s = 11 \) is very close to this case and the corresponding results for the flux pattern are in agreement with theirs.

**3.2.2 The specular scattering limit**

To demonstrate how the band structure effects enter our phenomenological model, we now study the effect of changing the ratio \( K_1/K_2 \) for the specular scattering limit (\( s = 8 \)).
3.2. Systematic analysis

Figure 3.5: Extrapolation lengths $b$ of the two order parameter components $\eta_\perp$ (solid) and $\eta_\parallel$ (dashed) in the isotropic limit $K_1/K_2 = 3$ for all surface types. The boundary regions A, B, C, and D, the three representative cases $s \in \{8, 18, 23\}$ (see Fig. 3.3) and the specific extrapolation length $b = 0.54$ for the “diffuse reflection” [146] are indicated.

In Fig. 3.6 we show the flux pattern for different ratios $K_1/K_2$ going from the isotropic limit $K_1/K_2 = 3$ (upper left) to the inverted value $K_1/K_2 = 1/3$ (lower right). Only a quarter disk is shown due to the $C_4$ symmetry. The radius is $R = 40\xi_0$ and the angles $\theta = \{0, \pi/2\}$ correspond to the basal plane crystal axes, with $\{0, \pi/4\}$ corresponding to the orientations called ‘straight’ and ‘zig-zag’ by Bouhon and Sigrist [104]. Concerning the color scheme, deep blue is $\min B_z \equiv B_\downarrow < 0$, deep red the corresponding positive value $-B_\downarrow > 0$ and yellow is $\max B_z \equiv B_\uparrow > -B_\downarrow > 0$. Both the minimal and maximal value are taken over all parameters and surface types, $(r, \theta, K_1/K_2, s)$, but both occur for the specular scattering $(s = 8)$ at the inverted ratio $K_1/K_2 = 1/3$, and at the angles $\theta = \pi/4$ and $\theta = 0$, respectively.

To discuss the results for the magnetic flux pattern as shown in Fig. 3.6, we start with the isotropic limit $K_1/K_2 = 3$ (upper left). This density plot shows exactly the same result as the curve for $s = 8$ in the middle plot of Fig. 3.4. For any ratio $K_1/K_2$ away from the isotropic limit, the flux pattern becomes angular dependent. Decreasing the ratio, the angular dependence becomes more and more pronounced. At $\theta = \{0, \pi/2\}$, the direction of the basal plane crystal axes, the value of the flux increases (in agreement with Ashby and Kallin [96]), while it decreases at the diagonal $\theta = \pi/4$. The result at the ratio $K_1 = K_2$ does not have any distinct properties. However, at a lower ratio $K_1/K_2 \approx 2/3$, a region of negative flux appears at the angle $\theta = \pi/4$, offset from the surface such that a ring of positive flux still goes around the whole disk. At an even lower ratio $K_1/K_2 \approx 0.54$, this region of negative flux extends to the surface and thus the angular current becomes negative at the diagonal $\theta = \pi/4$. This confirms the current reversal proposed by Bouhon and Sigrist [104], also for self-consistent solution to the full Ginzburg Landau free energy functional. Their analysis, however, suggested that the current reversal should appear for
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Figure 3.6: The magnetic flux $B_z(r, \theta)$ for the specular scattering limit $s = 8$ at different ratios $K_1/K_2$. Negative flux is blue, with deep blue being the minimum $B_\downarrow$. The corresponding positive value $-B_\downarrow$ is colored deep red and the maximum $B_\uparrow$ is yellow. Details for the subplot $K_1/K_2 = 1/3$ (bottom right) with current reversal are shown in Fig. 3.7.

all ratios $K_1/K_2 < 1$, while here we find that the region of negative flux first appears at a lower ratio than that, and the negative surface current only at an even lower value. This is because of the curvature of the surface leading to noticeable effects for the disk of finite size. From the full equation for the angular current, Eq. (A.14), now for specular scattering with $\eta_\perp(R) = 0$, and at the surface $r = R$, we find for $\theta = 0$ and $\pi/4$

$$
\frac{J_\theta}{2c\gamma} = \Im \left[ K_3 \partial_r \eta_\parallel \eta_\perp^* - K_1 \eta_\parallel \frac{\partial \eta_\perp^*}{R} \right]_{r=R,\theta=0} - \gamma A_\theta K_1 |\eta_\parallel|^2 \tag{3.13a}
$$

$$
\frac{J_\theta}{c\gamma} = \Im \left[ (K_1 - K_2) \partial_r \eta_\parallel \eta_\perp^* - \tilde{K} \eta_\parallel \frac{\partial \eta_\perp^*}{R} \right]_{r=R,\theta=\pi/4} - \gamma A_\theta \tilde{K} |\eta_\parallel|^2 \tag{3.13b}
$$

where $\tilde{K} = K_1 + K_2 + 2K_3 = K + 2K_3$ is constant when tuning $K_1/K_2$. For a straight surface $R \to \infty$, and when $K_1 = K_2$, the ‘source’ part of the second equation vanishes. Therefore, the ‘screening’ part also vanishes and there is current reversal for any $K_1 < K_2$, as proposed by Bouhon and Sigrist. The precise behavior for finite $R$ cannot be inferred from the boundary condition above, it is only accessible from a full self-consistent solution of the complete model. We have, however, also analyzed the results for a disk of larger radius $R = 240\xi_0$ and find that the negative flux and surface currents do appear at higher ratios, closer to the limit $K_1 = K_2$.

Finally, at the inverted ratio $K_1/K_2 = 1/3$, the angular dependence of both the absolute value and the direction of both the flux and the angular current is most pronounced. This result is shown in detail in Fig. 3.7 with both a density plot of the flux pattern and a vector plot of the full current $\mathbf{J} = \{J_r, J_\theta\}$. The direction of the current pointers is $\hat{\mathbf{J}}$, but their size is scaled by $|\mathbf{J}|^{1/3}$ to better illustrate the flow by enhancing the small values.
3.2. Systematic analysis

Finally, we systematically analyze the flux pattern for the whole range of surface types $s$ and ratios $K_1/K_2$ as defined above. The full results for the detailed shape of the flux pattern are shown in the appendix to this chapter, Sec. 3.4.3, with a density plot $B_z(r, \theta)$ for each case. Here, we focus on the presence of current reversal, the radially integrated flux, and the total flux. The corresponding quantities, extracted from the full results, are shown in Figs. 3.8 and 3.9. The vertical axis lists the 31 surface types $s$ and along the horizontal axis the ratio $K_1/K_2$ changes from the isotropic value $K_1/K_2 = 3$ (top) to the fully inverted value $K_1/K_2 = 1/3$ (bottom). However, equal steps are taken in $(K_1 - K_2)/(K_1 + K_2)$, see the numerical details in Sec. B.2.1.

Symmetry arguments

Let us start by mentioning two for our purpose useful symmetries of the magnetic field. The first concerns its symmetry properties in real space, while the second describes a symmetry concerning the tuning parameters from the Ginzburg Landau functional.

First, the arguments of the Ginzburg Landau functional $\eta$ and $(A_r, A_\theta)$, and the derived magnetic quantities $B_z$ and $(J_r, J_\theta)$, are periodic in $\pi/2$, because we still assume an underlying $C_4$ symmetry. In addition, each function $^1$ is even [or odd] in the angular variable with respect to the basal plane crystal axes at $\theta = 0$ and $\theta = \pi/2$, and the angular derivative $\partial_\theta$ [or the function value] at those angles is zero. Therefore $^2$, the functions are also

---

1 For the vector potential this naturally only holds in a proper gauge.
2 A function $f(x)$ periodic in $P$, $f(x) = f(x+P)$, and even or odd, $f(x) = \pm f(-x)$, is also even or odd with respect to $P/2$ because $f(x) = f(x-P) = \pm f(P-x) \Leftrightarrow f(P/2 + \lfloor x - P/2 \rfloor) = \pm f(P/2 - \lfloor x - P/2 \rfloor)$. 

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even [or odd] with respect to the diagonals $\theta = \pi/4$ and $\theta = 3\pi/4$, and $\partial \theta$ or [or the function value] is zero also at $\theta = \pi/4$. Consequently, the functions can be expanded as Fourier series in $\cos(4n\theta)$ [or $\sin(4n\theta)$]. For the magnetic quantities, the flux $B_z$ and the angular current $J_\theta$ are even, while the radial current $J_r$ is odd. In particular, $B_z$ can be expanded in $\cos(4n\theta)$, which is used below, and see Sec. B.2.1 with Fig. B.2.

Second, due to symmetries of the free energy\(^3\), the flux is an odd function of the Ginzburg-Landau coefficients in the following sense

$$ B_z(r, \theta, K_1/K_2, g_1, g_3 = 0) = -B_z(r, \theta, K_2/K_1, g_1, g_3 = 0). \tag{3.14} $$

In particular, it vanishes identically when $K_1 = K_2$ and $g_3 = 0$ (see also Refs. [96, 97]).

Current reversal

Extending the discussion of the current reversal to all surface types $s$ and all ratios $K_1/K_2$, in Fig. 3.8 (a) we analyze the combinations of current directions of the angular current at the surface, $J_\theta(R)$, comparing the direction at the crystal axis and at the diagonal, $\{\text{sgn} J_\theta(0), \text{sgn} J_\theta(\pi/4)\}$. Each sign may be positive (+), negative (−), or zero (0). While it can be shown that the angular current vanishes identically at the surface for some of the cases, the zero sign is obviously never reached exactly numerically. We therefore introduce a cut-off $|J_\theta| < 10^{-4}$, for which we label the sign 0. For our numerical results $J_\theta(R, 0) \geq J_\theta(R, \pi/4)$, such that only 6 of the 9 possible sign combinations appear. Those can be grouped as three equal-sign combinations, and three current-reversed combinations. While the combinations $\{+, 0\}$ and $\{0, -\}$ should appear at every transition from $\{+, +\}$ to $\{+, -\}$ and $\{-, -\}$ to $\{+, -, -\}$, respectively, such fine-tuned results are rarely captured and the few cases labeled $\{+, 0\}$ only appear because of the cut-off described above.

We find that the current reversal as described above for the limiting specular scattering case $s = 8$ appears throughout regions A and B. In the full pair breaking limit $s = 18$, $J_\theta(R) = 0$ vanishes identically for all ratios $K_1/K_2$, as seen from plugging the direct boundary condition $\eta_{\|}(R) = \eta_{\|}(R) = 0$ at the surface $r = R$ into the full form for the angular current Eq. (A.2.2), not only when restricted to the isotropic limit. The angular current is, however, only pushed inside, and remains finite locally, see Fig. 3.4.

In region C, the odd symmetry from Eq. (3.14) also holds. The current vanishes identically throughout the disk when $K_1 = K_2$, and flows in the opposite direction when $K_1 < K_2$.

In region D, we find a patch of current reversal even for $K_1 > K_2$, suggesting there may be other cases with current reversal for surface types inside the triangle of the range $G$, which have not been analyzed systematically.

Radially integrated flux and total flux

Here, we consider the radially integrated magnetic flux $\mathcal{B}(\theta) = \int r dr B_z(r, \theta)$ and the total flux $\Phi$. The integrated flux $\mathcal{B}(\theta)$ is in general still angular dependent. Let us first focus on specific angles. In Fig. 3.8 (b) we show the result at $\theta = 0$, the basal plane crystal axis,

\(^3\) For weak-coupling with $K_3 = K_4$, the free energy obeys the mathematical symmetry relation $\mathcal{F}[\eta_x, \eta_y, D_x, D_y, K_1, K_2] = \mathcal{F}[\eta_x, \eta_y, D_y, D_x, K_2, K_1]$. Switching $D_x \leftrightarrow D_y$ also changes the sign of the magnetic flux $B_z$, because $\varepsilon_{ijk} \varepsilon_{kij} = -\varepsilon_{ijk}$ in $\nabla \times \mathbf{A}$, such that $B_z(K_1, K_2) = -B_z(K_2, K_1)$. Including the surface term, this still holds when $g_3 = 0$.\)}}
3.2. Systematic analysis

and in (c) at the diagonal $\theta = \pi/4$. The color scale is chosen with the same principle as for $B_z$ but with the min and max now taken for $B$. The two extremal values, however, are still reached for $s = 8$ at the inverted ratio $K_1/K_2 = 1/3$, the maximum at $\theta = 0$, and the minimum at $\theta = \pi/4$.

For a straight surface along the basal plane crystal axis, the total flux per unit length is related to $B(0)$ of the disk geometry, and for straight surfaces along the diagonal to $B(\pi/4)$, up to corrections because of the curvature of the disk.

In addition, we perform a Fourier analysis of the radially integrated flux $B$. The symmetry properties of the magnetic flux $B_z$ (see above) also hold for $B$, which can therefore be expanded in $\cos(4 \theta)$ as

$$B(\theta) = \int_0^R r \, dr \, B_z = \sum_{j=0}^\infty B_j \cos(4 j \theta). \quad (3.15)$$

The total flux $\Phi$ through the whole disk is given by the zeroth expansion coefficient

$$\frac{\Phi}{2\pi} = \int_0^{2\pi} \frac{d\theta}{2\pi} \int_0^R r \, dr \, B_z = B_0. \quad (3.16)$$

Additional details are given in Sec. B.2.1 and Fig. B.2. We find that from the higher order expansion coefficients $B_1$ is the most significant, while $B_2$ still provides a small correction. All higher orders are negligible.

In Fig. 3.9 (a-c) we show $B_0$, $B_1$, and $B_2$. We find that the angular dependence increases with decreasing $K_1$ and is most pronounced near the specular scattering limit $s = 8$. In region C, surprisingly, there is no angular dependence (within numerical accuracy) of the magnetic signals, while the order parameter components remain angular dependent.

Altogether, we find that in region A, $B(0)$ first increases with decreasing $K_1$ and is maximal at $s = 8$. In region B, it decreases as $s \to 18$, and also starts to decrease with decreasing $K_1$, vanishing in a non-trivial region, until it is even inverted. On the other hand, $B(\pi/4)$ is more or less the same for a given $K_1/K_2$ all throughout A and B, while the total flux $\Phi$ always decreases with decreasing $K_1$, also going through a non-trivial region of vanishing total flux at finite local field, until it is inverted. In the full pair breaking limit $s = 18$, and all through region C, the field is odd with respect to the ratio according to $B_z(K_1/K_2) = -B_z(K_2/K_1)$, see Eq. (3.14), and thus vanishes identically everywhere when $K_1 = K_2$. As there is (almost) no angular dependence of the flux, $B(0)$, $B(\pi/4)$, and $\Phi$ coincide and decrease (increase) with increasing $s$ for $K_1 > K_2$ ($K_1 < K_2$), even crossing zero at the fine-tuned proximity case $s \approx 22.8$ (see above). Finally, region D basically interpolates between the end of C and the beginning of A, for which $B(\pi/4)$ has to change sign again. There is another non-trivial region of vanishing total flux at finite local field.

Discussion

The scope of results is striking. The flux may be (compared to the Matsumoto and Sigrist [95] reference scenario, $s = 8$ and $K_1/K_2 = 3$) enhanced or reduced, inverted or reversed, or even vanishing. The local field can be heavily angular dependent (the stronger the higher $g_3$ and the more inverted the ratio $K_1/K_2$) or rotationally symmetric (isotropic...
Figure 3.8: Selected quantities extracted from the full results: (a) combinations of the current directions; and the angular dependent radially integrated flux $B(\theta)$ at (b) $\theta = 0$ and at (c) $\theta = \pi/4$. Color scheme for (b) and (c) in Fig. 3.9.
Figure 3.9: Selected quantities extracted from the full results: Fourier analysis of the radially integrated flux. (a) total flux $B_0 = \Phi/(2\pi)$; (b) the first component $B_1$; and (c) $B_2$ almost vanishing everywhere such that higher orders are negligible.
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cases and when \( g_3 = 0 \), and have a variety of shapes. For many cases, the integrated or total value does not contain any information about the local shape. The current may flow in the same but either direction around the disk, or there may be current reversal. While some of these results are supported analytically or can be explained phenomenologically, others are more unexpected.

In particular, the vanishing total flux and the current reversal are not isolated and fine-tuned results. They appear for a large range of parameters depending on both the surface type and the band structure effects captured by the ratio \( K_1/K_2 \). When considering a straight surface only, there too is always an extended region of vanishing total flux. Still, the local field is finite in almost all but some highly symmetric cases.

3.3 Conclusion

To summarize, in our detailed and systematic analysis of the magnetic flux pattern appearing spontaneously at the surface of a disk-shaped sample we find an extreme sensitivity of the shape and the magnitude of the flux pattern on the ratio \( K_1/K_2 \) capturing band structure effects, and on the surface type \( s \), in combination with the surface orientation. We therefore conclude that this magnetic flux is not a universal feature of chiral \( p \)-wave superconductors. This is a fundamentally different behavior than for the topologically protected quasiparticle edge current mentioned in Sec. 1.4.1, which would be accessible in experiments for example through the quantized thermal Hall conductivity [87, 88]. We have also recovered the current reversal proposed by Bouhon and Sigrist [104]. In addition, we have compared our results to those of other previous work and are always in excellent agreement. Further support for the numerical results comes from selected analytical arguments.

A possible extension would be to consider \( g_i(r) \) varying around the disk or along the \( c \)-direction. Also, we have only treated a sharp surface, while an actual surface layer could be studied, and the adjacent material could be treated in a more controlled way. However, given the variety of resulting flux patterns given the small set of parameters considered, even more advanced models probably hold little additional information.

Most interestingly, we found that there are several non-trivial ranges where the radially integrated or even the total flux vanishes due to cancellation, although the local magnetic fields do not vanish. However, the extension of the flux pattern is on the order of the screening length, which may be relevant for the experimental detection by devices which have a considerably coarser spatial resolution than this. It is difficult to assess which parameter range is most probable for the material \( \text{Sr}_2\text{RuO}_4 \). While experimental accuracy has improved considerably over the last few years, making the bound very low and restricting the range within our scan dramatically, we would like to make clear that the comparison of experimental results with the magnitude of the flux found for the isotropic case with specular scattering is not necessarily conclusive. Given our results, in conjunction with other theoretical work such as Refs. [89, 97, 101, 102], the experimental absence of the edge current is not a decisive argument against the chiral \( p \)-wave character of this material.
3.4 Appendix

In this appendix we comment on the temperature dependence of the surface flux pattern in Sec. 3.4.1, discuss the flux pattern appearing at impurities in Sec. 3.4.2, and also provide the detailed results for the surface flux pattern for the full parameter range in Sec. 3.4.3.

3.4.1 Temperature dependence

Here we additionally discuss the temperature dependence of the flux pattern. Above, we have always used $T = 0$. While for a straight surface the results at higher temperatures are just rescaled versions of those at zero temperature, as can be seen straightforwardly from the temperature-dependent dimensionless form in Eq. (1.19) where only $\kappa$ enters, this does not apply for a curved surface. We focus on the most anisotropic result, the specular scattering limit $s = 8$ and the inverted ratio $K_1/K_2 = 1/3$ with current reversal as shown in detail in Fig. 3.7. The numerical results for temperatures $t = T/T_c = \{0, 0.2, 0.4, 0.6, 0.8, 1\}$ are shown in Fig. 3.10. The 6 plots on the left all have the same color scheme, as introduced for Fig. 3.6. At $\theta = 0$, as expected, as the temperature increases, the magnitude of the flux decreases linearly and the screening length increases like $1/\sqrt{1-t}$. At $\theta = \pi/4$, however, while the basic scaling behavior is similar, the size of the negative flux region decreases and already vanishes at $t \approx 0.867$. This is illustrated by showing the density plot for $t = 0.8$ in a rescaled color scheme on the right.

![Figure 3.10: Temperature dependence of the magnetic flux $B_\perp$ for the specular scattering surface type $s = 8$ at the inverted ratios $K_1/K_2 = 1/3$. The density plot for $t = 0.8$ is also shown with a rescaled color scheme to illustrate the changed shape of the flux distribution.](image)

We therefore conclude that the shape of the flux pattern changes with increasing temperature. This is understood straightforwardly because increasing the characteristic length scales is an effect related to decreasing the radius, for which we expect a qualitative change. For $t \approx 1$, the flux does not even go to zero near the center of the disk, in agreement with Refs. [98, 103] who have studied very small-sized disk-shaped samples.
3.4.2 Flux at impurities

Additionally, we briefly address non-magnetic impurities. These also distort the order parameter, leading to spontaneous currents which induce a local magnetic flux pattern. In the spirit of an effective critical temperature and using the simplest model possible, we consider an isotropic impurity as a drop in the critical temperature

\[ T_{c}^{\text{eff}} = T_{c}(1 - \tau_{\text{imp}}\delta(r - r_{\text{imp}})) \tag{3.17} \]

where \( \tau_{\text{imp}} > 0 \) is the strength and \( r_{\text{imp}} \) the position of the impurity.

For impurities, translational invariance in the \( z \)-direction is broken. For the anisotropic layered quasi two-dimensional superconductor, the field decays rapidly in the \( z \)-direction as the induced currents mainly run in the basal plane layer where the impurity is located. Here, we ignore this \( z \)-dependence, only treating a single layer, which could alternatively be understood as considering a line defect along the \( c \)-axis. However, concerning the overall magnetic signal from a bulk sample we have to keep in mind that the surface is continued in the \( z \)-direction, while the impurities are not.

**Isolated impurity**

We consider a single isolated impurity in an infinite sample and numerically compute the resulting magnetic flux pattern and order parameter tuning the ratio \( K_{1}/K_{2} \) for the range described above in Sec. 3.1.2, and additionally tuning the strength of the impurity, \( \tau_{\text{imp}} \).

As for the surface coefficients \( g_{i} \), we expect that there is a cut-off value of the strength \( \tau_{\text{imp}} \) for which the order parameter is essentially suppressed to zero at the impurity and where the resulting peak magnitude saturates. Further, the total flux for such an impurity vanishes. The computational details can be found in Sec. B.2.1, where we point out some difficulties in resolving the basically circular impurity using a square mesh, and mention additional numerical problems, because of which the details of the results have to be taken with caution, while the overall trend is certainly captured.

Fig. 3.11 shows the magnetic field and current distribution around the impurity in the isotropic limit \( K_{1}/K_{2} = 3 \) and for the maximally considered strength \( \tau_{\text{imp}} = 50\xi_{0}^{2} \), see below. In this limit there is no angular dependence as expected. The shape of the magnetic field \( B_{z}(r)/B_{\text{peak}} \) is shown normalized by its peak value on the left. The dependence of this value on \( \tau_{\text{imp}} \) and \( K_{1}/K_{2} \) will be discussed below. The flux is strongly peaked at the impurity site \( r = 0 \) (yellow) and is compensated by a negative tail on larger distances (blue) such that the total magnetic flux vanishes within the numerical accuracy as expected. The small inset shows an overview density plot of the flux peak. On the right, the peak is shown in detail with a density plot of the flux overlaid with a vector plot of the current.

We find that the magnetic flux is essentially suppressed on a length scale \( \xi_{0} \) rather than the screening length \( 2.6\xi_{0} \). This is because it is primarily connected with an induced \( \eta_{-} \) component, while the bulk only has a \( \eta_{+} \) component, and the actual London screening only becomes important on a larger length scale, as described in similar theoretical work by Okuno et al. [148], to which we refer for further details.

