Superconducting phase transitions in hybrid superconducting systems with ferromagnets and spin-orbit coupling

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Declaration

This thesis is the result of my own work and includes nothing which is the outcome of work done in collaboration, except as specified in the preface of each chapter. It is not substantially the same as any work that has already been submitted for any degree or other qualification. This thesis does not exceed the prescribed word limit for the Physics and Chemistry Degree Committee.

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This PhD thesis investigates theoretically the proximity-coupling of superconductivity with ferromagnetism and/or spin-orbit coupling (SOC) in hybrid superconductor systems. The results are summarised in three results chapters which assess the proximity effect in hybrid superconductor systems through calculations of the superconducting phase transition (i.e., the critical temperature $T_c$ and critical fields $h_{c1}$ and $h_{c2}$).

Chapter 3 investigates a ferromagnetic (F) strip on a thin film superconductor (S) with interfacial Rashba SOC in the Ginzburg-Landau formalism. In the presence of SOC, $h_{c1}$ has a positive vortex contribution and a negative contribution from the interaction between vortices and SOC. Since the latter is negative, SOC lowers $h_{c1}$. When the SOC is strong enough, $h_{c1}$ becomes zero and vortices are generated in the absence of a magnetic field.

Chapter 4 considers the phase diagram of a thin film S with SOC in the Usadel formalism. Comparing infinite films with and without SOC, the SOC renormalises the magnetic field, effectively increasing $h_{c2}$. In finite sized samples, singlet-to-triplet conversion results in spin magnetisation at the sample edges. This edge effect suppresses the phase transition. Due to the sample size-dependence, the transition can be controlled in shape-anisotropic samples by rotating the applied magnetic field direction.

Finally, chapter 6 explores an s-wave superconductor (S) / chiral p-wave superconductor (P) junction in the Bogoliubov-de Gennes lattice model. In a S/P junction, the singlet Cooper pairs in S cannot mix with the triplet Cooper pairs in P and $T_c$ of both layers remains the same. However, in a S/F/P junction, F converts singlet pairs to triplet pairs, which boosts the P $T_c$. By rotating the F layer magnetisation, the singlet pairs convert into a different type of triplet pair state that cannot enter P and $T_c$ is unaffected. Hence, in a S/F/P junction, P $T_c$ is magnetisation-orientation-dependent.
Acknowledgements

From the outside Cambridge may look like a small town with stunning historical buildings, but it’s so much more than that. It is in fact its people – friendly, ambitious, open-minded, from all over the world – that makes Cambridge a truly wonderful and inspiring place. I am incredibly grateful to have had the opportunity to study at the University of Cambridge and call Cambridge my home for four years. This would not have been possible without my amazing college, St John’s College, who have provided me with housing, formal dinners, exciting parties and events, great facilities and friends that I hold very dear. I will always think back fondly of Cambridge and St John’s College. Souvent me souvient, as Lady Margaret herself would have said.

During the first two years of my PhD I spent a lot of time in the lab. The lab, sometimes fun, often-times frustrating, would not have been the same without our wonderful research group. Always friendly and willing to help out a clumsy mathematician. I really enjoyed the lunches, biscuit competitions, climbing expeditions, conferences and pub trips together. I would like to thank the group members Anand, Angelo, Ben, Bence, Carla, James, Juliet, Graham, Guang, Hisa, Kohei, Lauren, Sachio and Shahbaz (in alphabetical order because I cannot pick favourites, but my favourite is Graham). And of course, Nadia, because without her, the lab would have been complete chaos, instead of only a little chaotic.

Although my labwork has led to several co-authored papers, non of it is discussed in this thesis. Instead, this thesis focuses on the theory work that is now published in three peer-reviewed papers, each in collaboration with a different senior author. The first project was led by Prof. Alexander Buzdin, who co-supervised me during the first year of my PhD. It is both inspiring and daunting to see a physicist who actually uses the pure mathematics (closely related to magic tricks) to evaluate limits of complicated summations. The second project was done under co-supervision of Dr. Xavier Montiel, who has always been very kind, patient and encouraging. For him, the results are the starting point of a project, instead of the end goal. This approach has given me a profound understanding of the project and why the equations work the way they do. The third project was supervised by Prof. Jacob Linder, someone I had previously been in contact with due to a confusion about our names (Linde and Linder are the same in Japanese). Jacob is the most efficient and muscular professor I know and has an incredible talent for coming up with exciting projects with promising results. I had the pleasure of visiting his group in the beautiful city of Trondheim. I would like to thank Sasha, Xavier and Jacob for teaching me and I am so proud of our publications together.