Next, we investigate how the peak value \( B_{\text{peak}} \) depends on the strength of the impurity, still restricted to the isotropic limit. This is shown in Fig. 3.12 on the left. As expected, for strong enough impurities the peak value saturates, and the order parameter is completely...
Figure 3.11: Magnetic flux pattern \( B_z(r) \) around a single isolated isotropic impurity in the isotropic limit \( K_1/K_2 = 3 \) with no angular dependence, normalized by its peak value \( B_{\text{peak}} \). The strength of the impurity is \( \tau_{\text{imp}} = 50\xi_0^2 \) for which the order parameter is fully suppressed. The colors are such that red to yellow indicate increasing positive flux, while blue is the much smaller negative screening flux. In the vector plot, the pointers are in the direction of \( \hat{J} \), but scaled by \(|J|^{1/3}\). The total flux \( \Phi_{\text{imp}} \) vanishes within the numerical accuracy as expected.

suppressed (not shown). On the right we also show how the shape of the flux pattern changes with increasing \( \tau_{\text{imp}} \). For small values (black lines), the shape of the impurity changes considerably, while it saturates for higher values (red lines).

For ratios away from the isotropic limit \( K_1/K_2 \) it seem that there is a slight anisotropy of the flux pattern. While this comes unexpected at first, it can probably be explained by the fact that this suppression is more connected to the induced \( \eta_- \) order parameter rather than the screening currents.

Of primary interest, anyway, is the peak value \( B_{\text{peak}} \). In Fig. 3.13 on the left this value is shown for tuning the ratio \( K_1/K_2 \) at \( \tau_{\text{imp}} = 10\xi_0^2 \), where the peak has saturated, see Fig. 3.12 on the left. We find an almost linear behavior in \((K_1 - K_2)/(K_1 + K_2)\), see also discussion in Sec. 3.1.2. The symmetry relation from Eq. (3.14) also applies here, and in particular the field vanishes identically when \( K_1/K_2 = 1 \). The shape of the flux pattern is shown on the right, for two different directions \( \theta = 0 \) parallel to the crystal axis, and for the diagonal \( \theta = \pi/4 \). For \( \theta = 0 \), the shape only varies little for different \( K_1/K_2 \), while the shape at the diagonal \( \theta = \pi/4 \) varies more.

**Conclusion**

While changing the ratio \( K_1/K_2 \) is a system-wide effect and the flux at both the surface and the impurity are affected, the flux at the surface is further influenced by the surface type \( s \), while the peak value of the flux at the impurity depends on the strength of the impurity.
Figure 3.12: Dependence of the magnetic flux peak at the impurity on the strength $\tau_{\text{imp}}$ in the isotropic limit $K_1/K_2 = 3$. (left) The peak value $B_{\text{peak}}$ plotted against $\tau_{\text{imp}}$, saturating for a strong enough impurity when the order parameter is fully suppressed. (right) The normalized flux $B_z(r)/B_{\text{peak}}$ for different $\tau_{\text{imp}}$, with the three highest values, at which the peak value has saturated, indicated in red in the insets, to demonstrate that the shape has also saturated within the numerical accuracy.

Figure 3.13: Dependence of the magnetic flux peak on the ratio $K_1/K_2$ for an impurity with strength $\tau_{\text{imp}} = 10\xi_0^2$, at which the peak value has saturated, see Fig. 3.12. (left) The peak value $B_{\text{peak}}$ plotted against $K_1 - K_2 [K]$, with a linear fit. (right) The normalized flux $B_z(r,\theta)/B_{\text{peak}}$ for the different $K_1 - K_2$, except $K_1 = K_2$ where it vanishes identically.
3.4. Appendix

$\tau_{\text{imp}}$, saturating when the order parameter is fully suppressed. We stress again, however, that some numerical issues require further investigation. Also, regarding the overall signal, we have to remember that the impurities are not continued in the $z$-direction.

We conclude that the behavior at impurities is therefore only partially related to what happens at the surface, which is important for reconciling the experimental absence of the edge current with the observed intrinsic magnetism from $\mu$SR experiments. There, the flux at domain walls or other defects also plays a role, but the flux in those situations should also only partially be related to what happens at the surface, following from a similar treatment.

3.4.3 Detailed flux pattern for the full parameter range

In this appendix, the full numerical results for the detailed shape of the flux pattern are shown over the whole parameter range. For each combination of $s$ and $K_1/K_2$, arranged in a grid as illustrated below in Fig. 3.14, a density plot of $B_z(r, \theta)$ is provided. The 31 surface types are split into four parts over the next pages, as indicated in Fig. 3.14, and with the surface type $s = 0$ repeated at the end.

![Density plots $B_z(r, \theta)/H_{c2}$](image)

Figure 3.14: Density plots $B_z(r, \theta)$ for each value of the parameters $s$ and $K_1/K_2$, arranged in a grid which is cut into four parts shown enlarged over the next four pages and where the color scheme is as for Fig. 3.6.
Spontaneous surface flux pattern
Motivated by the observation of an anomalous temperature dependence of the critical current in Pb/Ru/Sr$_2$RuO$_4$ devices as described in Sec. 1.4.2, here we study cylindrical Josephson junctions between a chiral p-wave and a conventional s-wave superconductor. Such junctions may be either in a topological trivial or frustrated state, depending on the winding of the p-wave state.

First, we describe the phenomenological sine-Gordon model in detail. We then analyze the different mechanisms limiting the critical current for the different topological states of the junction. In particular, we show that in the frustrated state of the junction only an inhomogeneous coupling strength leads to a finite critical current, breaking the rotationally degeneracy of the initial position of the line-shaped flux pattern appearing spontaneously in this configuration. The associated pinning-depinning transition of the flux line is also studied in detail.

Second, we discuss the phase diagram for the evolution of the different possible states of the junction, from the filamentary nucleation in the 3-Kelvin phase to the chiral bulk state, and for different strengths of the proximity-induced superconductivity inside the Ru-inclusion.

This chapter is based on S. B. Etter, H. Kaneyasu, M. Ossadnik, and M. Sigrist, PRB 90, 024515 (2014) [149] and H. Kaneyasu, S. B. Etter, T. Sakai, and M. Sigrist, PRB 92, 134515 (2015) [127]. The work on the frustrated junction was started in a semester project (2010) and was part of my Master thesis (2011).
4.1 Phenomenological model

We first describe our setup for modeling the Pb/Ru/Sr$_2$RuO$_4$ devices. We then introduce the coupling term between the $s$-wave and the chiral $p$-wave superconductor and formulate the representations of the order parameter in the distinct topological states of the junctions. Finally, these ingredients are combined in a sine-Gordon model of the extended Josephson junction which allows us to treat all possible situations within a single framework.

4.1.1 Model system

As illustrated in Fig. 4.1, the Ru inclusion is modeled as a cylinder of height $h$ and radius $R$ with the $z$-axis parallel to the $c$-axis of the tetragonal bulk. The Pb film does not appear explicitly in this setup. Assuming that the current enters through the top of the cylinder only, as described in Sec. 1.4.2, it is modeled as a current $I$ applied at the top, along the axis of the cylinder, which can equivalently be viewed as an external circular magnetic field $H$ applied to the top surface of the cylinder. In addition, neglecting both the proximity effect and the filamentary nature before the bulk transition, we assume homogeneous superconductivity throughout the system. The interface between the cylindrical $s$-wave superconductor and the chiral $p$-wave bulk is then treated as an extended Josephson junction and it is natural to use cylindrical coordinates. We note that the neglected features are not important for the discussion focusing on the limiting mechanism of the Josephson current through the interface, which we consider the weakest link for supercurrent flow in the whole device.

Figure 4.1: Model of the Pb/Ru/Sr$_2$RuO$_4$ Josephson junctions with a single Ru inclusion of cylindrical shape of radius $R$ and height $h$, surrounded by the Sr$_2$RuO$_4$ bulk. The contact through the Pb film is modeled by a current $I$ applied along the $z$-axis at the top, equivalent to an external circular magnetic field $H$. 
4.1.2 Josephson coupling

Focusing on the Josephson effect alone, we assume that the order parameters as such are rigid and only let the phase between the two superconductors vary along the interface. We develop an effective model for this situation, based on the free energy of the interface

\[ F_{\text{int}} = d \int_0^{2\pi} Rd\theta \int_0^h d\int_{\text{int}}(\theta, z). \] (4.1)

The effective width \( d = \lambda_{R_u} + \lambda_{\text{bulk}} + d_0 \) contains the London penetration depths of the two materials \( \lambda_{R_u,\text{bulk}} \) and the actual width of the interface \( d_0 \), which vanishes for the eutectic material, \( d_0 \approx 0 \). For the interface free energy density relevant are the energy of the magnetic self-field \( B \), confined within the range \( d \), and the Josephson coupling energy taking into account that the even-parity spin-singlet \( \psi_s \) and odd-parity spin-triplet order parameter \( \eta \) have to be matched through spin-orbit coupling \[115\], see also Sec. 2.1.3. Thus, by symmetry,

\[ f_{\text{int}}(\theta, z) = \frac{B^2}{8\pi} - \frac{K_c}{d} [\psi_s^* (\hat{z} \cdot (\hat{n} \times \eta)) + \text{c.c.}], \] (4.2)

with \( K_c \) a real coupling constant and \( \hat{n} = \hat{r} \) the normal of the interface.

4.1.3 Trivial and frustrated topology

To proceed, we first describe the two topologically distinct situations relevant for this junction, see also Fig. 1.6. The trivial states include the A- and the A’-phase. However, as follows from Eq. (4.2), only the order parameter component parallel to the interface couples to the s-wave order parameter to lowest order. Therefore, only the state nucleating in the A-phase at \( T_{J_K} \) is relevant and we neglect the component perpendicular to the interface nucleating at a lower temperature in the A’-phase. This topologically trivial order parameter is represented by

\[ \eta^{(A)} = \Delta_p \hat{z} \times \hat{n}. \] (4.3)

As mentioned above, we ignore the radial dependence of the gap amplitude \( \Delta_p \) because of its filamentary nature and use the value at the interface only. The topologically frustrated states include both the inhomogeneous B-phase and the chiral bulk phase. Again ignoring the spatial dependence of the gap amplitude and in addition assuming an isotropic system where the phase winding contains the only angular dependence, see Eq. (2.9) and the corresponding discussion, the order parameter in cylindrical coordinates is given by

\[ \eta^{(B)}(\theta) = \eta_p \hat{r} + \eta_\theta \hat{\theta} = \Delta_p (1, \pm i)e^{iN\theta}, \] (4.4)

where \( N = \pm 1 \) is the winding number of the order parameter around the inclusion. Finally, fixing the global phase of the p-wave order parameter by choosing a proper gauge, we define the Josephson phase \( \phi(\theta, z) \) through the order parameter on the s-wave side,

\[ \psi_s(R, \theta, z) = \Delta_s e^{i\phi(\theta, z)}, \] (4.5)

which is variable along the interface. Again, for the gap amplitude we use the value at the interface only. As mentioned above, we neglect that the proximity effect from Pb would
Topologically frustrated Josephson junction

yield a rather strong $z$-dependence and assume a constant gap amplitude throughout. This heavily simplifies our model, while the essential features important for the discussion of the limiting mechanism are still fully captured. We assume periodic boundary conditions around the interface for this Josephson phase,

$$\phi(\theta + 2\pi, z) = \phi(\theta, z),$$

(4.6)

while the possibility of an Abrikosov-like vortex in the center of the inclusion, where the phase winding is picked up by the $s$-wave order parameter, has been discussed by Kaneyasu and Sigrist in Ref. [116], see also the review of previous theoretical work in Sec. 1.4.2.

4.1.4 Sine-Gordon model

Using the standard procedure to derive the sine-Gordon model for the phase of an extended Josephson junction, see Sec. 1.2.2, we formulate for the free energy density

$$f_{sg}(\theta, z) = \frac{2(2\pi)^3}{\Phi_0^2} f_{int}(\theta, z) = \frac{1}{2} \left\{ \left( \frac{\partial\phi}{\partial z} \right)^2 + \left( \frac{\partial\phi}{R\partial\theta} \right)^2 \right\} - \frac{1}{\lambda_J^2} \cos[\phi(\theta, z) - N\theta]$$

(4.7)

with the Josephson penetration depth $\lambda_J$ defined as

$$\lambda_J^2 = \frac{\Phi_0^2}{4(2\pi)^3 d K_c |\eta_s||\eta|}$$

(4.8)

and with the winding number extended to both phases

$$N = \begin{cases} 0 & \text{phase A,} \\ \pm 1 & \text{phase B.} \end{cases}$$

(4.9)

The local Josephson critical current density per area is given by

$$J_c = \frac{4\pi c}{\Phi_0 K_c |\eta_s||\eta|} = \frac{c\Phi_0^2}{8\pi^2 d \lambda_J^2}.$$  

(4.10)

By variation with respect to the phase $\phi(\theta, z)$ we obtain the differential equation

$$\frac{\partial^2 \phi(\theta, z)}{R^2 \partial \theta^2} + \frac{\partial^2 \phi(\theta, z)}{\partial z^2} = \frac{1}{\lambda_J^2} \sin[\phi(\theta, z) - N\theta].$$

(4.11)

The boundary conditions are determined by the externally applied current $I$, injected through the top of the cylinder ($I > 0$). The cross-sectional current density is given by

$$J = -\frac{I}{\pi R^2} \dot{z} \Theta(z - h) \Theta(R - r),$$

(4.12)

The current can also be translated into a circular magnetic field (see Fig. 4.1) on top of the cylinder

$$H = \frac{2I}{cR} \dot{\theta}.$$  

(4.13)
4.2 Limiting mechanisms for the critical current

Combining this with the standard relation between the flux density and the phase on the interface, Eq. (1.26), we write the boundary conditions for the upper \((z = h)\) and lower \((z = 0)\) boundary,

\[
\frac{\partial \phi}{\partial z} \Big|_{z=h} = \frac{4\pi d}{c\Phi_0 R} I \equiv I, \quad (4.14a)
\]

\[
\frac{\partial \phi}{\partial z} \Big|_{z=0} = 0. \quad (4.14b)
\]

For future convenience we abbreviate the expression of the first condition by the parameter \(I\) in the following. The second condition corresponds to a vanishing current through the bottom of the cylinder, since we assume that all current leaves the Ru-inclusion through the interface. The solution which we discuss in the following could be extended by mirror symmetry at the plane \(z = 0\) to a cylinder of height \(2h\) with a current of the same magnitude entering the cylinder also through the bottom at \(z = -h\).

4.2 Limiting mechanisms for the critical current

We first discuss the topologically trivial state of the junction and review the standard limiting mechanism of Josephson junctions. For the topologically frustrated state of the junction we review the line-shaped flux pattern appearing spontaneously at zero applied current. We then proceed to the case with a finite applied current and show that a finite supercurrent can only be stabilized if we allow an inhomogeneous Josephson coupling that varies along the interface in the angular direction. Finally, we present a full solution computed numerically for each situation in an overview to compare the different mechanisms.

4.2.1 Review of the topologically trivial junction

In topologically trivial state of the junction, including both the A- and A’-phase, there is no phase winding and \(N = 0\) in the Josephson coupling part of Eqs. (4.7) and (4.11). Here, the standard discussion of an extended junction applies as introduced in Sec. 1.2.2. The existence of a Josephson coupling as detected in the experiment relies on the observation of the usual anomaly in the current-voltage relation of the junction, and indicates the existence of a superconducting condensate on both sides of the interface [113].

With the vanishing phase winding \(N = 0\), the phase depends only on \(z\), i.e. \(\phi(\theta, z) = \phi(z)\), and it is constant along \(\theta\) with the periodic boundary conditions fulfilled automatically. The current flows radially through the interface, \(J = J_r(z)\hat{r}\), yielding a circular magnetic field \(B = B_\theta(z)\hat{\theta}\) which equals \(H\) at \(z = h\) and penetrates on the length scale of the Josephson penetration depth \(\lambda_J\). Our cylindrical geometry can therefore be translated into a one-dimensional extended junction with boundaries at \(z = 0\) and \(h\). The behavior of the junction for this situation has been discussed by Owen and Scalapino [150].

Considering the case of a long cylinder, \(h \gg \lambda_J\), the current is concentrated at the top of the cylinder with a peak positioned roughly at the depth \(\lambda_J\), leading to a ring-shaped current pattern as shown in Fig. 4.2, together with the circular magnetic field. As formulated by Owen and Scalapino, we are in the ‘0 to 1 vortex mode’ and the current peak can be thought of as ‘half’ a current vortex present. Here, the Josephson current
is limited by the nucleation of a vortex at the top of the cylinder which then moves down, driven by the Lorentz force, and yields a voltage. Alternatively, the critical current corresponds (through the boundary condition) to the effective lower critical field \( H_{c1} \) for the penetration of vortices into the junction from the top [3],

\[
H_{c} = \frac{2I_c}{cR} = \frac{8\pi}{c}\lambda_J J_c \propto J_c^{1/2}.
\]  

(4.15)

For short cylinders, \( h \ll \lambda_J \), the current flows nearly uniformly and the critical current is

\[
I_c = 2\pi Rh J_c = I_{c0}.
\]

(4.16)

4.2.2 The frustrated junction

We now turn to the topologically frustrated state of the junction, including the B-phase and the chiral bulk, where the phase winding does not vanish and \( N = \pm 1 \). Here, the situation is fundamentally different. For the trivial case discussed above we were able to minimize the free energy \( f_{SG} \), Eq. (4.7), in both the gradient and the coupling part simultaneously at any point on the interface simply by choosing the constant phase \( \phi(\theta, z) = 2\pi n \).

This is not possible anymore with a finite winding number. Although keeping the phase constant everywhere still optimizes the gradient part, this leaves a coupling part

\[
- \frac{1}{\lambda_J^2} \cos[\phi - \theta]
\]

(4.17)

varying between \(-1/\lambda_J^2\) and \(+1/\lambda_J^2\) around the cylinder. On the other hand, optimizing the coupling term by choosing \( \phi(\theta, z) = ± \theta + 2\pi n \) leads to the problem of a non-vanishing
4.2. Limiting mechanisms for the critical current

gradient part
\[
\frac{1}{2} \left( \frac{\partial \phi}{R \partial \theta} \right)^2 = \pm \frac{1}{2R^2}.
\] (4.18)

This is a typical situation of frustration, where the Josephson coupling energy can only be optimized at the expense of magnetic energy and vice versa.

**Spontaneous line-shaped flux pattern**

We first consider the situation where no external current is applied, \( I = 0 \), such that the magnetic flux pattern described below is said to appear spontaneously. At zero applied current, the junction is translationally invariant along the \( z \)-axis and we again have a one-dimensional problem. Now, however, the system is independent of the height of the junction, and the phase depends only on \( \theta \) and is constant along \( z \), \( \phi(\theta, z) = \phi(\theta) \). This case was discussed before in Ref. [116].

The minimization of the free energy including the periodic boundary condition \( \phi(\theta + 2\pi) = \phi(\theta) \) has an analytic solution with the phase given by
\[
\phi(\theta, a) = \pi - 2\text{am}\left( \frac{K(m)}{\pi} (\theta - a), m \right) + \theta \mod 2\pi,
\] (4.19)

where \( \text{am}(x, m) \) is the Jacobi amplitude function and \( K(m) \) the complete elliptic integral of the first kind. The Jacobi parameter \( m \in [0, 1) \) is determined inversely via
\[
\frac{R}{\lambda_J} = \sqrt{m} K(m). \tag{4.20}
\]

The parameter \( a \in [0, 2\pi)_{\text{periodic}} \) denotes an undetermined shift of the position of the phase, as illustrated in Fig. 4.3, where we show the phase for different values of \( a \). The phase can be shifted along the identity by any angle without changing the energy. This degeneracy stems from the rotational symmetry of the circularly cylindrical junction and assuming an overall isotropic system.

Both the magnetic field and the radial current flowing through the interface are finite,
\[
B = B_z(\theta, a) \hat{z} = \frac{\Phi_0}{2\pi d} \frac{\partial \phi}{R \partial \theta} = \frac{\Phi_0}{2\pi dR} \left( 1 - \frac{2K(m)}{m} \cdot \text{dn} \right),
\] (4.21)

and
\[
J = J_r(\theta, a) \hat{r} = \frac{c}{4\pi R} \frac{\partial B_z}{\partial \theta} = \frac{c\Phi_0}{8\pi^2 d R^2} \frac{\partial^2 \phi}{\partial \theta^2} = \frac{c\Phi_0}{8\pi^2 d R^2} \frac{2mK(m)^2}{\pi^2} \cdot \text{cn} \cdot \text{sn},
\] (4.22)

where \( \text{cn} \), \( \text{dn} \) and \( \text{sn} \) are the Jacobi elliptic functions with the same argument as the Jacobi amplitude function in the phase above. For these magnetic quantities the effect of the degeneracy \( a \) is a simple shift around the cylinder. Note that this solution does not resolve the spatial dependence within the range \( d \) perpendicular to the interface where the screening currents run. Obviously, the total flux vanishes,
\[
\int_0^{2\pi} R d\theta B_z(\theta) = \frac{\Phi_0}{2\pi d} (\phi(2\pi) - \phi(0)) = 0,
\] (4.23)
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Figure 4.3: Josephson phase in the frustrated state of the junction $N = \pm 1$ at zero applied current (analytical result). The Josephson penetration depth is $\lambda_J = 0.5R$ and the chirality is positive ($N = +1$). There is a rotational degeneracy and the phase can be shifted along $\theta - \pi$ (dashed) due to the complete rotational symmetry of the circularly cylindrical junction by any angle without changing the energy. The solution for $a = \pi$ is shown in red.

and also no net current flows through the interface,

$$\int_0^{2\pi} R d\theta J_r(\theta) = \frac{c}{4\pi} (B_z(2\pi) - B_z(0)) = 0, \quad (4.24)$$

as is expected when no external current is supplied.

These expressions describe a current vortex centered at $\theta = a$ around a negative magnetic flux peak having a width of $\Delta \theta \propto \lambda_J/R$. The stronger the Josephson coupling, and therefore the smaller $\lambda_J$, the stronger and more concentrated this flux peak becomes. In the extreme limit this would be a flux line enclosing approximately one negative flux quantum $-\Phi_0$, which is compensated by a positive counter flux spread over the remaining part of the interface. In Fig. 4.4 we show the magnetic flux and current pattern for the state with positive chirality ($N = +1$) and $a = \pi$ at a Josephson penetration depth of $\lambda_J/R = 0.5$. Extending the solution along the cylinder in the $z$-direction, we find a line-shaped flux pattern on the interface of the inclusion, parallel to the axis of the cylinder.

**Finite applied current**

We now examine the behavior of the frustrated state of the junction if a non-vanishing external current is applied, $I > 0$. To analyze this situation we assume that $\lambda_J \gg R, h$ such that $\epsilon = R^2/\lambda_J^2$ is small while $h$ and $R$ are comparable. We then expand the phase obtained from solving the sine-Gordon equation (4.11) in $\epsilon$,

$$\phi(\theta, z) = \phi_0 + \sum_{k=1}^{\infty} \epsilon^k \phi_k(\theta, z), \quad (4.25)$$
4.2. Limiting mechanisms for the critical current

Figure 4.4: Flux pattern and radial current density in the frustrated state of the junction $N = \pm 1$ at zero applied current (numerical result). The Josephson penetration depth is $\lambda_J = 0.5R$ and the chirality is positive ($N = +1$). There is a flux line and a current vortex centered at $a = \pi$. The total flux through the cylinder and the net current through the interface are zero. The inset shows the circular cross-section of the cylinder with the sign of the flux and the position of the current vortex indicated.

where $\phi_0$ is a constant, as we will show below, and the remaining terms are small perturbations. The boundary conditions are

$$
\sum_k \epsilon^k \frac{\partial \phi_k}{\partial z} \bigg|_{z=0} = \begin{cases} 
I & z = h, \\
0 & z = 0.
\end{cases}
$$

(4.26)

First, we consider the lowest order only. Inserting the expansion into the differential equation, the coupling part vanishes and we obtain

$$
R^2 \nabla^2 \phi_0 = R^2 \left( \frac{1}{R^2} \frac{\partial^2 \phi_0}{\partial \theta^2} + \frac{\partial^2 \phi_0}{\partial z^2} \right) = 0,
$$

(4.27)

which can only be solved by $\phi_0$ being a constant with the boundary condition $\partial_z \phi_0 \bigg|_{z=0,h} = 0$, since at this order there is no Josephson contact and thus no current can flow. We then continue with the higher orders $k > 0$. By expansion in $\epsilon$ we obtain differential equations of the Poisson form

$$
\nabla^2 \phi_k(\theta, z) = q_k(\theta, z),
$$

(4.28)

The source term $q_k(\theta, z)$ does not depend on $\phi_k(\theta, z)$, nor on $\epsilon$, but it does depend on the resulting $\phi_{k'}(\theta, z)$ from lower orders $k' < k$ (iterative approach). We also obtain Neumann boundary conditions at the edges of the cylinder

$$
\frac{\partial \phi_k}{\partial z} \bigg|_{z=0} = \begin{cases} 
c_k & z = h, \\
0 & z = 0,
\end{cases}
$$

(4.29)
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which combine, together with Eq. (4.26), to the condition

$$\mathcal{I} = \sum_{k=1}^{\infty} \epsilon^k c_k.$$  \hspace{1cm} (4.30)

The periodic boundary conditions in $\theta$ still apply,

$$\phi_k(\theta + 2\pi, z) = \phi_k(\theta, z).$$  \hspace{1cm} (4.31)

For a solution to exist, the compatibility condition for the Neumann problem, following directly from Gauss’s divergence theorem, requires that

$$c_k = \frac{1}{2\pi R} \int_0^{2\pi} R d\theta \int_0^h dz \, q_k(\theta, z).$$  \hspace{1cm} (4.32)

Let us consider the actual equations order by order. We start with the first order in $\epsilon$,

$$R^2 \nabla^2 \phi_1 = \sin(\phi_0 - \theta).$$  \hspace{1cm} (4.33)

This is obviously only compatible with $c_1 = 0$ since $\phi_0$ is a constant. The solution is then given by

$$\phi_1(\theta, z) = -\sin(\phi_0 - \theta),$$  \hspace{1cm} (4.34)

where any integration constant can be absorbed in the constant $\phi_0$ as part of the complete solution $\phi$. Using this solution in turn for the equation of next order in $\epsilon$, we obtain,

$$R^2 \nabla^2 \phi_2 = \phi_1(\theta, z) \cos(\phi_0 - \theta) = -\sin(\phi_0 - \theta) \cos(\phi_0 - \theta)$$  \hspace{1cm} (4.35)

which is again only compatible with $c_2 = 0$. The solution is now given by

$$\phi_2(\theta, z) = \frac{1}{4} \sin(\phi_0 - \theta) \cos(\phi_0 - \theta).$$  \hspace{1cm} (4.36)

This solution can again be used to derive the next order in a hierarchy of Poisson differential equations that are all compatible with the Neumann boundary conditions only if $c_k = 0$ for all orders $k$. Therefore, no solution exists for a finite value of $\mathcal{I}$.

This result is supported by our numerical analysis which also does not converge to a stable solution. Rather, we obtain solutions varying in ‘time’, that is, with continuing iteration steps. Referring to the resistively shunted junction model, see for example Ref. [43], this is due to a dissipative contribution from a junction resistance $R_J$ besides the Josephson channel. We take this effect into account by an additional term in the sine-Gordon equation (4.11),

$$-\frac{\tau}{\hbar} \frac{\partial^2 \phi}{\partial t^2} + \frac{\partial^2 \phi}{R^2 \partial \theta^2} + \frac{\partial^2 \phi}{\partial z^2} = \frac{1}{\lambda_J^2} \sin(\phi - \theta),$$  \hspace{1cm} (4.37)

with $\tau = 2d/(c^2 R h)/R_J$ the basic Josephson time constant and where we ignoring any capacitative effects.

Assuming that the externally applied current is small, we approximate the solution in zeroth order in $\epsilon$ as

$$\phi_0(\theta, z, t) = \frac{\mathcal{I}}{\hbar \tau} t + \frac{\mathcal{I} z^2}{\hbar 2} + \ddot{\phi}_0,$$  \hspace{1cm} (4.38)
4.2. Limiting mechanisms for the critical current

where \( \tilde{\phi}_0 \) is a constant. The boundary condition for a finite current is then already satisfied by \( \phi_0 \), and we approximate all the other \( \phi_k \) with \( k \geq 1 \) by ignoring the \( z \)-dependence and using \( c_k = 0 \). The (constant) voltage is given by

\[
V = \frac{\Phi_0}{2\pi c} \frac{\partial \phi}{\partial t} = \frac{\Phi_0 I}{2\pi c \tau h} = R_J I, \tag{4.39}
\]

which corresponds to Ohmic behavior. The temporal dependence of the higher order components \( \phi_k \) is oscillatory and ignored here by taking a time average. This rather simple approximation of the extended model already incorporates the basic observation from the numerical solution of the full problem that the flux pattern moves around the cylinder, as the phase \( \phi \) is essentially linear in \( t \). Thus, we conclude that there does exist a solution of the sine-Gordon equation for any finite current, but with a time-dependent phase \( \phi \) corresponding to a resistive current flow.

Consequently, the homogeneous frustrated junction does not support any finite supercurrent. This is because the position of the spontaneous magnetic flux and current pattern induced by the frustration is not fixed, but can be shifted by any angle without changing the energy. Therefore, any finite current will drive the flux pattern by the Lorentz force. Dissipative dynamics then lead to a steady state situation with a constant time-averaged voltage. This will obviously also happen in the other limit, \( \lambda_J \ll R, h \).

4.2.3 The inhomogeneous frustrated junction

We now change the situation by removing the rotational symmetry, which is the underlying reason why the frustrated junction does not support any supercurrent. Maintaining the cylindrical geometry of our model, this can be implemented by introducing an angular dependent Josephson coupling \( \tilde{J}_c(\theta) \) by adding a modulation

\[
\frac{1}{\lambda_J^2} \rightarrow \frac{1}{\lambda_J^2} \{1 + m(\theta)\} \tag{4.40}
\]

with the restrictions that \( m(\theta) > -1 \), \( m(\theta + 2\pi) = m(\theta) \), and

\[
\int_0^{2\pi} d\theta m(\theta) = 0, \tag{4.41}
\]

whereby the \( J_c \) of Eq. (4.10) shall now be the angle-averaged coupling constant. The differential equation then reads

\[
R^2 \nabla^2 \phi = \epsilon\{1 + m(\theta)\} \sin(\phi - \theta), \tag{4.42}
\]

while the boundary conditions remain the same.

Again considering \( \epsilon \) small, we use the expansion from Eq. (4.25) to analyze the effect of the modulated \( \lambda_J \). For \( \phi_0 \) we still obtain a constant while the equation for the first order in \( \epsilon \) is now

\[
R^2 \nabla^2 \phi_1 = \frac{\partial^2 \phi_1}{\partial \theta^2} + R^2 \frac{\partial^2 \phi_1}{\partial z^2} = \{1 + m(\theta)\} \sin(\phi_0 - \theta). \tag{4.43}
\]

Now, the compatibility condition leads to

\[
c_1 = \frac{h}{R^2} \tilde{m}(\phi_0), \tag{4.44}
\]
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where

\[ \tilde{m}(\phi_0) = \int_0^{2\pi} \frac{d\theta}{2\pi} m(\theta) \sin(\phi_0 - \theta) = (m_1 \sin \phi_0 - m_2 \cos \phi_0) \] (4.45)

with

\[ \tilde{m} = m_1 + im_2 = \int_0^{2\pi} \frac{d\theta}{2\pi} m(\theta)e^{i\theta}. \] (4.46)

We then find the complete solution

\[ \phi_1(\theta, z) = \varphi(\theta, \phi_0) + \frac{\tilde{m}(\phi_0)}{2R^2} z^2, \] (4.47)

where \( \varphi(\theta, \phi_0) \) is the particular solution of the differential equation

\[ \frac{\partial^2 \varphi}{\partial \theta^2} = \{1 + m(\theta)\} \sin(\phi_0 - \theta) - \tilde{m}(\phi_0). \] (4.48)

It is obvious that we can satisfy the boundary conditions for finite currents \( I \neq 0 \) as long as \( \tilde{m}(\phi_0) \) is not zero. Neglecting higher orders, the compatibility condition leads to

\[ I = \epsilon \frac{\partial \phi_1}{\partial z} \bigg|_{z=h} = \frac{h}{\lambda_I} \tilde{m}(\phi_0) \] (4.49)

which corresponds to the current-phase relation

\[ I(\phi_0) = 2\pi R h J_c \tilde{m}(\phi_0) = I_{c0} \tilde{m}(\phi_0), \] (4.50)

where \( I_{c0} \) is given by Eq. (4.16) as the integral of the critical current density \( J_c \) over the interface. With \( |\tilde{m}(\phi_0)| < 1 \) for all \( \phi_0 \) this current \( I(\phi_0) \) is always smaller than \( I_{c0} \) and its maximum, the renormalized critical current, is given by

\[ I_c = I_{c0} \max_{\phi_0} \tilde{m}(\phi_0) = I_{c0} |\tilde{m}| = I_{c0} \sqrt{m_1^2 + m_2^2} < I_{c0}. \] (4.51)

Strictly speaking we have to take into account the variable Josephson coupling also in the trivial state of the junction used as a reference. However, in the limit \( \lambda_J \gg R, h \) the junction is ‘short’ in both directions. The resulting current density simply adjusts to the local critical current density like \( J_r(z, \theta) = J_{r,0}(z)(1 + m(\theta)) \) with \( J_{r,0} \) the result of the homogeneous case. Thus, the critical current of the inhomogeneous trivial junction is the same as for the corresponding homogeneous case with the same average Josephson coupling. This is also confirmed by the numerical results.

We conclude that the inhomogeneous frustrated junction does support a finite supercurrent, up to the renormalized critical current. Because of the angular dependent Josephson coupling, the initial position of the magnetic flux and current pattern at zero applied current is now fixed. Considering the junction dynamics, the mechanism involved here is

\[ \text{Eq. (4.45) can also be written } \tilde{m}(\phi_0) = \Re \left[ \tilde{m} e^{-i\phi_0} \right]. \text{ Then } |\tilde{m}(\phi_0)| = |\tilde{m} e^{-i\phi_0}| \leq |\tilde{m}|, \text{ from which the first part of Eq. (4.51) follows. Introducing } M(\theta) = m(\theta) + 1 \text{ with } M(\theta) \geq 0 \text{ and } \tilde{m} = \tilde{M}, \text{ we find } |\tilde{m}| = |\tilde{M}| = \int d\theta/(2\pi) |M(\theta) e^{i\theta}| \leq \int d\theta/(2\pi) |M(\theta) e^{i\theta}| = \int d\theta/(2\pi) M(\theta) \theta = \int d\theta/(2\pi) (m(\theta) + 1) = 1, \text{ from which the second part of Eq. (4.51) follows, excluding the equality which only holds when } m(\theta) \equiv 0. \]
4.2. Limiting mechanisms for the critical current

\[ B = (B_\theta(\theta, z), B_z(\theta, z)) \]

Figure 4.5: Deformed flux pattern in the frustrated state \( N = \pm 1 \) of the inhomogeneous junction at the renormalized critical current (numerical result). The Josephson penetration depth is \( \lambda_J = 0.5R \) and the chirality positive \( (N = +1) \). The height of the cylinder is \( h = 3R \) and in terms of the Josephson penetration depth \( h = 6\lambda_J \). The inhomogeneity is created by introducing an angular dependent Josephson coupling implemented by modulating the coupling strength with \( m(\theta) = 0.2\cos(\theta) \), see Fig. B.3. The flux line now has a fixed initial position at the minimum of the modulation, here at \( \pi \). At a finite applied current it is shifted away in the direction of the Lorentz force (here counter-clockwise). Due to screening the current flows through the interface mainly at the top. Thus, the flux line is bent near the top where the Lorentz force is strongest.

Based on the Lorentz force effect. As the applied current is increased, the flux pattern is shifted away from this stable position and its orientation along the \( z \)-axis is no longer straight. Since the current is screened inside the junction, away from the top surface of the cylinder (in analogy with the topologically trivial junction), the phase now also depends on \( z \) and the flux line is shifted farther away from its initial position near the top edge of the cylinder where the current is injected and the Lorentz force therefore is the strongest. Naturally, this pinning effect also governs the dynamics in the limit \( \lambda_J \ll R, h \), where it is even stronger, as we will discuss below. This deformation is illustrated in Fig. 4.5 where we show the magnetic field \( B = B_\theta \hat{\theta} + B_z \hat{z} \) on the interface of the junction with the flux peak compensated by a weak but broad counter flux. Even at a finite applied current, the flux line pattern does not move because it is pinned by the junction inhomogeneity.

Once the applied current is larger than the renormalized critical current, the resulting Lorentz force is strong enough to overcome this pinning potential. This corresponds to a depinning transition of the magnetic flux and current pattern which then starts to move, resulting in dissipation with a non-vanishing voltage in the same way as discussed above.
4.2.4 Summary

To summarize, we have found a mechanism limiting the critical current for the topologically frustrated state of the Josephson junction which is fundamentally different from the standard limiting mechanism. Introducing the inhomogeneous Josephson coupling, the supercurrent is limited by the depinning transition of the spontaneously appearing flux pattern. The associated renormalized critical current is always below the critical current of the trivial state of the junction.

The different behavior of the junction in the topologically trivial and frustrated state, at zero and at finite applied current, and with a constant or modulated coupling strength is confirmed numerically. The sine-Gordon free energy given in Eq. (4.7), supplemented with a boundary term corresponding to the direct boundary conditions given in Eq. (4.14), is minimized numerically using the method described in Sec. 2.2.2. Details on the numerics are given in Sec. B.2.2. With our iteration process it is rather easy to test whether a solution exists or not, as the iteration either converges (pinned flux pattern) or runs without convergence (depinned flux pattern), leading to a solution varying in time as discussed above.

The results for the inhomogeneous junction are summarized graphically in Fig. 4.6, where we show both the flux and current pattern on the full cylindrical interface for the topologically trivial and the frustrated state of the junction at zero applied current at just at the critical current.

4.3 The pinning effect

We now discuss in detail the pinning effect emerging in the frustrated state of the inhomogeneous junction, focusing on the difference between the two limits of weak and strong coupling. The weak coupling limit, where $\lambda J \gg R, h$, is also referred to as a ‘short’ Josephson junction, and was used in the approximative approach outlined above. The strong coupling limit, where $\lambda J \ll R, h$, is also referred to as a ‘long’ Josephson junction, and the flux pattern becomes a well-localized flux line with broad counter flux.

We give analytical arguments for the behavior of the pinning energy and the critical current in both limits, while the interpolation between them is possible numerically.

4.3.1 Pinning energy

The first quantity we address is the pinning energy, a measure of the depth of the pinning potential associated with a given structure of the inhomogeneous Josephson coupling at zero applied current. Defining the coupling anisotropy again as in Eq. (4.40), we label the free energy density $f_{SG}[m(\theta)]$ through the presence of a modulation $m(\theta)$. We then define the pinning energy as

$$E_{\text{pin}} = \int_0^{2\pi} Rd\theta \int_0^h dz \{f_{SG}[m(\theta) \equiv 0] - f_{SG}[m(\theta)]\}. \quad (4.52)$$

We first consider the weak coupling limit where the above solutions can be used. No
4.3. The pinning effect

The pinning effect

- topologically trivial
- topologically frustrated

zero applied current

just at the critical current

Figure 4.6: Overview of the different behavior of the inhomogeneous Josephson junction in both the topologically trivial and frustrated state and both at zero and at the critical applied current. The Josephson penetration depth is \( \lambda_J = 0.5R \) and the chirality positive \( (N = +1) \). The height of the cylinder is \( h = 3R \) and in terms of the Josephson penetration depth \( h = 6\lambda_J \). The coupling strength is modulated with \( m(\theta) = 0.2\cos(\theta) \).

current \( I = 0 \) means \( \tilde{m}(\phi_0) = 0 \). To linear order in \( \epsilon \) we then find

\[
E_{\text{pin}} \approx \frac{2\pi Rh}{\lambda_J^2} |\tilde{m}| \propto J_c. \tag{4.53}
\]

Turning next to the strong coupling limit we have to consider a different solution of the sine-Gordon equation (4.11). As shown in Ref. [116], a good approximation for the phase \( \phi \) in a homogeneous junction with no applied current is given by the soliton solution

\[
\phi(\theta, z) = \theta - 4 \arctan \left( e^{(\theta - u)\Lambda} \right), \tag{4.54}
\]

where \( \Lambda = R/\lambda_J \gg 1 \). The parameter \( u \) determines the (variable) position of the flux line along \( \theta \), which for no applied current is also the center of the spontaneous current vortex. The soliton is localized enough to satisfy the periodic boundary condition in \( \theta \).

For the inhomogeneous junction case we assume the same basic soliton shape but with the initial position \( u_0 \) being fixed by the presence of the coupling anisotropy. It is then straightforward to calculate the pinning energy for this case as

\[
E_{\text{pin}} \approx \frac{4h}{\lambda_J} (-m(u_0)) \propto \sqrt{J_c}, \tag{4.55}
\]

where \( u_0 \) is the position of the minimum of \( m(\theta) \). As expected, the spontaneous current vortex is centered on the minimum of the pinning potential where the Josephson coupling strength is the weakest.
Figure 4.7: Numerical results of the pinning energy for the four sample modulations summarized in Table B.2. We show $\lambda J^2 E_{\text{pin}}$ in units of $2\pi Rh$ against $\lambda J$ and also indicate the limiting behavior. In the weak coupling limit $\lambda J \gg R, h$, the pinning energy saturates to a constant value given (in these units) by the renormalization factor $|\hat{m}|$, which is half the first cosine coefficient, and is 0.125 for $m_a,d$, 0.25 for $m_b$, and vanishes for $m_c$. In the strong coupling limit $\lambda J \ll R, h$, the pinning energy increases linearly with the slope proportional to the minimum of the modulation which is the same for $m_{a,c}$ and for $m_{b,d}$.

These limiting behaviors are well reproduced in our numerical treatment as illustrated in Fig. 4.7, where we show the full numerical results for the pinning energy for different sample modulations and specifically indicate the limiting behavior found through the analytical considerations above. We have chosen four sample modulations $m(\theta)$ based on cosines of different amplitudes and orders, capturing the main different possible behaviors. They are described in detail in Sec. B.2.2, summarized in Table B.2, and illustrated in Fig. B.3. There is an obvious regime change at $\lambda J \sim R$.

In summary, we find

$$\lambda J^2 E_{\text{pin}} \propto \begin{cases} 
\lambda J & \lambda J \ll R, h, \\
\text{const.} & \lambda J \gg R, h.
\end{cases}$$

(4.56)

4.3.2 Critical current

Next, we investigate the critical current itself, again considering the two limits. The same type of scaling we found for $E_{\text{pin}}$ is also visible here. The weak coupling limit has already been discussed above and in Eq. (4.51) we found

$$I_c \approx \frac{e \Phi_0 Rh |\hat{m}|}{4\pi d \lambda J^2} = I_{00} |\hat{m}| \propto J_c,$$

(4.57)

which depends directly on the modulation.

We then turn to the strong coupling limit\(^2\). When calculating the pinning energy we found that the initial position of the phase soliton from Eq. (4.54) is at the point of the

\(^2\) For this analysis I acknowledge substantial contributions by my collaborator Matthias Ossadnik.
4.3. The pinning effect

weakest coupling, i.e. the minimum of \( m(\theta) \). To analyze this limit further we now suggest treating the pinned magnetic flux line as an elastic string in a potential landscape. With a non-vanishing external current applied, this string will deform while the basic soliton shape is preserved. This leads to the simple approximation,

\[ \phi(\theta, z) = \theta + v(z) - 4 \arctan \left( e^{[\theta-u(z)]/\Lambda} \right), \]

where \( u(z) \) is the displacement of the flux line in the \( \theta \)-direction and \( v(z) \) a \( z \)-dependent phase shift. Based on the solution for the trivial state, and confirmed by the effective approach described in Sec. 4.6.1, we approximate \( v(z) \) as

\[ v(z) = \frac{\pi \lambda J}{4R} e^{(z-h)/\lambda J I}, \]

which already fulfills the boundary conditions for the applied current in Eq. (4.14). The boundary condition for the displacement \( u(z) \) is therefore \( \partial_z u(z) = 0 \).

Note that \( v(z) \) has an influence only very close to \( z = h \) within a range of \( \lambda J \ll h \). Below, we may therefore use an approach with an effective boundary condition for \( u(z) \),

\[ u'(h) = \frac{\pi \lambda J}{4R I}, \]

and neglect the influence of \( v(z) \). A detailed derivation of this effective strong coupling model can be found in the appendix to this chapter, Sec. 4.6.1.

We then insert the ansatz from Eq. (4.58) into the free energy and by making the approximations mentioned above we obtain the following effective functional for \( u(z) \),

\[ F^*[u] = \int_0^h dz \left[ \frac{1}{2} (u'(z))^2 + \frac{1}{2R^2} m(u(z)) \right]. \]

From this we find the variational equation

\[ u'' - \frac{1}{2R^2} m'(u) = 0. \]

This can also be viewed as the equation of motion for a particle whose position is given by a single coordinate \( u \) in a potential \( V(u) = -m(u)/2R^2 \) with \( z \) playing the role of time. The boundary conditions then correspond to the velocities at the ‘times’ \( z = 0 \) and \( h \). The stable initial position at \( u = u_0 \) is a maximum of the potential \( V(u) \). For non-vanishing \( I \) and \( h \gg \ell \) (see the length scale defined in Eq. (4.88)) we then interpret the situation as follows. At \( z = 0 \) the particle ‘starts’ at \( u(z = 0) \approx u_0 \) corresponding to the top of the potential. At the ‘time’ \( z = h \) the particle ends up at a position \( u(h) = u_1 \) of lower potential energy and has gained the ‘kinetic energy’

\[ \frac{(u'(h))^2}{2} = \left( \frac{\pi \lambda J I}{4\sqrt{2}R} \right)^2 = V(u_0) - V(u_1) = \frac{m(u_1) - m(u_0)}{2R^2}. \]

The maximum of this ‘kinetic energy’ corresponds to the maximum possible gain of potential energy,

\[ \Delta m = \max_{u_1} (m(u_1) - m(u_0)) = \max_{\theta} m(\theta) - \min_{\theta} m(\theta), \]
such that the maximal value of $I$ for which there is a solution of the variational equation (4.62) is given by

$$I_c = \frac{4\pi}{\lambda_J} \sqrt{\Delta m}.$$  \hspace{1cm} (4.65)

The critical current is therefore

$$I_c = 8R\lambda_J J_c \sqrt{\Delta m} \propto \sqrt{J_c},$$  \hspace{1cm} (4.66)

which scales similarly as the topologically trivial junction in this limit, see Eq. (4.15),

$$I_c = 4\pi R\lambda_J J_c.$$  \hspace{1cm} (4.67)

Before comparing the different results, we again have to consider how the modulation affects the situation in the trivial state of the junction limited by the standard mechanism and used as a reference. In the limit $\lambda_J \ll R, h$ the junction is ‘long’ in both directions and not only the local critical current density $J_c$ changes but the Josephson penetration depth $\lambda_J$ is modified as well. Where $J_c$ is locally enhanced, $\lambda_J$ becomes shorter. Since both these values influence the current density, there is not a simple current redistribution any more and the critical current is lower than in the basic homogeneous case since the region of weaker coupling strength (now on a length scale larger than the Josephson penetration depth) can provide an entry point for a vortex at the top. This is confirmed by numerics. Since also in the frustrated state the penetration of Josephson vortices from above provides the ultimate limit, there exist situations for the inhomogeneous junction where the critical current from the trivial state lies below the theoretical critical current for the frustrated state. Then, the effective critical current for the frustrated state would rather be the one from the standard mechanism. This, again, is confirmed by numerics. However, such situations only exist for very long junctions with a very strong and broad modulation.