I am grateful to the co-authors on my publications: Jordi Weggemans for his contribution to the phase diagram project, Graham Kimbell for his help with optimising the numerics and Lina Johnsen for helping me all around, welcoming me to Trondheim, having amazing insights and a critical view.

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Nomenclature

Acronyms

2DEG  Two-dimensional electron gas
BCS  Bardeen-Cooper-Schrieffer
D  $d$-wave superconductor
F  Ferromagnet
GL  Ginzburg-Landau
h.c.  Hermitian conjugate
LOFF  Larkin-Ovchinnikov-Fulde-Ferrell
N  Normal metal
P  $p$-wave superconductor
S  Conventional $s$-wave superconductor
SOC  Spin-orbit coupling

Roman

$a, a_0$  Standard Ginzburg-Landau coefficient
$\hat{A}$  Spin-orbit field matrix
$\vec{A}$  Vector potential
$\vec{A}_q$  Fourier transform of the vector potential
$\vec{A}_q^{\text{vor}}$  Fourier transform of the vector potential due to vortices
$\vec{A}_q^{\text{soc}}$  Fourier transform of the vector potential due to spin-orbit coupling
$b$  Standard Ginzburg-Landau coefficient
$\mathbf{B}, \vec{B}$  Applied magnetic field
$B_{p_x}^c, B_{p_y}^c$  Critical field corresponding to $p_x$- and $p_y$-wave symmetry
$B_{ik}^\dagger, B_{jk}$  Basis vector containing the single-particle creation and annihilation operators
$c$  Speed of light
$c_{k\alpha}^\dagger, c_{k\alpha}$  Single-particle creation, annihilation operator in momentum space
$c_{is}^\dagger, c_{is}$  Single-particle creation, annihilation operator in two-dimensional real space
$c_{i\alpha k\alpha}^\dagger, c_{i\alpha k\alpha}$  Single-particle creation, annihilation operator with one real and one momentum coordinate (obtained by applying the Fourier transform to $c_{is}^\dagger, c_{is}$)
\begin{itemize}
\item $d$ \hspace{1cm} Intervortex distance
\item $\vec{d}$ \hspace{1cm} $\vec{d}$-vector describing the spin-triplet state
\item $d_F, d_N, d_S$ \hspace{1cm} Thickness of a ferromagnet, normal metal, superconductor
\item $D$ \hspace{1cm} Diffusion coefficient (general)
\item $D_F, D_N, D_S$ \hspace{1cm} Diffusion coefficients in a ferromagnet, normal metal and superconductor
\item $\hat{D}$ \hspace{1cm} Gauge-invariant momentum operator
\item $e$ \hspace{1cm} Electron charge
\item $E$ \hspace{1cm} Energy: in the dispersion relation or the energy eigenvalue
\item $\vec{E}$ \hspace{1cm} Electric field
\item $E_{\pm}$ \hspace{1cm} Spin-split energy
\item $E_{\text{ex}}$ \hspace{1cm} Exchange energy
\item $E_F$ \hspace{1cm} Fermi energy
\item $E_{\text{int}}$ \hspace{1cm} Interaction energy between vortices and spin-orbit coupling
\item $E^0_{\text{int}}$ \hspace{1cm} Pre-factor in the interaction energy between vortices and spin-orbit coupling
\item $E_k$ \hspace{1cm} Kinetic energy
\item $E_{nk}$ \hspace{1cm} Energy eigenvalues of matrix $H_k$
\item $E_p$ \hspace{1cm} Potential energy
\item $E_U$ \hspace{1cm} Constant contribution to the total energy from the on-site interaction
\item $E_V$ \hspace{1cm} Constant contribution to the total energy from the nearest-neighbour interaction
\item $E_{\text{Vor}}$ \hspace{1cm} Vortex energy
\item $f$ \hspace{1cm} Free energy density in Chapter 3, anomalous Green’s function in Chapter 4, or a general function (throughout)
\item $f(E_{nk})$ \hspace{1cm} Fermi-Dirac distribution
\item $\tilde{f}$ \hspace{1cm} Particle-hole conjugate of the anomalous Green’s function
\item $f_s$ \hspace{1cm} Singlet-component of the anomalous Green’s function $f$
\item $\tilde{f}_t$ \hspace{1cm} Triplet-component of the anomalous Green’s function $f$
\item $F$ \hspace{1cm} Total free energy in Chapter 3, general pair correlation function in Chapter 6
\item $\vec{F}$ \hspace{1cm} Lorentz force
\item $F_0$ \hspace{1cm} Free energy in the normal state
\item $F_{i \pm x, j \pm y}$ \hspace{1cm} Pair correlations corresponding to the nearest-neighbours in $x, y$ of lattice site $i$