In summary, we find the same basic scaling behavior for the critical current at a fixed height as for the pinning energy

$$\lambda_J^2 I_c \propto \begin{cases} \lambda_J & \lambda_J \ll R, h, \\ \text{const.} & \lambda_J \gg R, h. \end{cases}$$  \hspace{1cm} (4.68)

As before these limiting behaviors are well reproduced in our numerical treatment. The scaling behavior at a fixed height $h$ is shown in Fig. 4.8 where we again also indicate the limiting behavior and using the same sample modulations $m(\theta)$ as before.

### 4.4 Filamentary nucleation and evolution of the 3-Kelvin phase

The two different limiting mechanisms for the critical current established above can explain the presence of two distinct curves in the observed anomalous behavior of the critical current in Pb/Ru/Sr$_2$RuO$_4$ junctions [113], as discussed in Sec. 1.4.2. The next step is a discussion of the succession of the different states of the junction, illustrated in Fig. 1.6. While in Ref. [112], Kaneyasu et al. found a first order transition from the A-phase directly to the B-phase at a temperature well above the bulk critical temperature, the observed
4.4. Filamentary nucleation and evolution of the 3-Kelvin phase

Figure 4.8: Numerical results of the critical current at a height $h = 5R$ for the four sample modulations summarized in Table B.2. We show $\lambda^2 J_c/h$ in units of $\Phi_0 R^4/4\pi d$ against $\lambda J$ and indicate the limiting behavior. The critical current basically behaves like the pinning energy. In the weak coupling limit $\lambda J \gg R, h$, the critical current saturates to a constant value again given (in these units) by the renormalization factor $|\hat{m}_l|$, which is half the first cosine coefficient, and is 0.125 for $m_{a,d}$, 0.25 for $m_b$, and vanishes for $m_c$. In the strong coupling limit $\lambda J \ll R, h$, the critical current increases linearly with the slope now proportional to the square root of the amplitude of the modulation which is the same for $m_{a,c}$.

4.4.1 Phenomenological model

To address this issue, we have to take into account the spatial dependence both along the $z$-axis (proximity effect) as well as perpendicular to the interface in the radial direction (filamentary nucleation). For this we have to consider the full Ginzburg Landau free energy functional. Here, we formulate the most simple model possible that still includes all the main features. We neglect the actual structure of the proximity-induced superconductivity along the $z$-direction and treat the layers of Sr$_2$RuO$_4$ as independent. Rather, we minimize the free energy for different fixed absolute values of the induced $s$-wave order parameter and then combine the results in a phase diagram. To study the radial dependence perpendicular to the interface, the 3-Kelvin phase is described by an effective critical temperature, introduced in Ref. [112], for the enhanced critical temperature near the inclusion

$$T_c(r) = T_c + \frac{T_0 - T_c}{\cosh \left( \frac{r-R}{d} \right)},$$

(4.69)
where $T_c$ is the bulk critical temperature, $T_0 = T_c(R)$ the maximum value at the interface, $R$ the radius of the of the inclusion and $d$ the width of the filament assumed smaller than the coherence length $\xi_0$. We work in the isotropic limit such that the only angular dependence of the order parameter in the chiral $p$-wave state is the phase winding, while the order parameter in the $A$- and $A'$-phase has no angular dependence at all. The convenient representation is therefore $\eta = (\eta_r(r), i\eta_\theta(r))e^{iN\theta}$, which can describe all phases. The coupling to the $s$-wave order parameter is as described above for Eq. (4.2). Because the perpendicular component cannot couple, it is suppressed at the interface, described by an additional surface term. The interface free energy can then be written as

$$
\mathcal{F}_{\text{int}} = \int_0^{2\pi} R d\theta \left[ K_r |\eta_r|^2 - 2 K_\theta |\eta_\theta| |\psi_s| \cos(\phi - \theta) \right] - 2 \pi R \left[ K_r |\eta_r(R)|^2 - 2 K_\theta |\eta_\theta(R)| |\psi_s| \delta_{0,N} \right],
$$

(4.70)

where $K_r$ and $K_\theta$ are two phenomenological parameters, related to the basic coupling constant $K_c$ given in Eq. (4.2) above and the surface term coefficients $g_i$ discussed in Eq. (3.4) in the previous chapter. The angular integration for the last line is performed assuming $\psi_s = |\psi_s|e^{i\delta}$ with no angular dependence. While this coupling term neglects the actual structure of the phase difference $\phi(\theta)$ for the topologically frustrated state of the junction discussed at length above, it incorporates the main effect of frustration that in this state the coupling energy cannot be fully optimized anymore because of the phase mismatch. We also neglect the self-fields and any applied fields in this simple analysis.

Having integrated out the angular direction and neglecting the $z$-direction, the situation is reduced to a one-dimensional radial problem. All expansion coefficients take the values from the isotropic limit, see Sec. 2.1.2. The total free energy, labeled with the winding number $N$ determining the topological state, and for $\eta = (\eta_r(r), i\eta_\theta(r))e^{iN\theta}$, is given by

$$
\mathcal{F}[N] = \int_R^\infty r dr \left[ a(T - T_c(r)) \left( |\eta_r|^2 + |\eta_\theta|^2 \right) + \frac{b}{8} \left\{ 3|\eta_r|^4 + 3|\eta_\theta|^4 + 4|\eta_r|^2|\eta_\theta|^2 - \eta_r^2\eta_\theta^2 - \eta_\theta^2\eta_r^2 \right\} + K \{ \ldots \} \right] + R \left[ K_r |\eta_r(R)|^2 - 2 K_\theta |\eta_\theta(R)| |\psi_s| \delta_{0,N} \right],
$$

(4.71)

where the $\ldots$ stand for the gradient terms for polar coordinates and the above parametrization. The free energy of the Ru inclusion is not important for our analysis of the difference of the free energies for distinct sectors of $N$.

There are three important phenomenological parameters in this model, the interface critical temperature $T_0$, the width of the enhanced critical temperature $d$, and the surface coefficient $K_r$. While their effects are not independent, they can be partly understood as follows.

First, the width $d$ adjusts the placement of $T_B$ between $T_A$ and $T_{A'}$. For very large $d$, the $A$-phase would almost not be sustained, because the $B$-phase is energetically much more favorable on the Sr$_2$RuO$_4$ side. However, for the 3-Kelvin phase $d$ is estimated below to around at most the coherence length $\xi_0$, and we use a value $d = 0.5\xi_0$ here,
4.4. Filamentary nucleation and evolution of the 3-Kelvin phase

as in the previous work [112]. Next, the interface critical temperature $T_0$ can be used to adjust the nucleation of the A-phase at $|\psi_s| = 0$ to $T_A|\psi_s|=0 = T_{3K} \approx 2T_c$. Finally, the surface coefficient $K_r$ can be used to adjust the transition to the B-phase $T_B$ at $|\psi_s| = 0$ to $T_B|\psi_s|=0 \approx 2.4$ K, at which an additional signal in the critical current has been observed [110], and following the previous work [112]. Changing $K_r$ also shifts $T_A'$. The basic coupling constant $K_0$ could actually be absorbed in $|\psi_s|$ and therefore does not qualitatively change the phase diagram. All four parameters are fixed throughout our analysis, and are listed in Sec. B.2.2. The strength of the s-wave order parameter $|\psi_s|$ scans through different proximity-induced situations, and $N$ sets the topology of the bulk order parameter.

4.4.2 Phase diagram

The free energy is minimized numerically for $N = 0$ and $N = 1$ at a given temperature $T$ and a given proximity-induced order parameter $|\psi_s|$. We use the method introduced in Sec. 2.2.2, while the computational details are given in Sec. B.2.2, where we in particular also explain how to determine the different transition temperatures from the numerical data. Because we completely ignore the structure of the phase difference in the topologically frustrated state of the junction, the free energy for finite phase winding $F[N = 1]$ does not depend on $|\psi_s|$ and only has to be computed for different temperatures.

We then analyze the resulting free energies and their difference $F[N = 0] - F[N = 1]$, to find which phase is realized. From this we construct the full phase diagram for $|\psi_s|$ versus $T$ as shown in Fig. 4.9.

First, we consider the free energy $F[N = 0]$ for the topologically trivial state $N = 0$, ignoring for now that $F[N = 1]$ may be lower. There are three transitions. From the normal state to the A-phase at $T_A$, where the parallel component nucleates; from the A-phase to the A’-phase at $T_A'$, where also the perpendicular component nucleates and time reversal symmetry is broken; and from the A’-phase to the bulk at $T_c$. The last transition is first order, because the bulk necessarily has $N = 1$, while the other two are second order at $|\psi_s| = 0$. For finite $|\psi_s| = 0$ the nucleation at $T_A$ is actually only a crossover (no discontinuity in the second derivative of the free energy). The onset of the 3-Kelvin phase strongly depends on the value of $|\psi_s|$, which can be seen straightforwardly from the free energy. On the other hand, the transition to the A’-phase is rather rigid, because $|\psi_s|$ does not couple to the perpendicular order parameter component, and it is also straightforward to see that this transition can be adjusted with $K_r$. The bulk transition is strictly determined by $T_c$.

Next, we analyze the difference $F[N = 0] - F[N = 1]$ to determine which topological state is actually realized. The transition from a phase with $N = 0$ to a phase with finite $N = \pm 1$ is always first order, because the topology changes. There are three possibilities, depending on the strength of the induced s-wave order parameter. At zero and low $|\psi_s|$, there is a direct transition from the A-phase to the B-phase, in agreement with the previous result of Ref. [112]. At an intermediate value of $|\psi_s|$, the perpendicular component first appears in the A’-phase, but there is still a transition to the B-phase before the bulk transition. Finally, at high values of $|\psi_s|$, the A’-phase extends all the way to the bulk transition. At the bulk critical temperature $T_c$ there would be a first order transition to the bulk chiral.
Figure 4.9: Phase diagram of $|\psi_s|$ versus $T$ for the evolution of the 3-Kelvin phase, see Fig. 1.6 for an illustration of the three different phases. The normal state is colored light blue, the topologically trivial state with $N=0$ is white, and the topologically frustrated state with a finite phase winding $N=1$ is colored light red. The filamentary A-phase nucleates at $T_A$ (blue), the perpendicular order parameter in the phase with no winding $N=0$ nucleates at $T_A'$ (cyan), while the first order transition to the B-phase with finite winding $N=1$ is at $T_B$ (red). The extension of $T_B$ beyond the bulk critical temperature $T_c$ is a purely numerical effect because of the finite system size and is therefore indicated light red only.

$p$-wave state, while for the numerical results $T_B$ extends beyond $T_c$ because of the finite system considered.

This succession of the different phases is a direct result of the way we have constructed the coupling term. Even though the model is extremely simple and many effects have been approximated or neglected, we have confirmed the overall picture that a strong proximity-induced superconductivity in the Ru inclusion extends the topologically trivial phase with $N=0$ until the bulk transition, to avoid the unfavorable frustrated state. More details on this project can be found in our publication [127].

4.5 Conclusion

Recent experiments have studied the Josephson effect between a conventional superconducting Pb film and the presumably chiral $p$-wave superconducting bulk of Sr$_2$RuO$_4$ through Ru-metal inclusions [113]. Maeno et al. found an anomalous temperature dependence of the critical current. Here we have analyzed a model situation of a single cylindrical Ru-inclusion carrying a superconducting $s$-wave order parameter which is coupled through the interface to the $p$-wave order parameter in the bulk material Sr$_2$RuO$_4$. We have considered two topologies for the $p$-wave order parameter, the trivial and the chiral one, which appear in the 3-Kelvin phase and the bulk phase of Sr$_2$RuO$_4$, respectively.
4.5. Conclusion

Due to the cylindrical geometry the chiral topology leads to a frustrated junction, while the trivial one is not frustrated. This frustration causes a rather distinct behavior when an externally applied current runs through the junction.

While the topologically trivial junction behaves as expected for an extended Josephson junction in both the long and the short junction limit, the frustrated junction is characterized by the appearance of a spontaneous magnetic flux on the interface already at zero applied current. In the case of a rotationally symmetric junction this prevents the flow of a supercurrent since the flux pattern, driven by the Lorentz force, immediately starts to move, leading to dissipation. Only pinning the flux pattern through an inhomogeneous Josephson coupling and thus breaking the rotational symmetry stabilizes the supercurrent, now limited by a pinning-depinning transition. As long as moderate modulations are considered, the critical current is always smaller in the frustrated junction, even if the average coupling strength is the same as in the corresponding trivial junction for which the vortices involved in the dynamics are only created with increasing current and are not spontaneously present.

In our model we have simplified the modulation of the Josephson coupling by allowing only angular modulations and keeping it constant along the z-axis. This clearly leads to stronger pinning, analogous to columnar pinning for vortex lattices. As a further simplification the spatial dependence of the proximity induced superconducting order parameter in the Ru inclusion is ignored. However, we do not expect qualitative differences concerning the reduction of the critical current in the frustrated case, while the scaling behavior in the two junction limits may be different. Also, there exist extreme situations of very long junctions with a very strong modulation where the frustrated case is effectively limited by the standard mechanism.

In addition, we have presented a phase diagram showing that if there is a coupling to the proximity-induced order parameter in the Ru inclusion, the transition from the topologically trivial state with $N = 0$ to the topologically frustrated state with $N = 1$ is essentially reduced to the bulk transition temperature. We therefore propose that this is a possible way to explain the rather sharp drop in the critical current seen at the transition temperature $T_c \approx 1.5$ K, associated with a change in the topology of the $p$-wave order parameter. Thus, $T_c$ sets the boundary between the frustrated and trivial Josephson junction and also between the different topologies for the $p$-wave order parameter of the Sr$_2$RuO$_4$.

As a final note, throughout the above discussion we have assumed an isotropic system, except for the modulation making the coupling inhomogeneous. However, even away from the isotropic limit, as studied in the other chapters, the underlying mechanism would qualitatively still be the same. Actually, the coupling strength can become intrinsically anisotropic by considering $\eta_\parallel(r, \theta)$ with an angular dependence.
4.6 Appendix
In this appendix we derive the effective strong coupling model used above in Sec. 4.3.2.

4.6.1 Effective strong coupling model
We derive here\(^3\) the effective free energy functional \(F^*[u(z)]\) for the displacement \(u(z)\) of the spontaneous flux line. We insert the ansatz for \(\phi(\theta, z)\) from Eq. (4.58) into the sine-Gordon free energy from Eq. (4.7) including a modulation \(m(\theta)\) of the coupling strength. Averaging the different terms over \(\theta\) we find

\[
\left\langle \left( \frac{\partial \phi}{\partial z} \right)^2 \right\rangle_\theta = \left( \frac{1}{\cosh[\Lambda(\theta - u)]} \right)^2 \approx \frac{4\Lambda}{\pi} - 1, \tag{4.73}
\]

and

\[
\left\langle (1 + m(\theta)) \cos(\phi - \theta) \right\rangle_\theta = \left( (1 + m(\theta)) \cos v \left( 1 - \frac{2}{\cosh^2[\Lambda(\theta - u)]} \right) \right) - \left( (1 + m(\theta)) \sin v \frac{2 \sinh[\Lambda(\theta - u)]}{\cosh^2[\Lambda(\theta - u)]} \right) \approx \cos v \left( 1 - \frac{2}{\pi \Lambda} (1 + m(u)) \right) - \sin v \frac{1}{\Lambda^2} m'(u). \tag{4.74}
\]

Collecting all terms depending on \(u(z)\) and \(v(z)\) while dropping the constants and a global prefactor we find

\[
F[u, v] = \int_0^h dz \left[ \left( \frac{u'}{2} \right)^2 + \frac{1}{2R^2} m(u) \cos v + \frac{\pi \lambda_j}{4R} m'(u) \sin v + \frac{\pi \lambda_j}{4R} u' v' \right. \left. + \frac{\pi \lambda_j}{4R} \left( \frac{(v')^2}{2} - \frac{1}{\lambda_j^2} \cos v \right) \right], \tag{4.75}
\]

with the boundary conditions

\[
\begin{align}
&v'(h) = I, \quad v'(0) = 0, \tag{4.76a} \\
&u'(h) = 0, \quad u'(0) = 0. \tag{4.76b}
\end{align}
\]

First, we consider the leading terms in the variation of \(F\) with respect to \(v\),

\[
v'' = \frac{1}{\lambda_j^2} \sin v, \tag{4.77}
\]

which is solved approximately by

\[
v(z) = \lambda_j e^{(z-h)/\lambda_j I}, \tag{4.78}
\]

\(^3\) For this model I acknowledge substantial contributions by my collaborator Matthias Ossadnik.
which is consistent with the guess based on the solution from the trivial case in Eq. (4.59). This solution is confined in a very narrow region $h - \lambda_J \leq z \leq h$, where the variation of $F$ with respect to $u$ is

$$u'' = -\frac{\pi \lambda_J}{4R} v''.$$  

(4.79)

Integrating and taking into account the boundary condition we then obtain close to $z = h$

$$u'(z) = -\frac{\pi \lambda_J}{4R} \left\{ e^{(z-h)/\lambda_J} - 1 \right\}. \quad (4.80)$$

In the range $0 \leq z \leq h - \lambda_J \sim h^*$ we can therefore describe the behavior of $u(z)$ using the above functional with $v(z) \approx 0$,

$$F^*[u] = \int_0^{h^*} dz \left[ \frac{(u')^2}{2} + \frac{1}{2R^2} m(u) \right], \quad (4.81)$$

and with an effective boundary condition

$$u'(h^*) = \frac{\pi \lambda_J}{4R} I. \quad (4.82)$$

The additional bending of $u(z)$ in the range $h^* < z \leq h$ is neglected. This approach is used in Sec. 4.3 to discuss the pinning effect of the flux line, approximating $h^* \approx h$. In Fig. 4.10 we show both the full $u(z)$ and the linear extrapolation corresponding to the effective model with $h^* = h$.

While $u(z)$ captures the displacement of the flux line, the actual position $w(z)$ of the current vortex is given through the condition

$$J_r(w(z), z) = 0. \quad (4.83)$$

Our ansatz leads to

$$w(z) = u(z) + \lambda_J \log \left( \tan \left( \frac{v(z) + \pi}{4} \right) \right) \approx u(z) + \lambda_J \frac{v(z)}{2}. \quad (4.84)$$

The flux line displacement $u(z)$ and the current vortex $w(z)$ can be extracted from the numerical data through

$$u(z) = \min_{\theta} B_2(\theta, z), \quad (4.85)$$

and indirectly through

$$\phi(\theta, z) = \theta + \pi \text{ at } \theta = w(z), \quad (4.86)$$

using the current-phase relation. Both $u(z)$ and $w(z)$ are plotted in Fig. 4.10, highlighting the meaning of $h^*$.

Note that for solutions close to the minimum $u = u_0$ of $m(u)$ there is a natural length scale $\ell$ found through the parabolic approximation

$$F^*[u] = \int_0^{h^*} dz \left[ \frac{(u')^2}{2} + \frac{1}{4R^2} m''(u_0) u^2 \right], \quad (4.87)$$

and given by

$$\ell = \sqrt{\frac{2R^2}{m''(u_0)}}, \quad (4.88)$$

We assume that $\lambda_J \ll \ell \ll h^*, h$.  

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Figure 4.10: Flux line displacement \( u(z) \) and vortex position \( w(z) \) at the renormalized critical current \( I = I_c \) just before depinning. The Josephson penetration depth is \( \lambda_J = R/15 \), the height of the cylinder is \( h = 20R \), and in terms of the Josephson penetration depth it is \( h = 300\lambda_J \). The coupling strength is modulated by \( m(\theta) = 0.2 \cos(\theta) \) with the initial position of both the flux line and the current vortex being at \( \pi \). The inset shows a close-up of the region \( h - 3\lambda_J < z \leq h \) where \( u(z) \) and \( w(z) \) differ. For most of the height, however, both lines are the same. The inset also shows the linear extrapolation of \( u(z) \) after \( z = h^* = h - \lambda_J \), which is used in our effective model where we take the slope at this point, \( u'(h^*) \), as an effective boundary condition.
Chiral p-wave superconductors have two degenerate ground states, such that domains of opposite chirality can form as introduced in Sec. 1.4.3. Here, we such study domains along the c-direction.

In the first part, the stable configurations of the domain wall are discussed by deriving the energetically favorable phase differences, taking into account the anisotropy of the electronic structure. These have a non-trivial periodicity of $\pi$, such that the smallest supported vortex carries only half a flux-quantum. In the second part the structure of this vortex is examined. On the one hand, the results over the full range of anisotropies are computed numerically. On the other hand, the limiting behavior is explained using a phenomenological sine-Gordon model.

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This chapter is based on S. B. Etter, W. Huang, and M. Sigrist, in preparation.
5.1 Stable domain wall configurations

We start with a discussion of the basic behavior of domains of opposite chiralities along the c-axis, taking into account the anisotropy $\nu$ of the electronic structure introduced in Sec. 2.1.2 and illustrated in Fig. 2.2. Because these c-axis domain walls are translationally invariant in the basal plane, no in-plane derivatives enter. Therefore, this discussion is valid in general for the weak-coupling limit.

While the shape of the order parameter obviously changes across the domain wall, an overall phase might be acquired in addition. We first show which phase change minimizes the free energy, depending on the sign of the anisotropy $\text{sgn}(\nu)$ only. Next, we discuss and compare an approximative analytical and a numerical solution for the shape of the order parameter and the free energy, which both only depend on the magnitude of the anisotropy $|\nu|$.

5.1.1 Phase change across the domain wall

For the discussion of domain walls it is convenient to use the ±-representation for the order parameter, $\eta = (\eta_+, \eta_-)$, directly relating to the two degenerate chiral ground states, and to treat the complex order parameter components in an amplitude and phase parametrization, $\eta_\pm = |\eta_\pm| e^{i\phi_\pm}$, as described in Sec. 2.1.1. Using the gauge $A_z = \partial_z \phi_+$, only the phase difference $\varphi = \phi(z > z_{dw}) - \phi(z < z_{dw})$ enters the free energy, which is then given by

$$\mathcal{F}[\eta_+, \eta_-] = \int dz \left[ 2a(T - T_c) (|\eta_+|^2 + |\eta_-|^2) + (2b_1 + b_2) \left(|\eta_+|^4 + 4|\eta_+|^2|\eta_-|^2 + |\eta_-|^4\right) \right]$$

$$+ (4b_1 - 6b_2) \left(|\eta_+|^2|\eta_-|^2 \cos(2\varphi)\right) + 2K_5 ((\partial_z |\eta_+|)^2 + (\partial_z |\eta_-|)^2 + |\eta_-|^2 (\partial_z \varphi)^2),$$

(5.1)

neglecting any variations in the phase far away from the domain wall, where one component vanishes identically and the phase can vary freely without any cost in energy. All in-plane derivatives and vector potentials vanish due to the assumed translational invariance.

The free energy from Eq. (5.1) is clearly minimized when $\varphi = \text{const}$, such that $\partial_z \varphi = 0$. The c-axis domain wall (at $z = 0$) is then modeled by the boundary conditions

$$\begin{align*}
(\eta_+, \eta_-) &= (|\eta_0|, 0) \quad (z \to -\infty) \quad (5.2a) \\
(\eta_+, \eta_-) &= (0, |\eta_0| e^{i\varphi}) \quad (z \to \infty), \quad (5.2b)
\end{align*}$$

where $|\eta_0|^2 = -a(T - T_c)/(4b_1 - b_2 + b_3)$ is the bulk value. Symmetry considerations lead to the general structure $(\eta_+(z), \eta_-(z)) = |\eta_0| \left(u(z), u(-z) e^{i\varphi}\right)$, with $u(z)$ real and positive, but not necessarily symmetric with respect to the domain wall, and with the boundary conditions $u(z \to -\infty) = 1$ and $u(z \to \infty) = 0$.

Taking into account the anisotropy of the electronic structure $\nu$ to determine the expansion coefficients of the Ginzburg Landau free energy functional for weak-coupling, the only term left depending on the phase change $\varphi$ is given by

$$f_\varphi = 2(2b_1 - 3b_2)|\eta_+|^2 |\eta_-|^2 \cos(2\varphi) = 2\nu b_1 |\eta_+|^2 |\eta_-|^2 \cos(2\varphi).$$

(5.3)
The sign of the anisotropy thus determines the energetically favorable phase change $\varphi$ across the domain wall, which is given by

$$
\varphi = \begin{cases} 
0 \mod \pi & \nu < 0 \\
\pi & \nu = 0 \\
\pi \mod \pi & \nu > 0.
\end{cases}
$$

(5.4)

In the isotropic limit $\nu = 0$, the phase difference is fully degenerate, corresponding to the absence of any Josephson-like coupling between the two domains. This limit describes a completely rotationally invariant system where the Cooper pair orbital angular momentum is a good quantum number and must be conserved during the tunneling event. Pair tunneling is then strictly prohibited between the two domains of opposite chirality, in agreement with these results. Once the rotational symmetry is broken for finite anisotropies $|\nu| > 0$, due to both band and gap structure effects, the angular momentum is no longer a good quantum number and the Cooper pair tunneling is allowed. The two domains are coupled and a finite Josephson current can flow parallel to the $c$-axis. The domain wall thus constitutes an effective Josephson junction. Given the non-trivial $\pi$-periodicity of the discrete allowed values for the phase difference, we explore the possibility of a half-quantum vortex in such junctions in Sec. 5.2.

5.1.2 Shape of the order parameter across the domain wall

To find the shape of the order parameter across the domain wall, we plug the resulting phase change $\varphi$ from Eq. (5.4) into the functional from Eq. (5.1). The resulting free energy, and thus the shape of the order parameter, only depend on the magnitude of the anisotropy $|\nu|$. Following the approach of Sigrist and Agterberg [119], see also Ref. [120], we approximate $|\eta|^2 = |\eta_b|^2$ and use the ansatz $(\eta_+, \eta_-) = |\eta_b| (\sin(\chi(z)), \cos(\chi(z)) e^{i\varphi})$. The boundary conditions from Eq. (5.2) translate to $\chi(z \to -\infty) \to \pi/2$ and $\chi(z \to \infty) \to 0$, and the free energy simplifies to

$$
F = \int d z \left[ 2 a (T - T_c)|\eta_b|^2 + b |\eta_b|^4 + \frac{b|\eta_b|^4}{2} (1 - |\nu|) \sin^2(2\chi) + 2 K_5 |\eta_b|^2 (\partial_z \chi)^2 \right].
$$

(5.5)

Variation with respect to $\chi$ leads to the sine-Gordon type partial differential equation

$$
\partial_z^2 \chi(z) = \frac{b|\eta_b|^2 (1 - |\nu|)}{4 K_5} \sin(4\chi(z))
$$

(5.6)

with the standard solution, using $\xi_c(T) = \sqrt{K_5/(b|\eta_b|^2)}$,

$$
\chi(z) = \arctan \left( \exp \left( -\sqrt{1 - |\nu|} \frac{z}{\xi_c} \right) \right).
$$

(5.7)

The width of the domain wall therefore scales as $\xi_c/\sqrt{1 - |\nu|}$. Plugging this solution back in, we find the free energy density per unit in-plane area

$$
F - F_0 = \frac{3}{\sqrt{2}} b |\eta_b|^4 |\xi_c| \sqrt{1 - |\nu|},
$$

(5.8)
Figure 5.1: The shape of the amplitude of the order parameter and its two components across the $c$-axis domain wall for the different anisotropies $|\nu| \in \{0, 0.3, 0.5, 0.7, 0.9, 0.95\}$. The shape only depends on the absolute value of the anisotropy $|\nu|$, and the width of the domain wall explodes for $|\nu| \to 1$. The total absolute value $|\eta|$ is suppressed at the domain wall, the most for $\nu = 0$.

where $F_0$ is the bulk free energy without any domain wall. The cost of the domain wall is largest in the isotropic limit $\nu = 0$, where the two domains are decoupled, as discussed above. In the limit $|\nu| \to 1$, the domain wall comes at no cost at all and its width stretches to infinity, because for a square-shaped system the two order parameter components are decoupled. Compared to the in-plane domain wall depending on $\xi_{ab}$, the $c$-axis domain wall depends on $\xi \ll \xi_{ab}$ and is thus energetically much more favorable.

We also compute the shape of the amplitude of the order parameter components and the free energy of the domain wall self-consistently by minimizing the full free energy numerically at fixed values of the phase difference $\phi$. We use the method introduced in Sec. 2.2.2, while the computational details are given in Sec. B.2.3.

In Fig. 5.1 we show both the amplitude of the two components, $|\eta_+|$ (red) and $|\eta_-|$ (blue), and the total absolute value $|\eta|$ (black), all at $\nu = 0$ (thick). In addition, we indicate the results at higher values of $\nu$ (thin), where we observe the described increase of the width of the domain wall with increasing $\nu$, stretching to ‘infinity’ as $|\nu| \to 1$. This effect is limited here by the finite numerical system size. The total absolute value is suppressed at the domain wall to lower the weight of the coupling term. This suppression is the largest for $\nu = 0$ and decreases with increasing $\nu$. For the approximative solution we neglected this effect and assumed $|\eta| = |\eta_b|$ everywhere. These results for $|\eta_+|$ and $|\eta_-|$ agree with the above-mentioned symmetry $(\eta_+, \eta_-) \propto (u(z), u(-z))$.

In Fig. 5.2 we show the numerical results for the free energy density of the domain wall for $\phi = \{0, \pi/2\}$ (empty and filled dots), together with the approximative analytical solution from Eq. (5.8) (solid black line), as function of the anisotropy $\nu$. We also indicate a fit to the numerical data (red line) and its linear expansion (dashed red line), used below in Sec. 5.2.2. First, we confirm the energetically favorable phase changes $\phi$ as given in Eq. (5.4). Second, the qualitative agreement of the numerical and approximative analytical solution is good, with the quantitative difference between them largest at $\nu = 0$, when $|\eta|^2$
5.1 Stable domain wall configurations

Figure 5.2: Free energy density per unit area of the c-axis domain wall comparing the approximative analytical solution (solid black line) with the numerical data for \( \varphi = 0 \) (empty dots) and \( \varphi = \pi/2 \) (filled dots). The former phase difference minimizes the free energy when \( \nu < 0 \), and the latter when \( \nu > 0 \). We also indicate a fit to the numerical data (solid red) and its linear expansion for small \(|\nu| \ll 1\) (dashed red), used in Sec. 5.2.2.

is suppressed the most at the domain wall. Third, the symmetry \( F[\nu, \varphi] = F[-\nu, \varphi + \pi/2] \) always holds, even for the non-minimizing branch.

Finally, let us briefly comment on comparing the numerical (exact) result of the shape of the order parameter with the approximative analytical solution. Using the symmetry \((\eta_+, \eta_-) \propto (u(z), u(-z)e^{i\varphi})\) we can access the error that we make in the approximation by rewriting the exact result as \((\eta_+, \eta_-) = |\eta| (\sin(\chi(z)) \epsilon(z), \cos(\chi(z)) \epsilon(-z)e^{i\varphi})\). The error \(\epsilon(z)\) is largest at the domain wall, where the overall amplitude \(|\eta|^2\) is suppressed the most, which we approximated by the constant value \(|\eta_0|^2\) everywhere. However, just at \(z = 0\) the errors of \(\eta_+\) and \(\eta_-\) coincide by symmetry (both are \(\epsilon(0)\)). Therefore, extracting \(\arctan(|\eta_+|/|\eta_-|)\) of the numerical values achieves the best coincidence with the approximative \(\chi\), because the two errors cancel just where they are biggest, in contrast to extracting, for example, \(\arccos(|\eta_+|)\). This is illustrated in Fig. 5.3.

5.1.3 Bogoliubov-deGennes approach

In the Ginzburg Landau framework discussed above we have taken into account the band structure and gap function details with the single anisotropy parameter \(\nu\) for a weak-coupling approach, entering in the expansion coefficients of the free energy functional. Consistent results were also obtained from the study of a Bogoliubov-deGennes approach for the \(\gamma\)-band on a square lattice, analyzed by Wen Huang. For the two different pairings \(\Delta \propto (\sin k_x + i \sin k_y)\) and \(\Delta \propto (\sin k_x \cos k_y + i \cos k_x \sin k_y)\) he computed the value of the anisotropy \(\nu\), and the domain wall energy as a function of the phase change \(\delta E(\varphi)\), for different fillings. The energetically favorable values for the phase change as given above in Eq. (5.4) are recovered for both forms of the gap function. Further details can be found in our forthcoming publication.
5.2 Half-quantum vortex

For bulk vortices in conventional or one-component superconductors, the phase of the order parameter winds by an integer multiple of $2\pi$ around the singularity at the line defect. For multi-component superconductors, on the other hand, each order parameter component can wind separately, such that more intricate structures with fractionally quantized vortices are possible \[51\]. The different components, however, are always coupled and closely related. Therefore, simply changing the relative phase throughout the system is not energetically favorable and bulk fractional vortices are not energetically stable\(^1\). A special situation occurs at domain walls where the relative phase already changes anyway. Here, fractional vortices can be stabilized and lead to interesting phenomena \[118, 119\].

The $c$-axis domain wall considered above also supports such fractional vortices, but limited to carrying (integer multiples of) half a flux quantum (HQV). This is seen straightforwardly from the non-trivial $\pi$-periodicity of the phase change across the domain wall from Eq. (5.4) and the underlying $\cos(2\varphi)$ coupling term, such that a $\pi$-kink is the smallest possible increase of the phase change between two stable states.

Here, the structure of such HQVs is explored. The in-plane translational symmetry is now broken and all gradient terms have to be taken into account. The anisotropy $\nu$ can also be used to parametrize the ratios of the gradient term expansion coefficients, see Eq. (2.25), but only in a quasiclassical approach, while the discussion of the previous section holds in general for weak-coupling. For negative anisotropies\(^2\) $\nu < 0$, the values $\varphi = 0$ and $\varphi = \pi$ are the two degenerate phase changes. A line defect on the domain wall is introduced along the $y$-direction at $(x, z) = (0, 0)$, with the boundary conditions $\varphi = 0$ for $x \to -\infty$ and $\varphi = \pi$ for $x \to \infty$, as illustrated in Fig. 5.4. In addition, we set a phase shift of $\pm \pi/2$ for $z \gtrless 0$ along the $x$-direction to connect the two stable domain wall states. In

\(^1\) This holds for axial structures, while core-splitted vortices can appear, where the singularities for the two components are spatially separated, see Sec. V.B.2 in Ref. \[55\].

\(^2\) Treating $\nu > 0$ is analogous, but with the HQV oriented at an angle $\theta = \pi/4$ in the basal plane.
5.2. Half-quantum vortex

Figure 5.4: Setup of the half quantum vortex $B_y$ with $J_{xz}$ on the $c$-axis domain wall (blue) with all resulting states of the order parameter $(\eta_+, \eta_-)$ indicated. The anisotropy is $\nu < 0$, with the allowed phase differences across the junction of 0 and $\pi$ (blue arrows). Phase shifts $\pm \pi/2$ (red arrows) perpendicular to the domain wall connect the two stable configurations.

The resulting states of the order parameter $(\eta_+, \eta_-)$ are indicated in Fig. 5.4. The domain wall at $z = 0$ separates $\eta_+$ for $z < 0$ from $\eta_-$ for $z > 0$. The line defect on the domain wall at $x = 0$ separates the phase changes $\varphi = 0$ for $x < 0$ from $\varphi = \pi$ for $x > 0$. Going clockwise around the HQV, the order parameter takes the following values. First, starting at $x < 0$ and $z < 0$ in the $\eta_+^+$-domain, $(\eta_+, \eta_-) = \eta_b(1, 0)$. Crossing the domain wall upwards along the $z$-direction without a phase change, the order parameter at $x < 0$ and $z > 0$ is $(\eta_+, \eta_-) = \eta_b(0, 1)$. With the $\pi/2$-phase shift along the $x$-direction, the order parameter at $x > 0$ and $z > 0$ is $(\eta_+, \eta_-) = \eta_b(0, i)$. Crossing the domain wall again, down along the $z$-direction, now the phase change is $\pi$ and the order parameter at $x > 0$ and $z < 0$ is $(\eta_+, \eta_-) = \eta_b(-i, 0)$. Finally, with another $\pi/2$-phase shift along the $x$-direction, the initial value is recovered.

The winding of a single component out of the two-component order parameter is not apparent straightforwardly. To see this feature, the order parameter is represented as

$$\eta = (\eta_1, \eta_2) = \frac{1}{\sqrt{2}}(\eta_x - \eta_y, \eta_x + \eta_y) = \frac{1}{\sqrt{2}}((1 - i)\eta_+ + (1 + i)\eta_-, (1 + i)\eta_+ + (1 - i)\eta_-),$$

which corresponds to the representation for an in-plane rotation by $-\pi/2$, as can be seen from a comparison with Eq. (3.1). These two components are illustrated in Fig. 5.5 with a three-dimensional plot of their amplitude and a colored density plot of their phase beneath.
Figure 5.5: The two order parameter components $\eta_1$ and $\eta_2$ from the representation given in Eq. (5.9). The three-dimensional plots show the absolute value and the colored density plots indicate the phase of each component around the HQV at $(x, z) = (0, 0)$, extracted from numerical data for $\nu = -0.11$. The $\eta_1$ component winds by $2\pi$ and is suppressed to zero at the singularity of the HQV, while the $\eta_2$ component has no phase winding but is enhanced at the HQV. Both components are suppressed at the domain wall.

What is the size of such a HQV? Perpendicular to the domain wall it is screened efficiently by in-plane currents on the length scale $\lambda_{ab}$. The extension along the domain wall, however, is a more complicated issue. As discussed above, the maximal current through the domain wall strongly depends on the anisotropy $\nu$. In the isotropic limit $\nu = 0$, no current can flow, while there is a finite current parallel to the $c$-axis for any anisotropy $|\nu| > 0$. Treating the domain wall as an effective Josephson junction, we find that this critical current approximately scales as $J_c \approx |\nu|$ (details see Eq. (5.13) below). The size of a Josephson vortex is determined by the Josephson penetration depth $\lambda_J \propto 1/\sqrt{J_c}$, see Sec. 1.2.2, such that the extension of the HQV should approximately scale as $\lambda_J \approx 1/|\nu|$. Therefore, near the isotropic limit $|\nu| \ll 1$, the vortex explodes along the domain wall. For higher values of $|\nu|$ we have to consider that in addition, for layered superconductors, the superconducting anisotropy $\gamma_s = \xi_{ab}/\xi_c$ leads to different screening lengths $\lambda_{ab}$ and $\lambda_c \gg \lambda_{ab}$ for screening currents parallel and perpendicular to the layers, respectively, as discussed in Sec. 2.1.2 and illustrated in Fig. 2.1. Therefore, while for conventional Josephson junctions usually $\lambda_J \gg \lambda_L$, for the situation considered here, these two length scales are of comparable size already at a very small value of $\nu \approx 0.04$ (see Eq. (5.19) below). Once $\lambda_J < \lambda_c$, non-local Josephson electrodynamics have to be considered, as reviewed in Ref. [48]. The long-range screening behavior is then Abrikosov-like, on the length scale $\lambda_c$, while the core remains Josephson-like and has a new characteristic length $l = \lambda_J^2/\lambda_c < \lambda_J$.

The detailed structure of the HQV is computed by self-consistently minimizing the free energy numerically using the method described in Sec. 2.2.2. Because of the two different length scales $\lambda_c$ and $l$ entering, the numerics are rather involved, as described in detail in the appendix in Sec. B.2.3. To facilitate the computations, a value of $\gamma_s = 10$ is used below, while the $\gamma_s = 20$ found in the literature for Sr$_2$RuO$_4$ [62] was used above. We first present and discuss the numerical results for a single HQV to confirm the general setup. Next, we analyze the overall phenomenology for treating the domain wall as an effective Josephson...
5.2. Half-quantum vortex

The numerical minimization of the free energy leads to the detailed shape of the order parameter and the vector potential around the HQV. Here it is convenient to use the real and imaginary parts of the order parameter components $\eta_x$ and $\eta_y$ as arguments for the free energy. For the vector potential, because of the assumed translational invariance along the $y$-direction, we use the partial gauge $A = (A_x, 0, A_z)$, but see comment below.

Different quantities extracted from the result for the order parameter at an anisotropy $\nu = -0.11$ are shown in Fig. 5.6, with the position of the HQV at $(x, z) = (0, 0)$ indicated by a black dot. The relative phase between the $x$- and the $y$-component of the order parameter is shown on the top left. It is $+\pi/2$ for $z > 0$ and $-\pi/2$ for $z < 0$, in accordance with the setup. This confirms the presence of the domain wall even with the HQV. The total absolute value $|\eta|^2$ is shown on the top right. As discussed above, it is suppressed at the domain wall. Now, it is additionally suppressed at the HQV. The global phase $\phi_x = \arg \eta_x$ is shown on the bottom left. The phase changes $\varphi = 0$ for $x < 0$ and $\varphi = \pi$.
The magnetic structure of the HQV is analyzed in Fig. 5.7. A density plot of the magnetic field $B_y(x, z)$ is shown on the top, with an inset zooming in on its center, where a vector plot of the current field $(J_x, J_z)$ is also shown. As described above, depending on the anisotropy $\nu$, there are two length scales describing the HQV, one for its long-range behavior and one for $x > 0$ are confirmed, as are the two phase shifts of $\pm \pi/2$ along the $x$-direction for $z \geq 0$. Finally, the $\pi$-kink in the phase difference between the $\eta_+$ and the $\eta_-$ component along the domain wall, $\varphi = \phi_- - \phi_+$, is shown on the bottom right. This quantity is associated with the Josephson phase difference when treating the domain wall as an effective Josephson junction.

Figure 5.7: The magnetic structure of the HQV at $(x_0, z_0)$ for $\nu = -0.11$. (top) Magnetic field $B_y$ with a zoom into the center, also showing the current $J_{xz}$. (bottom left) Flux $\Phi$ contained in a box of width $2w$ and covering all of the $z$-direction. The width $w_{\text{box}}$ of a box containing $0.49\Phi_0$ is also indicated in the field plot. (bottom right) Profile of the current $J_z$ across the domain wall (solid) and its inverse (dashed).
for the core. A measure of the full size of the HQV is given by the flux through a strip from \( x = -w \) to \( x = +w \), and extending along the whole system in the \( z \)-direction

\[
\Phi(w) = \int_{-\infty}^{\infty} dz \int_{-w}^{w} dx B_y(x, z),
\]

(5.10)
as shown on the bottom left. We then define \( w_{\text{box}} \) from the width \( 2w_{\text{box}} \) of the strip containing 0.49\( \Phi_0 \), indicated in \( \Phi(w) \) and also in the density plot of the flux. A measure for the core is defined through the current across the domain wall, \( J_z(x, 0) \), as shown on the bottom left. The size of the core of the vortex is then defined as the position \( x_{\text{max}} \) of the maximal current across the domain wall \( J^\text{max}_z \), which we associate with the critical current of the domain wall. In addition, \( -J_z(-x) \) is shown (dashed), which indicates that the current is slightly asymmetric, while the total current \( \int_{-\infty}^{\infty} dx J_z(x, 0) \) still integrates to zero within the numerical accuracy. However, while an underlying translational symmetry in the \( y \)-direction was assumed with \( A_y = 0 \) everywhere, the structure of the order parameter actually also leads to a source current \( J_y(x, z) \), as can easily be derived from the Ginzburg Landau free energy functional. The self-screening of this source current was neglected, which could explain this feature. In any case, this asymmetry does not affect the overall discussion below.

To summarize, the HQV was introduced and stabilized in our numerical analysis. The parameters \( w_{\text{box}} \), \( x_{\text{max}} \) and \( J^\text{max}_z \) have been defined to describe the magnetic properties of the HQV, measuring the full size, the core size and the critical current, respectively. The structure of the HQV over the full range of anisotropies is discussed in the next section, based on an analysis of these three parameters.

### 5.2.2 Junction phenomenology

Here we discuss in detail the behavior of the HQV at different anisotropies \( \nu \). The three parameters \( w_{\text{box}}, x_{\text{max}} \) and \( J^\text{max}_z \) introduced above are extracted from the numerical results over the full range of anisotropies. In addition, they are estimated analytically near the isotropic limit and in the strongly anisotropic limit. We start with a discussion of the critical current obtained from the current-phase relation by treating the domain wall as an effective Josephson junction. Next, we analyze the two limits using the standard and the non-local sine-Gordon model. Finally, we compare the different results.