\item $F_{i \pm x(S), j \pm y(S)}$ \hspace{1cm} Pair correlations corresponding to the nearest-neighbours in $x, y$ of lattice site $i$, obeying anti-symmetric spin exchange
\item $F_{i \pm x(T), j \pm y(T)}$ \hspace{1cm} Pair correlations corresponding to the nearest-neighbours in $x, y$ of lattice site $i$, obeying symmetric spin exchange
\item $F_{ij}^{\uparrow}$, $F_{ij}$ \hspace{1cm} Pair correlation between electrons with opposite spin at lattice sites $i$ and $j$
\item $F_{ij \pm k}$ \hspace{1cm} Pair correlation between electrons with opposite spin at lattice sites $i_x$ and $j_x$ with momentum $k$ (obtained by applying the Fourier transform to $F_{ij}$)
\item $F_{p_x}, F_{p_y}$ \hspace{1cm} Pair correlations with $p_x$, $p_y$-wave symmetry
\end{itemize}
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<thead>
<tr>
<th>Nomenclature</th>
<th>Description</th>
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<tr>
<td>$F_{d,i}$, $F_{p_{x,i}}$, $F_{p_{y,i}}$</td>
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<td>$\tilde{F}<em>{d</em>{x_{1,2}}, p_{x_{1,2}}, p_{y_{1,2}}}$</td>
<td>Anomalous Green’s function describing the creation of a Cooper pair</td>
</tr>
<tr>
<td>$g$</td>
<td>Spectroscopic splitting factor, or the single-particle Green’s function</td>
</tr>
<tr>
<td>$\tilde{g}$</td>
<td>Particle-hole conjugate of the single-particle Green’s function</td>
</tr>
<tr>
<td>$\tilde{g}$</td>
<td>Spin-dependent part of the single-particle Green’s function</td>
</tr>
<tr>
<td>$g(\tilde{R}, \omega_n)$</td>
<td>Green’s function in spin $\otimes$ particle-hole space</td>
</tr>
<tr>
<td>$g(\tilde{R}, \tilde{p}_{F}, E)$</td>
<td>Energy-integrated Green’s function in the quasiclassical approximation</td>
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<td>$g_0$</td>
<td>Isotropic part of the Green’s function in the dirty limit in Chapter 2, or the spin-independent part of the single-particle Green’s function $g$ in Chapter 4</td>
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<tr>
<td>$g_1$</td>
<td>Linear part of the Green’s function in the dirty limit</td>
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<tr>
<td>$G$</td>
<td>Green’s function (general)</td>
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<td>$\hat{G}$</td>
<td>Green’s function matrix in Nambu $\otimes$ spin space</td>
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<tr>
<td>$G(\tilde{r}_1, \tilde{r}_2, E)$</td>
<td>Gor’kov Green’s function</td>
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<tr>
<td>$G_{s_{1,2}}(\tilde{r}_1, t_1, \tilde{r}_2, t_2)$</td>
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<td>$\tilde{G}<em>{s</em>{1,2}}(\tilde{r}_1, t_1, \tilde{r}_2, t_2)$</td>
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<td>$\tilde{h}$</td>
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<td>$h^0_{\text{soc}}$</td>
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<td>$\tilde{h}_{\text{vor}}$</td>
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<tr>
<td>$\tilde{h}_x, \tilde{h}_y$</td>
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<td>$H$</td>
<td>Total Hamiltonian</td>
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<td>$H_0$</td>
<td>Single-electron Hamiltonian</td>
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<tr>
<td>$H_D$</td>
<td>Dresselhaus spin-orbit coupling Hamiltonian</td>
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<tr>
<td>$H_h$</td>
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<tr>
<td>$H_{ijk}$</td>
<td>Total momentum- and space-dependent Hamiltonian in $B_{ik}$ basis</td>
</tr>
<tr>
<td>$H_K$</td>
<td>Total momentum-dependent Hamiltonian in $W_k$ basis</td>
</tr>
<tr>
<td>$H_{\mu}$</td>
<td>Chemical potential Hamiltonian</td>
</tr>
<tr>
<td>$H_R$</td>
<td>Rashba spin-orbit coupling Hamiltonian</td>
</tr>
</tbody>
</table>
Nomenclature