#### Current-phase relation

Treating the domain wall as an effective Josephson junction, the Josephson phase difference is given by \( \varphi(x) = \phi_- - \phi_+ \) and the current-phase relation is found through the domain wall energy, see Eq. (5.3), neglecting any additional contributions due to the in-plane gradient coupling terms. The free energy of the domain wall, depending on the phase difference, is then given by Eq. (5.8)

\[
\mathcal{F}_{\text{dw}}(\varphi) = \frac{3}{\sqrt{2}} b n_x^2 \xi_c \sqrt{1 + \nu \cos(2\varphi)}.
\]

(5.11)
The current density across the domain wall, see Eq. (1.24), is therefore

\[
J_z(\varphi) = \frac{2\pi c}{\Phi_0} \partial_\varphi \mathcal{F}_{\text{dw}} = \frac{3 c \Phi_0}{\sqrt{2} 8(2\pi)^2 \xi_0 \lambda_c} \frac{-\nu \sin(2\varphi)}{\sqrt{1 + \nu \cos(2\varphi)}}.
\]

(5.12)
and approximating for small anisotropies $|\nu| \ll 1$ we find the critical current density

$$J_c \approx \frac{3 c \Phi_0}{\sqrt{2} 8 (2\pi)^2 \xi_{ab} \lambda_{ab} \lambda_c} |\nu|,$$

(5.13)

recovering that $J_c(\nu = 0) = 0$, as discussed above.

However, this expression for the free energy of the domain wall, Eq. (5.11), was computed in the scope of the approximative analytical solution Eq. (5.7) assuming $|\eta|^2 = 1$. In Fig. 5.2 and the subsequent discussion we found, however, that the assumption $|\eta|^2 = 1$ and the resulting domain wall energy are the least valid for small $\nu$, while here we expand using exactly that limit. Therefore, instead of using Eq. (5.11) for the domain wall energy directly, we fit the numerical solution with $\mathcal{F}_{\text{fit}}(x)$, as indicated in Fig. 5.2 (red line). Linearizing this fit for small anisotropies $|\nu| \ll 1$ (dashed red line), we still have $J_c \propto |\nu|$, but with a different slope, $J_{c,\text{fit}} \approx 0.5 J_c$. This value $J_{c,\text{fit}}$ is used throughout the discussion below. We note that the critical current at higher $|\nu|$ is actually larger than the value obtained from linearizing, because the slope of the free energy gets steeper, and the next order $\sin(4 \varphi)$ has the same sign.

To bring the critical current of the domain wall in relation to a situation without a domain wall, we follow the standard procedure for the depairing current [4] and find the maximal current along the $c$-direction to be

$$J_{\text{dep}} = \frac{8c \gamma K_5 |\eta_b|^2}{3\sqrt{3} \xi_c} = \frac{c \Phi_0}{3\sqrt{3} (2\pi)^2 \xi_{ab} \lambda_{ab} \lambda_c}.$$ 

(5.14)

For this result we have assumed an anisotropic yet continuous behavior of the layered superconductor, such that the anisotropic Ginzburg-Landau theory is applicable, as discussed in Sec. 2.1.2. We note, however, that this is the ultimate limit, and is not the upper limit for the critical current of the HQV on the domain wall, as we will see below.

In Fig. 5.8 we compare the maximal current extracted from the numerical data for the HQV, $J_{z,\text{max}}$ (black dots), as defined in Fig. 5.7; the linear expansion of the critical current $J_c$ from the analytic approximation of the domain wall energy as defined in Eq. (5.13) (black line); the linear expansion of the critical current $J_{c,\text{fit}}$ obtained from fitting the numerical result of the domain wall energy as shown in Fig. 5.2 (red line); and the depairing current $J_{z,\text{dep}}$ defined in Eq. (5.14) (dashed line). We find that for small $|\nu| \ll 0$ the maximum current of the HQV $J_{z,\text{max}}$ follows the critical current $J_{c,\text{fit}}$. This supports our treatment of the domain wall as an effective Josephson junction and using the current-phase relation as above, but also confirms that $J_{c,\text{fit}}$ has to be used rather than the approximate value $J_c$. At higher values of $|\nu|$, the maximum current of the HQV becomes smaller than this expected value $J_{c,\text{fit}}$, while from the higher order terms we would even have expected an increase, as noted above. The actual limiting value of $J_{z,\text{max}}$ requires further investigation, see also the discussion below.

In the following $J_{z,\text{max}}$ extracted from the numerical results for the HQV is used as the critical current of the junction. While the strongly anisotropic limit is described analytically below using a non-local sine-Gordon model, the critical current is always only an input, entering as a phenomenological property of the junction. It therefore cannot be determined using that model, but the value extracted from the numerical results has to
5.2. Half-quantum vortex

Figure 5.8: Maximum current passing across the domain wall at the HQV extracted from the numerical data (black dots), compared to the critical current obtained from the approximative analytical solution (black line) and from a linear expansion of the fit to the numerical solution for the free energy, $J_c^{\text{fit}}$ (red), see Fig. 5.2. Also indicated is the depairing current (dashed), the ultimate limit for the case with no domain wall in the first place. The inset zooms into the local limit $|\nu| \ll 0$, supporting the description as an effective junction.

be relied on. While it seems like circular reasoning to use the extracted value to fit other quantities, this still allows describing the shape of the HQV and determining whether it is Josephson or Abrikosov like, and what the extensions of its core and tail are, like in the local limit where the penetration depth is given by $\lambda_J \propto 1/\sqrt{J_c}$, even if $J_c$ is extracted from the results.

Isotropic limit

Near the isotropic limit $|\nu| \ll 1$ the field of the HQV is locally related to the phase difference at each point of the junction through the standard field-phase relation Eq (1.26), which for our geometry is given by

$$B_y(x) = \frac{\Phi_0}{2\pi d} \partial_x \phi(x),$$

(5.15)

where $d$ is the effective width of the junction. For the $c$-axis domain wall $d = 2\lambda_{ab}$. Together with the current-phase relation Eq. (5.12) we find the sine-Gordon equation, in analogy to Eq. (1.29) and the corresponding discussion,

$$J_c \sin(2\phi) = \frac{c}{4\pi} \frac{\Phi_0}{2\pi d} \partial_x^2 \phi(x)$$

(5.16)

which here has the solution

$$\phi(x) = 2 \arctan \left( e^{x/\lambda_J} \right),$$

(5.17)
and with the Josephson penetration depth $\lambda_J$ now given by

$$
\lambda_J = \sqrt{\frac{e\Phi_0}{16\pi^2 d J_c}}. \tag{5.18}
$$

The resulting current has a maximum value $J_z^{\text{max}} = J_c$ by construction and at the position $x_{\text{max}} = \text{arcsinh}(1)\lambda_J \equiv \tilde{\lambda}_J$. This is the single characteristic length measuring the extension of the HQV in the local limit.

With the expression for the critical current from the approximative analytical result for the domain wall energy as given in Eq. (5.13), and taking into account the additional factor when fitting the numerical result for the domain wall energy, $J_c^{\text{fit}} \approx 0.5 J_c$, we find

$$
\lambda_J \approx \sqrt{\frac{2\sqrt{2}}{3\kappa\gamma_s|\nu|}} \lambda_c. \tag{5.19}
$$

such that $\lambda_J = \lambda_c$ at $\nu_{\text{cross}} \approx 0.0363$, at which value the linear expansion is still applicable, see Fig. 5.2 and Fig. 5.8. For $\lambda_J < \lambda_c$ the standard sine-Gordon model is no longer valid, as $\lambda_c$ provides the fundamental screening length. We conclude that already for very small values of $|\nu|$ non-local effects as discussed in the next section come into play.

**Non-local limit**

When $\lambda_J < \lambda_c$, the field of the HQV depends on the phase difference at all points of the junction through a case-specific non-locality Kernel $G(x, z, x')$ as

$$
B_y(x, z) = \frac{\Phi_0}{2\pi} \int_{-\infty}^{\infty} G(x, z, x') \partial_{x'} \varphi(x') dx', \tag{5.20}
$$

see the review by Abdumalikov et al. [48]. The local case is recovered by $G(x, z, x') = \delta(x - x')/d$. The current-phase relation Eq. (5.12) still holds such that the non-local sine-Gordon model is given by

$$
J_c \sin(2\varphi) = \frac{c}{4\pi} \frac{\Phi_0}{2\pi} \partial_x \int_{-\infty}^{\infty} G(x, z, x') \partial_{x'} \varphi(x') dx'. \tag{5.21}
$$

For our setup we use the Kernel for vortices in layered superconductors with planar defects as described by Gurevich, Benkraouda, and Clem [151], which is given by a modified Bessel function

$$
G(x, z, x') = \frac{1}{2\pi \lambda_{ab} \lambda_c} K_0 \left( \sqrt{\frac{(x - x')^2}{\lambda_c^2} + \frac{z^2}{\lambda_{ab}^2}} \right). \tag{5.22}
$$

The field of the HQV can then approximately be written by (see Eq. (34) in Ref. [151])

$$
B_y(x, z) = \frac{\Phi_0}{4\pi \lambda_c \lambda_{ab}} K_0 \left( \sqrt{\frac{x^2}{\lambda_c^2} + \left( \frac{l}{\lambda_c} + \frac{|z|}{\lambda_{ab}} \right)^2} \right), \tag{5.23}
$$

with the characteristic length scale $l = \lambda_J^2/\lambda_c$

$$
l = \frac{c\Phi_0}{32\pi^2 \lambda_{ab} \lambda_c J_c} \approx \frac{2\sqrt{2}}{3|\nu|} \xi_{ab} = \frac{2\sqrt{2}}{3\kappa\gamma_s|\nu|} \lambda_c \ll \lambda_c, \tag{5.24}
$$

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where we have again used \( J_{\text{fit}}^c \) as above for Eq. (5.19), and where the last inequality only holds for large enough \( |\nu| \gg \nu_{\text{cross}} \) as given above. Note that this form for the field Eq (5.23) gives the correct asymptotics within this approach, but is not normalized correctly due to the core cut-off \( l \).

The maximal current is still \( J_{z}^{\text{max}} = J_{c} \) by construction, but the peak position is now at \( x_{\text{max}} = l \), such that \( l \) can be considered the core size of the HQV. The long-range behavior is Abrikosov-like and determined by \( \lambda_{c} \). There are now two important length scales of very different size, which complicates the numerical minimization, see discussion in Sec. B.2.3.

We note that the approach above follows the description of non-local Josephson electrodynamics for a line defect as studied by Gurevich [152] for isotropic systems. The same in-plane behavior is found from a description of vortices in layered superconductors as studied by Clem and Coffey [153], but where the out-of-plane behavior slightly differs, see Eq. (35) in Ref. [151] and the corresponding discussion. The out-of-plane behavior for the HQV as observed from the numerical data lies somewhere in between these two results. In the following, we focus on the in-plane behavior only.

**Discussion**

First, we discuss the different structures of the HQV in the local and the non-local limit. In Fig. 5.9, the numerical results (black) of the field \( B_{y}(x) \) (top row) and the phase difference \( \varphi(x) \) (bottom row) are shown for the anisotropies \( \nu = \{-0.004, -0.11, -0.4\} \). At each anisotropy we indicate the results for the local and for the non-local limit, using the extracted critical current \( J_{z}^{\text{max}} \) as the only input. For the field, the Josephson-like behavior is found from combining Eq. (5.17) with Eq. (5.15) (blue), and the Abrikosov-tail-Josephson-core structure is found from Eq. (5.23) (red). We find, as expected, that the HQV behaves like a full Josephson vortex in the local limit, while its tail changes to Abrikosov-like behavior in the non-local limit. Still, it retains the Josephson core, meaning that there is no normal core as for a full Abrikosov vortex. From our self-consistent numerical minimization we find that the order parameter does get additionally suppressed at the HQV, but not fully. For the phase difference, the Josephson-like behavior is directly found from Eq. (5.17), while for the non-local case we have used Eq. (26) from Ref. [151]. While the local limit gives a perfect fit, the correspondence in the non-local limit is not as good. This suggests that the Bessel Kernel used above is not fully applicable. This should not, however, come as a surprise, remembering that we are actually considering the \( c \)-axis domain wall and only treat it as an effective junction. Rather opposite, it is surprising how well all the asymptotics fit.

Next, we analyze the full size of the HQV. For this the measure \( w_{\text{box}} \) has been introduced, describing the size of the strip containing \( 0.49\Phi_{0} \), see Fig. 5.7. Considering the long-range Abrikosov behavior and fully neglecting the core structure, such that the field is normalized correctly, see the comment above, the HQV behaves just like a vortex in an anisotropic superconductor [129, 153] with the field given by

\[
B_{y}(x, z) = \frac{\Phi_{0}}{4\pi \lambda_{c} \lambda_{ab}} K_{0} \left( \sqrt{\frac{x^{2}}{\lambda_{c}^{2}} + \frac{z^{2}}{\lambda_{ab}^{2}}} \right).
\]  

(5.25)

The full integral over this expression is \( \Phi_{0}/2 \). In Fig. 5.10 we show the value of \( w_{\text{box}} \).
Figure 5.9: Flux pattern and phase difference of the HQV along the domain wall, comparing the numerical (black) results to the phenomenological descriptions for the local (blue) and the non-local limit (red).

extracted from the numerical results (black dots) and the limiting $w_A$ computed from the above expression for the Abrikosov behavior (red line), where only the two screening lengths $\lambda_{ab}$ and $\lambda_c$ enter. In addition, we indicate the numerical system size $2w_{\text{sys}}$ (dotted), changing with $|\nu|$ to accommodate the exploding HQV, see discussion in Sec. B.2.3. We find that for $|\nu| \ll 1$ the HQV explodes as predicted. In the strongly anisotropic limit, the long-range size of the HQV and therefore its tail length is indeed limited by the Abrikosov-like behavior, confirming the structural change of the HQV.

Finally, we analyze the core size $x_{\text{max}}$ of the HQV, that is, the position of the maximum current across the domain wall. In Fig. 5.11 the numerical results for $x_{\text{max}}$ (black dots) are shown, together with the position $\tilde{\lambda}_J$ based on the Josephson penetration depth ($\tilde{\lambda}_J = \text{arcsinh}(1)\lambda_J = x_{\text{max}}^{\text{local}}$) (red line), and the characteristic length of the non-local limit $l$ (blue line). For both, the critical current entering the expressions is the one extracted from the numerical results for the HQV $J_z^{\text{max}}$. In addition, the relevant screening length $\tilde{\lambda}_c = \text{arcsinh}(1)\lambda_c$ is indicated (dashed), as well as the value $\nu_{\text{cross}}$ of the anisotropy at which $\lambda_J \approx \lambda_c$. Finally, we also indicate the numerical step size $h$ (dotted), giving the resolution. We find that in the isotropic limit $|\nu| \ll 1$ the size of the vortex core is indeed given by $\lambda_J$, while it is determined by $l$ in the strongly anisotropic limit. We observe a crossover region around $\nu_{\text{cross}}$, where neither analytical description fits. This further supports the above description of the structural change of the HQV with increasing anisotropy and helps to explain the numerical difficulties described in Sec. B.2.3.

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Figure 5.10: Width $w$ of the box containing $0.49\Phi_0$ as a function of the anisotropy $\nu$ extracted from numerical data (black dots) with the lower limit given by the box size for an anisotropic Abrikosov vortex (red line) with screening lengths $\lambda_c$ and $\lambda_{ab}$. The increasing system size for decreasing $|\nu|$ is also indicated.

Figure 5.11: Position of the maximum current across the domain wall at the HQV, extracted from the numerical data (black dots), compared to $\tilde{\lambda}_J$ (black) for the local limit $|\nu| \approx 0$ and to $l$ (red) for the non-local limit $\nu \to -1$. For each we show both the case where $J_c$ is based on $J_c^{\text{fit}}$ (dashed) and on the $J_z^{\text{max}}$ (solid) extracted from the numerical data for the HQV vortex (black dots in Fig. 5.8). The screening length $\tilde{\lambda}_c$ (gray), the anisotropy $\nu_{\text{cross}}$ (dotted) and the mesh size $h$ (dashed) are also indicated.
5.3 Conclusion

In this project the structure of $c$-axis domain walls has been investigated. In the first part it was shown that a finite current can only flow across the domain wall if the anisotropy of the underlying electronic structure is taken into account. The stable configurations were found to depend on the sign of the anisotropy, but with the non-trivial periodicity of $\pi$. This was also confirmed in a Bogoliubov-deGennes approach, explored by Wen Huang.

The $c$-axis domain wall therefore supports half-quantized vortices, which were subsequently analyzed. The structure of these vortices depends critically on the anisotropy $\nu$, and different characteristic length scales emerge for different limits. When $|\nu| \ll 1$, the standard sine-Gordon model describes a Josephson-like structure. For $\nu \to 0$, the vortex explodes along the domain wall and the critical current vanishes. In the opposite limit, for large anisotropies, the vortex shrinks below the relevant screening length. Using a non-local sine-Gordon model, two characteristic length scales were identified. The Josephson character is retained in the core of size $l$, while the long-tail behavior is now Abrikosov-like, described by the screening length $\lambda_c$. These phenomenological descriptions and the numerical results are in good agreement.

The limiting value of $J_z^{\text{max}}$ when $|\nu| \to 1$ has not yet been fully explained. A first hint comes from the fact that in the non-local electrodynamics for the Josephson junction it is assumed that the core size $l \gg \xi_{ab}$, see Ref. [152]. Here, however, $l \approx \xi_{ab}$ when $J_c = 3\sqrt{3}/8J_{z}^{\text{dep}}$, found by combining Eq. (5.24) and Eq. (5.14). On the other hand, as the anisotropy increases, the order parameter at the HQV becomes more and more suppressed, and more of an Abrikosov character might also emerge in the core. It is therefore clear that $J_z^{\text{max}}$ will saturate as observed from the numerical results in Fig. 5.8, the actual value of this upper limit, however, requires further investigation.

To conclude, a rich phenomenology for $c$-axis domain walls was discovered when considering the phenomenological anisotropy parameter $\nu$. While these domain walls are energetically more favorable than the in-plane domain walls, they have not been systematically analyzed before.
In this thesis, magnetic phenomena at boundaries in chiral p-wave superconductors were explored using the phenomenological Ginzburg Landau approach. For each project, efforts were made to always provide both, analytical arguments for the limiting cases, together with a systematic numerical analysis of the full parameter range. In addition, the results were always analyzed in the context of experimental observations and previous theoretical work. Furthermore, beyond studying three phenomena in particular, we have described in detail the overarching methodology of formulating and subsequently minimizing the free energy functional. While specific conclusions and outlooks have been provided at the end of each chapter, here we close with a focused summary, an overall conclusion, and a general outlook.
Summary

First, we summarize the main results for each phenomenon. Next, we compile examples for each methodological concept, and finally recapitulate the process of minimizing the Ginzburg Landau functional.

The intrinsic magnetic phenomena

First, in Ch. 3, the sensitivity of the spontaneous surface magnetic flux pattern in disk-shaped samples has been discussed. It was shown how band structure effects can be included qualitatively, and how boundary conditions beyond specular scattering can be treated naturally. Each of these two effects has then been systematically analyzed, and it was found that the shape and magnitude, and in particular the direction of the flux pattern depend intricately on all considered parameters. From this we have concluded that the magnetic flux pattern is not a universal feature of chiral $p$-wave superconductors. Also, the current reversal proposed by Bouhon and Sigrist [104] was recovered. Further, the flux pattern at impurities was discussed and it was found that, while depending on the band structure effects in a similar way, the magnitude is equally governed by the ‘strength’ of the impurity, unrelated to what happens at the surface. These findings can explain the absence of any sign of the edge current in scanning probe measurements, while still reconcilable with the results from $\mu$SR experiments.

Second, in Ch. 4, the unconventional limiting mechanism for the critical current in topologically frustrated Josephson junctions has been analyzed. Pb/Ru/Sr$_2$RuO$_4$ devices as studied experimentally by Maeno et al. [113], were modeled as cylindrical Josephson junctions between a chiral $p$-wave and a conventional $s$-wave superconductor, with an external magnetic field applied at the top. On the one hand, it was shown that an inhomogeneous coupling strength pins the flux line appearing spontaneously in the phase-frustrated state, such that the critical current is limited by the corresponding pinning-depinning transition. On the other hand, a phase diagram of the different topological states of the junction influenced by the coupling to the proximity-induced superconductivity in the Ru-inclusions was presented. Combining these two effects can explain the observed anomalous dependence of the critical current in the Pb/Ru/Sr$_2$RuO$_4$ devices as a transition between the trivial and the frustrated state of the junction with different limiting mechanisms.

Third, in Ch. 5, the non-trivial features of $c$-axis domain walls supporting half-quantum vortices have been examined. First, it was shown that the phase difference across such domain walls depends on the sign of the anisotropy $\nu$ of the electronic structure, and takes discrete values with a periodicity of $\pi$, except for the isotropic limit where all values are allowed. Based on these results it was proposed that the domain wall supports vortices carrying only half a flux quantum. Treating the domain wall as an effective Josephson junction, the structure of these vortices was analyzed and found to critically depend on the magnitude of the anisotropy. In the isotropic limit, the vortex explodes and the junction character is lost, while for small anisotropies it can be describes as a standard Josephson vortex. However, in the strongly anisotropic limit, the Josephson penetration depth becomes smaller than the relevant screening length $\lambda_c$ of the layered superconductor. Non-local effects have to be considered, and there is a crossover to a vortex structure which only retains the Josephson character in the core, while its tail behaves like that of
Summary

an Abrikosov vortex. While some details require further consideration, we have provided a comprehensive description of the situation at c-axis domain walls.

Modeling a chiral p-wave superconductor

The methodology of formulating the Ginzburg Landau functional was described in detail in Ch. 2. Here, the introduced concepts are exemplified in view of the studied phenomena. First, choosing an appropriate representation of the order parameter is crucial such that the underlying effects are displayed clearly in a simplified free energy functional. For the disk-shaped sample and the nucleation at the Ru-inclusion, the polar representation \( \eta = (\eta_r, \eta_\theta) = (\eta_\perp, \eta_\parallel) \) was used, giving direct access to the order parameter component parallel and perpendicular to the boundary. For the c-axis domain wall, it was natural to use the chiral representation \( \eta = (\eta_+, \eta_-) \) giving direct access to the two degenerate ground states. Interestingly, once the half-quantum vortex is introduced on the domain wall, it is more convenient to work with \( \eta = (\eta_x, \eta_y) \), while the true nature of the half-quantum vortex, with a phase winding in one of the two components alone, only becomes apparent in the representation \( \eta = (\eta_{x-y}, \eta_{x+y}) \), which is rotated by \(-\pi/4\).

Next, the importance of the coordinate system is obvious. However, while especially the polar coordinates can lead to a rather lengthy expression for the full free energy functional, as displayed in Sec. A.2, it was demonstrated to be feasible to perform the coordinate transformations and the change of the representation, as well as the preparation of the terms needed for the numerical minimization, automatically using a computer algebra system capable of advanced symbolic operations.

Furthermore, the expansion coefficients in the free energy functional can be determined following the same scheme as for conventional superconductors. The sets of coefficients \( \{b_i\} \) and \( \{K_i\} \) incorporate, however, more complex physics on the phenomenological level and may reflect intricate microscopic properties of the electronic structure. For example, for the surface flux pattern the proposed current reversal was recovered by considering a variation in the ratio \( K_1/K_2 \), which was found by Bouhon and Sigrist [104] to change considerably with band filling in a lattice model. The behavior of the c-axis domain wall was shown to depend both on the sign and the magnitude of the anisotropy \( \nu \) of the electronic structure.

Finally, various boundary effects can be described straightforwardly using either additional terms or by considering an effective space- and component-dependent critical temperature. The corresponding parameters can be scanned systematically to analyze divers conditions within a single framework. Different surface types were studied for the disk-shaped sample, which critically determine the shape, the magnitude and the direction of the surface magnetic flux pattern. The coupling to an s-wave superconductor in a cylindrical Josephson junction was discussed, with the phase winding of the order parameter determining the topological state of the junction and thus the limiting mechanism of the critical current.

Analyzing the Ginzburg Landau functional

Setting up the Ginzburg Landau free energy functional is the first essential step. However, analyzing this functional is the main work. In this thesis, both analytical and numerical
tools have been used, which we comment on below.

While solving the full problem analytically is usually not feasible, a lot of insight can be gained from various analytical considerations. The allowed values for the phase difference across the c-axis domain wall were found from the appropriate form of the free energy alone. It was possible to explain several limits for the surface flux pattern in the disk-shaped sample only by looking at the boundary conditions or the equation for the angular current derived by variation, without actually solving the equations. For the topologically frustrated Josephson junction, the general need for an inhomogeneous coupling strength was demonstrated by considering a limiting case alone. Eventually, even if only a restricted limiting case can be solved analytically, this always supports the numerical results. While the computational results for the half-quantum vortex only converged rather poorly, this was immediately understood from the non-local sine-Gordon model with two different characteristic length scales.

However, at the heart of each project was the systematic numerical analysis of the full parameter range, and the proper graphical presentation of the results. In particular, the whole workflow from setting up the functional and the algorithm to computing and analyzing the solution was heavily automated. It was successfully demonstrated that the simple relaxed one-step Newton-Jacobi method is fully capable of minimizing even the most complex functionals.

**Conclusion and Outlook**

To conclude, we have exemplified the versatility of the Ginzburg Landau approach and the feasibility of analyzing the free energy functional even for intricate situations. In particular, it was demonstrated that effects due to details of the electronic structure can be included qualitatively, and that the full parameter range for a variety of boundary conditions is accessible systematically. It is the combination of both which helps understand issues not readily accessible in a microscopic framework.

The results of this thesis are compatible with the experimental observations which initially inspired the different projects. In particular, our result for the sensitivity of the surface flux pattern has in turn contributed to the discussion surrounding the elusive edge currents in \( \text{Sr}_2\text{RuO}_4 \), and we conclude that this should not be considered a decisive argument against chiral \( p \)-wave pairing. In addition, our results are consistent with those of previous theoretical work, also when other methods have been used.

While systematically scanning the relevant parameters is implemented straightforwardly numerically, the main limitation to this approach is interpreting which physical situation is actually described by these parameters. Some features were found to be robust over the full range of parameters, such as the unconventional limiting mechanism for the topologically frustrated Josephson junction. However, for results as sensitive to the parameter as the surface flux pattern in the disk-shaped sample, no predictions can be made.

In future work, the implementation of the algorithm could certainly be heavily optimized, including a parallelization of the secondary one-step Jacobi method, or an improvement of the memory management. Especially an adaptive or at least gauge-controlled non-uniform
mesh would be desirable and open the doors to consider less well-behaved geometries.

Beyond the three phenomena presented in this thesis, we have touched upon other features such as a thin film in an applied field, strain due to dislocations\textsuperscript{1}, or the behavior of a constriction\textsuperscript{2}. As demonstrated in my own Master thesis, even the time-dependent dissipative regime of a Josephson junction is somewhat accessible using the iterative Newton method. The approach presented here can surely be used in many other interesting situations. In particular, the topic of nucleation in thin films or the 3-Kelvin phase could be revisited in the light of the findings for the surface flux pattern, while it has so far always been discussed for specular scattering and the isotropic expansion coefficients. The situation is expected to change for different surface types, especially in combination with varying the ratio $K_1/K_2$.

While we have focused on chiral $p$-wave pairing, for which the Ginzburg Landau functional has one of the most complex forms, the described methodology can in general be adapted to any kind of pairing symmetry or could be extended to treat multiple bands.

In closing, I hope that this thesis and my detailed description of formulating and numerically minimizing the Ginzburg Landau functional encourages other researchers to use this beautiful method to explore unconventional phenomena. I am curious to see what surprises and secrets are waiting to be discovered.

\textsuperscript{1} Master thesis of Cedric Klinkert (2015).
\textsuperscript{2} Master thesis of Bastian Zinkl (2017).
Appendix
First, selected expressions of the Ginzburg Landau free energy functional for a chiral p-wave superconductor are compiled for different representations of the two-component order parameter, in different coordinates, and for general expansion coefficients. For the homogeneous terms, almost all the possible expressions are listed, while for the gradient terms only the $\pm$-representation in cartesian coordinates is discussed. Also, in each case the weak-coupling ratios discussed in Sec. 2.1.2 are plugged in to illustrate the resulting simplified formulations.

Second, for the specific case of the disk-shaped sample discussed in Ch. 3, the full proper boundary conditions for the two order parameter components and the full equation for the angular current are stated. These are the basis for the analytical arguments used in Sec. 3.2 to support and explain the numerical results.
A.1 Selected expressions

First, the expressions for the homogeneous terms are presented, and then for the gradient terms. The magnetic term only depends on the coordinate system, for which the standard expressions of the curl apply, and is not discussed.

A.1.1 Homogeneous terms

The structure of the homogeneous terms is only affected by the representation of the order parameter, but not by the coordinate system. Repeating Eq. (1.36) as a reference, we start with

$$ F_{\text{hom}}[\eta_x, \eta_y] = \int d^3r \left[ a \left( T - T_c \right) |\eta|^2 + b_1 |\eta|^4 + \frac{b_2}{2} \left( \eta_x^2 \eta_y^2 + \eta_x^2 \eta_y^2 \right) + b_3 |\eta_x|^2 |\eta_y|^2 \right]. \quad (A.1) $$

**Representation for the two chiralities**

For the $\pm$-representation we find as the most general expression

$$ F_{\text{hom}}[\eta_+, \eta_-] = \int d^3r \left[ 2a(T - T_c)(|\eta_+|^2 + |\eta_-|^2) 
+ b_1 \left( 4|\eta_+|^4 + 4|\eta_-|^4 + 8|\eta_+|^2|\eta_-|^2 \right) 
- b_2 \left( |\eta_+|^4 + |\eta_-|^4 - 4|\eta_+|^2|\eta_-|^2 + \eta_+^2 \eta_-^2 + \eta_-^2 \eta_+^2 \right) 
+ b_3 \left( |\eta_+|^4 + |\eta_-|^4 - \left( \eta_+^2 \eta_-^2 + \eta_-^2 \eta_+^2 \right) \right) \right]. \quad (A.2) $$

For weak-coupling with $b_3 = 2(b_2 - b_1)$, with the unit $b = 4b_1 - b_2 + b_3 = 2b_1 + b_2$, and with the anisotropy $\nu b = 2b_1 - 3b_2$, see Sec. 2.1.2, this simplifies to

$$ F_{\text{hom}}[\eta_+, \eta_-] = \int d^3r \left[ 2a(T - T_c)(|\eta_+|^2 + |\eta_-|^2) 
+ b \left\{ \left( |\eta_+|^4 + 4|\eta_+|^2|\eta_-|^2 + |\eta_-|^4 \right) + \nu \left( \eta_+^2 \eta_-^2 + \eta_-^2 \eta_+^2 \right) \right\} \right]. \quad (A.3) $$

The expression for the isotropic limit is given by that for $\nu = 0$.

**Representation for the parallel and perpendicular component**

For the $(\eta_\perp, \eta_\parallel)$-representation accessing the component perpendicular and parallel to a normal vector $\mathbf{n}$ in the basal plane, the most general expression is too lengthy and not illustrative. We directly provide that for weak-coupling, where it simplifies to

$$ F_{\text{hom}}[\eta_\perp, \eta_\parallel] = \int d^3r \left[ a(T - T_c)(|\eta_\perp|^2 + |\eta_\parallel|^2) 
+ \frac{b}{8} \left\{ 3|\eta_\perp|^4 + 3|\eta_\parallel|^4 + 4|\eta_\perp|^2|\eta_\parallel|^2 + \eta_\perp^2 \eta_\parallel^* \eta_\perp^* \eta_\parallel^2 
+ \nu \cos(4\theta(\mathbf{n})) \left( |\eta_\perp|^4 + |\eta_\parallel|^4 - 4|\eta_\perp|^2|\eta_\parallel|^2 - \eta_\perp^2 \eta_\parallel^2 - \eta_\perp^2 \eta_\parallel^2 \right) 
+ 2\nu \sin(4\theta(\mathbf{n})) \left( -|\eta_\perp|^2 + |\eta_\parallel|^2 \right) \left( \eta_\perp \eta_\parallel + \eta_\parallel \eta_\perp \right) \right\} \right]. \quad (A.4)
This is mostly useful in the isotropic limit $\nu = 0$. Also, it only makes sense for some specific choices of the normal $\mathbf{n}$. Either, a rotated straight surface with a fixed angle in the basal plane, or a circular geometry with $\mathbf{n} = \hat{r}$ and with $\theta$ the polar angle.

### A.1.2 Gradient terms

The gradient terms become very complicated very quickly, because they are affected by both the representation of the order parameter as well as by the coordinate system, and because there are many more coupled terms. We therefore only provide a few specific expressions, starting from

$$
\mathcal{F}_{\text{grad}}[\eta_+, \eta_-] = \int d^3 r \left[ \sum_{\alpha, \beta} \left( \frac{D_{\alpha} \eta_+}{\beta} + \frac{D_{\beta} \eta_-}{\alpha} \right)^2 \right] + \left\{ K_3 (D_x \eta_+)^* (D_y \eta_-) + K_4 (D_y \eta_+)^* (D_x \eta_-) + c.c \right\} 
\] = 0.

\] A.1. Selected expressions

For the ±-representation we find as the most general expression

$$
\mathcal{F}_{\text{grad}}[\eta_+, \eta_-] = \int d^3 r \left[ \left( K_1 + K_2 \right) \left( |D_x \eta_+|^2 + |D_y \eta_+|^2 + |D_x \eta_-|^2 + |D_y \eta_-|^2 \right) + \frac{1}{4} \left( (K_3 - K_4) \left( \frac{K_5}{2} \right) \right) \right] + \frac{1}{\gamma_s^2} \left( |D_z \eta_+|^2 + |D_z \eta_-|^2 \right).
$$

For weak coupling, $K_3 = K_4$, and the fourth line vanishes. In the quasiclassical approximation we may use the anisotropy parameter $\nu$, as discussed in Sec. 2.1.2. With the ‘unit’ $K_1 + K_2 = K$, with $K_1 - K_2 = K(1 + \nu)/2$, $K_3 = K_4 = K(1 - \nu)/4$, and by using $K_5 = K/(2\gamma_s^2)$ with the superconducting anisotropy $\gamma_s$, this simplifies to

$$
\mathcal{F}_{\text{grad}}[\eta_+, \eta_-] = \int d^3 r K \left[ \left( |D_x \eta_+|^2 + |D_y \eta_+|^2 + |D_x \eta_-|^2 + |D_y \eta_-|^2 \right) + \frac{1}{\gamma_s^2} \left( |D_z \eta_+|^2 + |D_z \eta_-|^2 \right) \right].
$$

(A.7)
In the quasiclassical approximation, see above, this simplifies to

Using again $J$ and the parallel current. These can be used for the disk-shaped sample with the component of the order parameter for the disk-shaped sample, and the full equation for the boundary conditions from the variation with respect to the order parameter component are given below, where their space dependence is omitted for readability.

$$F_{\text{grad}}[\eta_+, \eta_-] = \int d^3r \frac{1}{2} \left[ (K_1 + K_2 + K_3 - K_4) \left( |D_+\eta_+|^2 + |D_-\eta_-|^2 \right) + (K_1 + K_2 - K_3 + K_4) \left( |D_+\eta_-|^2 + |D_-\eta_+|^2 \right) + (K_1 - K_2 + K_3 + K_4) (D_+\eta_+)^*(D_-\eta_-) + c.c \right].$$

In the quasiclassical approximation, see above, this simplifies to

$$F_{\text{grad}}[\eta_+, \eta_-] = \int d^3r \frac{K}{2} \left[ \left( |D_+\eta_+|^2 + |D_-\eta_-|^2 \right) + \left( |D_+\eta_-|^2 + |D_-\eta_+|^2 \right) + \left( (D_+\eta_+)^*(D_-\eta_-) + \nu(D_+\eta_-)^*(D_-\eta_+)^* + c.c \right) \right].$$

Using again $D = (D_x, D_y)$ in the first line, we find

$$F_{\text{grad}}[\eta_+, \eta_-] = \int d^3r K \left[ \left( |D_+\eta_+|^2 + |D_-\eta_-|^2 \right) + \frac{1}{2} \left( (D_+\eta_+)^*(D_-\eta_-) + \nu(D_+\eta_-)^*(D_-\eta_+)^* + c.c \right) \right].$$

### A.2 Polar coordinates

Here we show the full proper boundary conditions for the parallel and perpendicular component of the order parameter for the disk-shaped sample, and the full equation for the parallel current. These can be used for the disk-shaped sample with $(\eta_\perp, \eta_\parallel) = (\eta_r, \eta_\theta)$ and $J_r(r, \theta)$, but can also be adapted for a straight rotated surface in the basal plane at an angle $\theta$ to the crystal axes by taking the limit $r, R \to \infty$. These expressions have been derived using symbolic computation, see also Sec. 2.2.1.

#### A.2.1 Boundary conditions for the order parameter

The boundary conditions from the variation with respect to the order parameter components are given below, where their space dependence $(R, \theta)$ is omitted for readability.

$$- 4(g_1 + g_3)\eta_\perp = (3K_1 + K_2 + 2K_3 + \cos(4\theta)(K_1 - K_2 - 2K_3)) \partial_r \eta_\perp \quad \text{(A.11a)}$$

$$+ (K_1 - K_2 + 2K_3 - \cos(4\theta)(K_1 - K_2 - 2K_3)) \left( \frac{\eta_\parallel}{R} + \frac{\partial_\theta \eta_\parallel}{R} \right)$$

$$- \sin(4\theta)(K_1 - K_2 - 2K_3) \left( \frac{\partial_\theta \eta_\parallel}{R} - \frac{\eta_\parallel}{R} + \partial_r \eta_\parallel \right)$$

$$- i \gamma A_\theta \left( (K_1 - K_2 + 2K_3 - \cos(4\theta)(K_1 - K_2 - 2K_3)) \eta_\parallel - \sin(4\theta)(K_1 - K_2 - 2K_3) \eta_\perp \right)$$

$$- i \gamma A_r \left( (3K_1 + K_2 + 2K_3 + \cos(4\theta)(K_1 - K_2 - 2K_3)) \eta_\perp - \sin(4\theta)(K_1 - K_2 - 2K_3) \eta_\parallel \right)$$
A.2. Polar coordinates

\[ -4(g_1 - g_3)\eta_\| = (K_1 + 3K_2 - 2K_3 - \cos(4\theta)(K_1 - K_2 - 2K_3))\partial_\eta_\| \] (A.11b)

\[ - (K_1 - K_2 + 2K_3 - \cos(4\theta)(K_1 - K_2 - 2K_3)) \left( \frac{\eta_\|}{R} - \frac{\partial_\eta_\perp}{R} \right) \]

\[ + \sin(4\theta)(K_1 - K_2 - 2K_3) \left( \frac{\partial_\eta_\|}{R} + \frac{\eta_\perp}{R} - \partial_\eta_\perp \right) \]

\[ - i\gamma A_\theta \left( (K_1 - K_2 + 2K_3 - \cos(4\theta)(K_1 - K_2 - 2K_3))\eta_\perp + \sin(4\theta)(K_1 - K_2 - 2K_3)\eta_\| \right) \]

\[ - i\gamma A_r \left( (K_1 + 3K_2 - 2K_3 - \cos(4\theta)(K_1 - K_2 - 2K_3))\eta_\| - \sin(4\theta)(K_1 - K_2 - 2K_3)\eta_\perp \right). \]

**Straight rotated surface in the basal plane**

In the limit of a straight surface at an angle \( \theta \), with translational invariance along the surface, we can always choose a gauge where \( A_\perp = 0 \). At the angle \( \theta = 0 \) we recover Eq. (2.27)

\[ - (g_1 + g_3)\eta_\| = K_1 \partial_\eta_\| - i\gamma A_y K_3 \eta_y \] (A.12a)

\[ - (g_1 - g_3)\eta_y = K_2 \partial_\eta_\perp - i\gamma A_y K_3 \eta_x. \] (A.12b)

For comparison, at the angle \( \theta = \pi/4 \) we find

\[ - 2(g_1 + g_3)\eta_\perp = (K_1 + K_2 + 2K_3)\partial_\eta_\perp - i\gamma A_\parallel (K_1 - K_2)\eta_\parallel \] (A.13a)

\[ - 2(g_1 - g_3)\eta_\parallel = (K_1 + K_2 - 2K_3)\partial_\eta_\parallel - i\gamma A_\parallel (K_1 - K_2)\eta_\perp. \] (A.13b)

**A.2.2 Angular current**

From the variation with respect to the vector potential we find the full Ginzburg-Landau equations for the currents, not restricted to the boundary. Of particular interest is the angular current \( J_\theta \), given by

\[ \frac{2}{c\gamma} J_\theta = (K_1 - K_2 + 2K_3) \Im \left[ \eta_\perp \partial_\eta_\|^* - \eta_\perp \partial_\eta_\|^* \right] \] (A.14)

\[ - \frac{1}{r} \Im \left[ (4(K_1 + K_2)\eta_\|^* - (K_1 + 3K_2 - 2K_3)\eta_\perp \partial_\eta_\|^* - (3K_1 + K_2 + 2K_3)\eta_\parallel \partial_\eta_\|^*) \right] \]

\[ - (K_1 - K_2 - 2K_3) \Im \left[ \eta_\perp \partial_\eta_\|^* - \eta_\perp \partial_\eta_\|^* + \frac{1}{r} (\eta_\perp \partial_\eta_\|^* - \eta_\parallel \partial_\eta_\|^*) \cos(4\theta) \right] \]

\[ - (K_1 - K_2 - 2K_3) \Im \left[ \eta_\perp \partial_\eta_\|^* - \eta_\perp \partial_\eta_\|^* - \frac{1}{r} (\eta_\parallel \partial_\eta_\|^* - \eta_\parallel \partial_\eta_\|^*) \sin(4\theta) \right] \]

\[ + \gamma A_r \left( (K_1 - K_2 + 2K_3 - \cos(4\theta)(K_1 - K_2 - 2K_3)) 2R \left| \eta_\parallel \right|^2 \right) \]

\[ - \sin(4\theta)(K_1 - K_2 - 2K_3) \left( |\eta_\perp|^2 - |\eta_\||^2 \right) \]

\[ + \gamma A_\theta \left( 2(K_1 + K_2) |\eta|^2 - (K_1 - K_2 + 2K_3 + \cos(4\theta)(K_1 - K_2 - 2K_3)) \left( |\eta_\perp|^2 - |\eta_\||^2 \right) \right) \]

\[ + \sin(4\theta)(K_1 - K_2 - 2K_3) 2R \left[ \eta_\perp \eta_\| \right]. \]
This appendix contains information about the numerical minimization of the Ginzburg Landau functional. In the first part, additional details for the implementation of the discretization scheme and the one-step relaxed Newton-Jacobi method are provided.

In the second part, computational details for each project are compiled. The physical, numerical and phenomenological parameters are listed, and specific features of each computational model are described. We also comment on the particular implementation and discuss numerical issues we encountered.
Numerical minimization

B.1 Implementation

While the algorithm has been described in detail in Sec. 2.2.2, here we give some additional comments about its implementation.

B.1.1 Derivatives of the Riemann sum

Once the function \( g(x, y) \) has been discretized as \( g_{ij} \) on each vertex of the mesh and the functional \( F[g(x, y)] \) has been approximated by a middle Riemann sum \( A(g_{ij}) \), this high-dimensional function has to be minimized. This corresponds to solving \( \partial A/\partial g_{ij} = 0 \).

Remembering the functional density \( F[m_{ij}, dx_{ij}, dy_{ij}] \equiv F_{ij} \) on each cell of the mesh, this innocent looking derivative in its full glory is given by

\[
\frac{\partial A}{\partial g_{ij}} = hs \left( \frac{\partial F_{ij}}{\partial g_{ij}} + \frac{\partial F_{i-1,j}}{\partial g_{ij}} + \frac{\partial F_{i,j-1}}{\partial g_{ij}} + \frac{\partial F_{i-1,j-1}}{\partial g_{ij}} \right)
= hs \left( \frac{\partial F_{ij}}{\partial m_{ij}} \frac{\partial m_{ij}}{\partial g_{ij}} + \frac{\partial F_{i-1,j}}{\partial m_{i-1,j}} \frac{\partial m_{i-1,j}}{\partial g_{ij}} + \frac{\partial F_{i,j-1}}{\partial m_{i,j-1}} \frac{\partial m_{i,j-1}}{\partial g_{ij}} + \frac{\partial F_{i-1,j-1}}{\partial m_{i-1,j-1}} \frac{\partial m_{i-1,j-1}}{\partial g_{ij}} \\
+ \frac{\partial F_{ij}}{\partial dx_{ij}} \frac{\partial dx_{ij}}{\partial g_{ij}} + \frac{\partial F_{i-1,j}}{\partial dx_{i-1,j}} \frac{\partial dx_{i-1,j}}{\partial g_{ij}} + \frac{\partial F_{i,j-1}}{\partial dx_{i,j-1}} \frac{\partial dx_{i,j-1}}{\partial g_{ij}} + \frac{\partial F_{i-1,j-1}}{\partial dx_{i-1,j-1}} \frac{\partial dx_{i-1,j-1}}{\partial g_{ij}} \\
+ \frac{\partial F_{ij}}{\partial dy_{ij}} \frac{\partial dy_{ij}}{\partial g_{ij}} + \frac{\partial F_{i-1,j}}{\partial dy_{i-1,j}} \frac{\partial dy_{i-1,j}}{\partial g_{ij}} + \frac{\partial F_{i,j-1}}{\partial dy_{i,j-1}} \frac{\partial dy_{i,j-1}}{\partial g_{ij}} + \frac{\partial F_{i-1,j-1}}{\partial dy_{i-1,j-1}} \frac{\partial dy_{i-1,j-1}}{\partial g_{ij}} \right)
= hs \left( \frac{1}{4} \left( \frac{\partial F}{\partial m} \right)_{ij} + \frac{1}{4} \left( \frac{\partial F}{\partial m} \right)_{i-1,j} + \frac{1}{4} \left( \frac{\partial F}{\partial m} \right)_{i,j-1} + \frac{1}{4} \left( \frac{\partial F}{\partial m} \right)_{i-1,j-1} \\
- \frac{1}{2h} \left( \frac{\partial F}{\partial dx} \right)_{ij} - \frac{1}{2h} \left( \frac{\partial F}{\partial dx} \right)_{i-1,j} - \frac{1}{2h} \left( \frac{\partial F}{\partial dx} \right)_{i,j-1} - \frac{1}{2h} \left( \frac{\partial F}{\partial dx} \right)_{i-1,j-1} \\
- \frac{1}{2s} \left( \frac{\partial F}{\partial dy} \right)_{ij} - \frac{1}{2s} \left( \frac{\partial F}{\partial dy} \right)_{i-1,j} - \frac{1}{2s} \left( \frac{\partial F}{\partial dy} \right)_{i,j-1} - \frac{1}{2s} \left( \frac{\partial F}{\partial dy} \right)_{i-1,j-1} \right).
\]  

While \( \partial A/\partial g_{ij} \) runs over all vertices (iterators \( i \in \{0, \ldots, n\} \) and \( j \in \{0, \ldots, m\} \)), only half the terms of the second and third equality appear at \( i \in \{0, n\} \) and \( j \in \{0, m\} \), but boundary terms might have to be added. For the example from Eq. (2.42), we have

\[
\frac{\partial A}{\partial g_{nj}} = s \left( \frac{\partial B_j}{\partial g_{nj}} + \frac{\partial B_{j-1}}{\partial g_{nj}} \right)
= s \left( \frac{\partial B_j}{\partial b_{nj}} \frac{\partial b_{nj}}{\partial g_{nj}} + \frac{\partial B_{j-1}}{\partial b_{n,j-1}} \frac{\partial b_{n,j-1}}{\partial g_{nj}} \right) \\
= s \left( \frac{1}{2} \left( \frac{\partial B}{\partial b} \right)_{nj} + \frac{1}{2} \left( \frac{\partial B}{\partial b} \right)_{n,j-1} \right),
\]  

where for the case of periodic boundary conditions in \( y \), with \( (j = 0) \equiv (j = m) \) such that \( (j = -1) \equiv (j = m - 1) \), the remaining iterator is \( j \in \{0, \ldots, m - 1\} \).
The partial derivatives $\partial F/\partial m$, $\partial F/\partial dx$, and $\partial F/\partial dy$, as well as $\partial B/\partial b$, have to be derived from the underlying form of the functional only once, see the first automatization step below. The notation $(\partial F/\partial m)_{ij}$ then refers to that derivative with the mean and difference values of the cell $(i, j)$ plugged in (notation see Fig. 2.3), where the iterators are $i \in \{0, 1, \ldots, n-1\}$ and $j \in \{0, 1, \ldots, m-1\}$. Next, these derivatives have to be added correctly to the full derivative, taking care of the signs,

$$
\begin{align*}
M &= \frac{1}{4} \left( \frac{\partial F}{\partial m} \right)_{ij} \quad \Rightarrow \quad \frac{\partial A}{\partial g_{ij}} + = hs (M - X - Y), \\
X &= \frac{1}{2h} \left( \frac{\partial F}{\partial dx} \right)_{ij} \quad \Rightarrow \quad \frac{\partial A}{\partial g_{i,j+1}} + = hs (M + X - Y), \\
Y &= \frac{1}{2s} \left( \frac{\partial F}{\partial dy} \right)_{ij} \quad \Rightarrow \quad \frac{\partial A}{\partial g_{i+1,j}} + = hs (M - X + Y), \\
\end{align*}
$$

adding the terms from $(\partial B/\partial b)_{nj}$ where applicable, which is the second step that can be automatized. The advantages of using these boundary terms rather than direct boundary conditions have been discussed in detail in Sec. 2.2.2.

For the diagonals of the Hessian, $\partial^2 A/\partial g_{ij}^2$ the procedure is analogous, but where mixed second derivates such as $\partial^2 F/\partial (m dx)\partial dx$ also have to be considered, because $g_{ij}$ appears in both $m_{ij}$ and $dx_{ij}$. While these usually do not appear for most expressions of the free energy functional, they should not be disregarded, as they can pop up in certain situations.

For example, when the order parameter representation for polar coordinates with a winding number is used also away from the isotropic limit, $(\eta_r, \eta_\theta) = \eta_b(f(r, \theta), ig(r, \theta))e^{iN\theta}$, the product rule leads to terms $\partial \eta_r = (\partial \theta f + iNf)e^{iN\theta}$. Or, such mixed second derivatives appear for the vector potential components in the magnetic term in polar coordinates.

For multiple input functions $F[g, f]$, the above procedure has to be extended accordingly. Note that the mixed derivatives $\partial^2 A/(\partial f \partial g)$ have already been discarded in the diagonalization of the Hessian for the one-step Newton-Jacobi method.

### B.1.2 Automatization and book-keeping

As mentioned several times, while the above procedure looks tedious, it is highly repetitive and the different steps can be automatized straightforwardly, which is largely a book-keeping exercise.

#### Preparing of the derivatives

Computing the derivatives $(\partial F/\partial m)$ automatically from the free energy functional can be done using symbolic computation. While this seems not too difficult to do by hand, there are situations when not even the free energy functional can be derived by hand. This was encountered for the disk-shaped sample, where the full free energy for the representation $(\eta_r, \eta_\theta) = \eta_b(f(r, \theta), ig(r, \theta))e^{iN\theta}$ with all arguments spelled out is given by

$$
F[\Re f(r, \theta), \Im f(r, \theta), \Re g(r, \theta), \Im g(r, \theta), A_r(r, \theta), A_\theta(r, \theta)].
$$

For the formulation of the free energy, a computer algebra system ensuring a proper handling of complex variables, capable of advanced symbolic computation and additionally able to do major simplifications makes this feasible. We have used Mathematica [135]. It is then straightforward to also compute all the derivatives automatically.
Numerical minimization

Adding the derivatives

For a free energy functional with many coupled terms, the crucial point is to compute each \((\partial F/\partial m)_{ij}\) only once, and then add them to the \(\partial A/\partial g_{ij}\) in the way described in Eq. (B.3), because the speed bottleneck are all the necessary point operations in substituting the \(g^k_{ij}\). This is the second step of the implementation, and can be automatized using class objects, and for our case of using C++ to implement the one-step Newton-Jacobi method, also virtual functions. This is described in detail in the excellent lecture notes by Piette [154], which were of great help to me.

Such a code takes time to set up at first, but can then be used repeatedly. The same underlying program was used to compute all the results from Ch. 3 and Ch. 5, and could easily be adapted to other situations.

B.2 Computational details

For each phenomenon, all the relevant parameters are listed. We distinguish physical parameters, for which fixed values are used, and while the results might depend on them, their variation is not further analyzed within these projects; numerical parameters, on which the results should not depend; and model parameters, which are varied systematically and studied thoroughly.

The only material parameters from \(\text{Sr}_2\text{RuO}_4\) used as input are the Ginzburg Landau parameter \(\kappa_{ab} = 2.6\) and the superconducting anisotropy \(\gamma_s = 20\), as described in Sec. 1.3.2. These values, taken from Ref. [62], are used unless specified otherwise, but are listed if the results are expected to depend on them in a qualitative way.

In addition, numerical issues are discussed and comments regarding the implementation are provided.

B.2.1 Spontaneous surface flux pattern

Physical parameters

- disk radius \(R = 40\xi_0\) (see comment in Sec. 3.2.2)
- Ginzburg Landau parameter \(\kappa = 2.6\)
- temperature \(T = 0\) (see Sec. 3.4.1 for \(T > 0\))

Numerical parameters

- inner radius \(r_0 = 10\xi_0\)
- radial system size \(r \in [r_0, R]\)
- angular system size \(\theta \in [0, \pi/2]\)
- radial mesh size \(n = 100\)
- angular mesh size \(m = 100\)
B.2. Computational details

Model parameters

The ratio $K_1/K_2$ is systematically changed from the isotropic limit $K_1/K_2 = 3$ to the inverted value $K_1/K_2 = 1/3$, with $K_1 + K_2 = K =$ const for a constant coherence length. The results are, however, computed for equal steps in $(K_1 - K_2)/(K_1 + K_2) \in \{0.5 - i0.1 | i = 0, \ldots, 10\}$, as described in Sec. 3.1.2. This is illustrated in Fig. B.1.

The spontaneous flux pattern at the surface is computed for 31 surface types $s \in \{0, \ldots, 30\}$, as indicated in Fig. 3.3, and which are summarized below in Table B.1.

For the region B, that is, crossing from the specular scattering limit on the diagonal $g_1 = g_3$ to the full pair breaking limit on the axis $g_3 = 0$, we follow $g_3 = 2g_0 - g_1$, with $g_0 \rightarrow \infty$. The value of $g_0$ does not have to be specified, because we explicitly set $\eta(R) = 0$ for the corresponding component(s) of the order parameter, but a cut-off has to be introduced. From the a-posteriori analysis of the extrapolation lengths the applicability of the chosen cut-off was confirmed, see Fig. 3.5. To exclude the origin, we follow $g_3 = 2g_m - g_1$ with $g_m = g_3(0) = 0.25$.

Gauge, initial values and boundary conditions for the vector potential

We use the ‘minimal’ gauge, where the vector potential only has the most necessary spatial dependences. This can be understood as follows. In the isotropic limit, we do not want any angular dependences except for the phase winding. This is achieved by setting $(\eta_r, \eta_\theta) = |\eta_\theta|(u(r), iv(r))e^{iN\theta}$ with both $u(r)$ and $v(r)$ purely real and no global phase on $|\eta_\theta|$, $A_r = 0$ everywhere, and $A_\theta(r)$ with $A_\theta \rightarrow 0$ in the bulk. The vanishing $A_r$ and the $A_\theta$ constant in $\theta$ still fulfill the odd/even symmetry property discussed in Sec. 3.2.3. Away from the isotropic limit, there is a general angular dependence, and $A_r$ becomes finite. However, the even/odd property still holds, as it could only be destroyed by another gauge.

We stress that all of the above is implemented only by starting with appropriate initial conditions and fixing the constant values in the bulk throughout the minimization, while all other values can change freely.

Figure B.1: Equal steps in $(K_1 - K_2)/(K_1 + K_2)$ versus the ratio $K_1/K_2$. 
Table B.1: The numerical values of the 31 surface types \( s \) indicated in Fig. 3.3 (black dots). When \( T_{\text{eff}}^\text{cl}/T_c = 1 - 2g_0 \), the corresponding order parameter component is set to zero explicitly at the surface, \( \eta(R) = 0 \).

<table>
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<th>( g_3/(\xi_0aT_c) )</th>
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<th>( T_{\text{eff}}^\parallel/T_c )</th>
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</table>
B.2. Computational details

Figure B.2: The radially integrated flux for the most anisotropic case, the specular scattering surface type $s = 8$ at the inverted ratio $K_1/K_2 = 1/3$. The radial Riemann sum (dots) is compared with the Fourier expansion to first order (blue) and to second order (red).

**Fourier analysis of the radially integrated flux**

The radial integral is computed directly from the numerical results, using the discretized values of the vector potential and approximating the integral by a Riemann sum. For an even number $m$ of mesh points in the angular direction we then perform a type-I discrete cosine transform (DCT-I) on the first half $m/2$ of mesh points.

This is illustrated in Fig. B.2. The radial Riemann sum (dots) is compared to the Fourier expansion to first order (blue) and to second order (red). The first order $B_1$ is the most significant, while the second order $B_2$ still provides a small correction. All higher orders are negligible. This is true for all surface types, as can be seen from Fig. 3.9 (c).

**Impurity**

The impurity is implemented by changing $T_c$ in the middle of a single cell. The value is determined through a fixed integrated value for the impurity, $\tau_{\text{imp}} = \tau_{\text{imp}}^{\text{num}}hs$, where $h = L_x/n$ and $s = L_y/m$ are the mesh spacings for a system of side length $L_i$ and $n$ and $m$ mesh points. Here, we use $n = m = 600$ and $L_x = L_y = 30\xi_0$ and the temperature is $t = 0$. The results for changing the ratio $K_1/K_2$ have been computed for a mesh of size $n = m = 400$ only.

There are two numerical issues. First, polar coordinates are not feasible due to the singularity at $r = 0$. However, to resolve the impurity, which is mostly rotationally symmetric, a high number of mesh points are necessary. Second, as mentioned already in Sec. 3.4.2, the convergence is rather bad, in particular the higher $\tau_{\text{imp}}$. We have used the standard $(\eta_x, \eta_y)$ representation for the order parameter. However, the system might be better described using $(\eta_+, \eta_-)$, because the bulk component of this representation gets suppressed.
at the impurity, while the other component is at first enhanced, and then also suppressed at the impurity. Extracting (for the case of positive chirality) the component \( \eta^- \) from our numerical results, we find that it is oscillatory around the impurity. This issue requires further investigation, and we will try to compute the results using the \( \pm \)-representation. Both these issues should not influence the overall result and conclusion, while details of the shape of the flux pattern may change.

### B.2.2 Topologically frustrated Josephson junction

Lengths are measured in units of the cylinder radius \( R \). The physical parameters listed below are for Figs. 4.2 to 4.6, while the values for the other figures are indicated in the corresponding captions. For Figs. 4.7 and 4.8, \( \lambda_J/R \in [0,6] \) is the model parameter and is varied systematically.

#### Physical parameters

- Josephson penetration depth \( \lambda_J = 0.5R \)
- Cylinder height \( h = 3R = 6\lambda_J \)

#### Numerical parameters

The angular system size is \( \theta \in [0,2\pi] \) and the axial system size is \( z \in [0,h] \).

<table>
<thead>
<tr>
<th>Physical parameters</th>
<th>Figs. 4.2 to 4.6</th>
<th>Fig. 4.7</th>
<th>Fig. 4.8</th>
<th>Fig. 4.10</th>
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<td>( n = 40 )</td>
<td>( n = 200 )</td>
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<tr>
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<td>no axial dependence</td>
<td>( m = 40 )</td>
<td>( m = 400 )</td>
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</table>

#### Inhomogeneous coupling strength

Modulations \( m(\theta) \) are introduced to make the coupling strength inhomogeneous, as described in Sec. 4.2.3. The requirements are \( m(\theta) > -1 \) such that the coupling strength is always positive, \( m(\theta + 2\pi) = m(\theta) \) for periodicity, and \( \int_0^{2\pi} d\theta m(\theta) = 0 \) such that the angle-averaged critical current remains the same. The modulation can therefore be written as a Fourier expansion

\[
m(\theta) = \sum_{k=1}^{\infty} (a_k \cos(k\theta) + b_k \sin(k\theta)).
\] (B.5)

The quantity \( \hat{m} \) introduced in Eq. (4.46) is then given by

\[
\hat{m} = c_{-1} = \frac{a_1 + ib_1}{2} \Rightarrow |\hat{m}| = \frac{\sqrt{a_1^2 + b_1^2}}{2}.
\] (B.6)

All modulations used are illustrated in Fig. B.3 with their function, characteristic quantities and relations listed in Table B.2. All modulations are even and have their minimum at \( \theta = \pi \). The modulation \( m_0(\theta) \) is used for the detailed results in Sec. 4.2. The other four modulations are chosen as the most simple functions capturing the main ingredients entering the different possible behaviors derived in Sec. 4.3.
B.2. Computational details

Figure B.3: The four sample modulations $m(\theta)$. We consider cosines with different amplitudes, a second order cosine, and a combination: $m_a = 0.25 \cos(\theta)$, $m_b = 2m_a = 0.5 \cos(\theta)$, $m_c = -0.25 \cos(2\theta)$, and $m_d = m_a + m_c$. As required, the integral over one period is zero. The renormalization factor $|\hat{m}|$ is given by half the first cosine coefficient and is the same for $m_a$ and $m_d$, while it vanishes for $m_c$. The minimum and thus the initial position is always $u_0 = \pi$. The minimum value $-m(\pi)$ is the same for $m_a$ and $m_c$, and for $m_b$ and $m_d$. The amplitude $\Delta m$ is the same for $m_a$ and $m_c$.

| name   | function                                      | $|\hat{m}|$ | min($m(\theta)$) | max($m(\theta)$) | relation  |
|--------|-----------------------------------------------|-----------|------------------|------------------|-----------|
| $m_0(\theta)$ | $0.2 \cos(\theta)$                             | 0.1       | -0.2             | 0.2              |           |
| $m_a(\theta)$ | $0.25 \cos(\theta)$                             | 0.125     | -0.25            | 0.25             |           |
| $m_b(\theta)$ | $0.5 \cos(\theta)$                             | 0.25      | -0.5             | 0.5              | $= 2m_a$  |
| $m_c(\theta)$ | $-0.25 \cos(2\theta)$                          | 0         | -0.25            | 0.25             |           |
| $m_d(\theta)$ | $0.25 (\cos(\theta) - \cos(2\theta))$         | 0.125     | -0.5             | 0.25 arctan $\sqrt{15}$ | $= m_a + m_c$ |

Filamentary nucleation and evolution of the 3-Kelvin phase

**Physical parameters**

radius of the inclusion $R = 5\xi_0$

**Numerical parameters**

radial system size $r \in [R, R + 20\xi_0]$  
radial mesh size $n = 300$

**Model parameters**

bulk critical temperature $T_c = 1.5$ K  
interface critical temperature $T_i(R) = T_0 = 4.9$ K  
perpendicular surface parameter $K_r = 0.3/(\xi_0aT_c)$  
basic coupling parameter $K_l = 0.3/(\xi_0aT_c)$  
width of the filament $d = 0.5\xi_0$
Numerical minimization

The coupling strength |ψs| is increased by Δ|ψs| = 0.0125 for |ψs| ∈ [0, 0.425], the scale of which is somewhat set by Kθ. For each value of |ψs|, we start at T = 1 K and initialize the order parameter to its constant bulk value at this temperature. We then increase the temperature by ΔT = 0.01, using each obtained solution in turn for the next temperature, until we reach T = 5. The increasing temperature direction is preferable because we cannot start from the initial value η ≡ 0 for both components and do not want to introduce any bias, while the constant bulk values are known.

The transition temperatures are determined as follows. For T_A there is a second order transition at |ψs(0)|, determining the onset T_{3K}. For finite |ψs(0)| there is only a crossover. The temperature of this is determined by computing the slope of max_r η_{θ}(T) at T_{3K} and at the upper limit T = 5 K, and taking the temperature at which they intersect. Close inspection of the shape of max_r η_{θ}(T) shows that this is an appropriate choice. The temperature T_A’ is simply taken as the value when max_r η_{θ}(T) > 0.03. The temperature T_B is determined from the free energy difference $\mathcal{F}[N = 0] − \mathcal{F}[N = 1] = 0$, doing a linear interpolation between the negative value on the right and the positive value on the left of the transition.

B.2.3 C-axis domain wall

The model parameter is the anisotropy ν.

Physical parameters

- Ginzburg Landau parameter $\kappa = 2.6$
- superconducting anisotropy (domain wall) $\gamma = 20$
- superconducting anisotropy (HQV) $\gamma = 10$

Numerical parameters

- z-axis system size $z \in [-\xi_0, \xi_0]$
- mesh size $m = 200$

Stabilizing the domain wall

First, we compute the result at $\nu = 0$, starting from the step functions $(|\eta_{+}|_{j}, |\eta_{-}|_{j})/|\eta_{b}| = (\Theta(m/2), 1 - \Theta(m/2 + 1))$ (for $m$ even) as the initial value, which puts the domain wall exactly on the mesh point $j = m/2$. The anisotropy $\nu$ is then increased in small steps $\nu += 0.05$, in turn using the previous result as the new initial value. The same procedure is performed for negative $\nu$, again starting from the solution at $\nu = 0$. Due to the inversion symmetry of the domain wall, it is stabilized in the center of the system, such that no fixed boundary conditions have to be provided during the minimization iterations. This has the advantage that a rather small finite system size is sufficient, even when the width of the domain wall grows for $|\nu| \to 1$ such that both order parameter components are finite at the boundary. In that case, even though the solution does not converge within the maximally allowed iteration steps, the resulting value of the free energy behaves as expected, $\mathcal{F}_{dw} \to 0$ for $|\nu| \to 1$, see Fig. 5.2.
Introducing and stabilizing the HQV

Here the standard $xy$-representation of the order parameter is used and we solve for the real and imaginary values of the complex components, $\eta = (\eta_x, \eta_y) \equiv (R_x + iI_x, R_y + iI_y)$. In order to introduce the HQV to the system and stabilize it, we perform several steps. This is done at a fixed intermediate value of $\nu = -0.15$, based on the result of which the other results are computed. First, the basic shape of the order parameter across the domain wall is computed for the phase difference $\varphi = 0$ and in the gauge $A = 0$, leading to the odd $I_y \equiv f(z)$ and to $R_x \approx 1$ with a slight increase near the domain wall, while $I_x = I_y = 0$. As above, the domain wall is positioned directly on a mesh point by using the initial values $I_y(z \leq 0) = \pm 1$ and $I_y(z = 0) = 0$. Second, the phase shift is introduced by setting $I_y = f(z)\sqrt{(1 + \tanh(x/\xi_0))/2}$ and $R_y = \sqrt{1 - I_y^2}$, where we neglect the slight increase of the total absolute value near the domain wall. Far away from the domain wall $f(z)^2 = 1$ and the phase shift is given by

$$\varphi(x) = \arctan\left(\frac{1 + \tanh(x/\xi_0)}{1 - \tanh(x/\xi_0)}\right).$$

(B.7)

From symmetry it follows that $I_x = I_y(-x, -z)$ and $R_x = \sqrt{1 - I_x^2}$. Third, we compute the full results including the vector potential components $A_x$ and $A_z$ with fixed boundary conditions for the shape across the domain wall far away from the phase shift. The width of the phase shift, however, is not fixed, yet assumed small enough compared to the system size such that all quantities can relax. Finally, in a fourth step, we release all boundary conditions. This is especially important when the HQV explodes as $\nu \to 0$.

Changing the anisotropy $\nu$ for the HQV

The size and structure of the HQV changes considerably across the range of $\nu$. In addition, in the strongly anisotropic limit described by the non-local sine-Gordon model, two different characteristic length scales emerge, the core size $l$ and the Abrikosov-tail size $\lambda_c$. The system has to be large enough to accommodate the full half flux quantum, see also the discussion of the box size. For a uniform regular mesh this means that a small step size $h$ is needed to resolve the core, while a high number of mesh points are needed to have large overall system size $n \cdot h$.

This was achieved by using a mesh of $m = 600$ points for a fixed system size along the $z$-direction of $z \in [-20, 20] \xi_0$, and by using $n = 600$ points in the $x$-direction, but changing the step size $h$ as a function of $\nu$. This is illustrated by indicating the overall growing system size (dotted line) in Fig. 5.10 showing the full size of the HQV, and by indicating the step size $h$ (dotted line) in Fig. 5.11 showing the core size of the HQV. Still, the convergence was slow and could have been better, especially in the two limits. Yet, the overall trend was confirmed in several runs under slightly different conditions, and the main effect was always recovered. The unresolved details are unimportant for our analysis.

Here in particular a non-uniform or even adaptive mesh would have been very useful. We tried a brute-force approach of a non-uniform mesh but ran into problems maintaining the gauge. This is certainly a point to revisit in future projects.
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   *Evolution of the filamentary 3-Kelvin phase in Pb-Ru-Sr$_2$RuO$_4$ Josephson junctions*

3. **S. B. Etter**, A. Bouhon, and M. Sigrist
   *Spontaneous surface flux pattern in chiral p-wave superconductors – revisited*

4. **S. B. Etter**, W. Huang, M. Sigrist
   *Half-quantum vortices on c-axis domain walls of chiral p-wave superconductors*
   In preparation.
Over the past seven years I had the opportunity to work with Manfred Sigrist for a semester project, my Master thesis, and this PhD thesis. I have profited enormously from his ideas and insight, and was continuously amazed how he could answer any questions I had. He gave me the freedom and support to cope with both having children and finishing my PhD. This was only possible with his trust, for which I am truly grateful.

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