$H_t$ Hopping Hamiltonian
$H_U$ Superconducting on-site interaction Hamiltonian
$H_V$ Superconducting nearest-neighbour interaction Hamiltonian
$H_Z$ Zeeman Hamiltonian
$i, j$ Lattice site
$j$ Electric current density
$j_0$ Pre-factor in the electric current density
$j_{soc}$ Current density contribution from spin-orbit coupling
$j_{soc}^0$ Pre-factor in the current density contribution from spin-orbit coupling
$j_{vor}$ Current density contribution from vortices
$\hat{J}$ Total angular momentum operator
$J_{ex}$ Exchange energy of two neighbouring spins
$k, \tilde{k}$ Momentum, momentum vector, wave vector
$k_L$ Momentum perpendicular to the interface
$k_B$ Boltzmann constant
$k_F$ Fermi momentum
$K$ Kernel function
$K_0$ Zero momentum term in the self-consistent expression of $\Delta_i$
$K_{x0}, K_{y0}$ Zero momentum term in the self-consistent expression of $F_i^{x \pm}, F_i^{y \pm}$
l Orbital angular momentum
$l$ A general length, used for integration
$\ell$ Mean free path
$\ell_{so}$ Spin-flip length
$L$ Ferromagnetic strip width in Chapter 3, superconductor size in Chapter 4
$\hat{L}$ Orbital angular momentum operator
$m$ Electron mass
$\tilde{m}$ Microscopic magnetic moment
$m_s$ Spin magnetic quantum number
$M, \tilde{M}$ Magnetisation
$M_0$ Normalisation factor for the magnetisation
$M_r$ Remnant magnetisation
$M_s$ Saturation magnetisation
$n$ An integer
$\hat{n}$ Unit normal vector
$n_{1\uparrow}, n_{1\downarrow}$ Number of spin-up, spin-down electrons at the Fermi level
$n_{is}$ Number operator counting the electrons in state $i$ with spin $s$
$n_s$ Density of superconducting electrons
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
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<tbody>
<tr>
<td>(N)</td>
<td>Number of vortices</td>
</tr>
<tr>
<td>(N(E))</td>
<td>Density of states</td>
</tr>
<tr>
<td>(N_x, N_y)</td>
<td>Total number of lattice points in the (x-, y)-direction</td>
</tr>
<tr>
<td>(N_{x,F}, N_{x,p}, N_{x,s})</td>
<td>Number of lattice points in the (x)-direction in the ferromagnet, (p)-wave superconductor, (s)-wave superconductor</td>
</tr>
<tr>
<td>(\tilde{p})</td>
<td>Momentum</td>
</tr>
<tr>
<td>(\tilde{p}_F)</td>
<td>Fermi momentum</td>
</tr>
<tr>
<td>(\hat{p}_F)</td>
<td>Unit vector in the direction of the Fermi momentum</td>
</tr>
<tr>
<td>(\tilde{q})</td>
<td>Coordinate in Fourier transform</td>
</tr>
<tr>
<td>(q_y)</td>
<td>Modulation factor of the plane wave function</td>
</tr>
<tr>
<td>(Q)</td>
<td>General order parameter in Landau theory</td>
</tr>
<tr>
<td>(r, \tilde{r})</td>
<td>Position, or relative coordinate</td>
</tr>
<tr>
<td>(R, \tilde{R})</td>
<td>Centre-of-mass coordinate</td>
</tr>
<tr>
<td>(s, \tilde{s})</td>
<td>Electron spin</td>
</tr>
<tr>
<td>(\hat{s}_i)</td>
<td>Unit vector in the direction of the electron spin at lattice site (i)</td>
</tr>
<tr>
<td>(s_i)</td>
<td>Spin density at lattice site (i)</td>
</tr>
<tr>
<td>(S)</td>
<td>Entropy, or an enclosed area used for integration, or the total spin momentum</td>
</tr>
<tr>
<td>(\hat{S})</td>
<td>Spin angular momentum operator</td>
</tr>
<tr>
<td>(S_x, S_y, S_z)</td>
<td>Spin projections along the (x), (y) and (z) axes</td>
</tr>
<tr>
<td>(t)</td>
<td>Time, or the hopping parameter</td>
</tr>
<tr>
<td>(t_{ij})</td>
<td>Hopping amplitude between lattice sites (i) and (j)</td>
</tr>
<tr>
<td>(\mathcal{T})</td>
<td>Time-ordering operator</td>
</tr>
<tr>
<td>(T)</td>
<td>Temperature</td>
</tr>
<tr>
<td>(T^*)</td>
<td>Tricritical point in magnetic field versus temperature phase diagram</td>
</tr>
<tr>
<td>(T_c)</td>
<td>Superconducting critical temperature (general)</td>
</tr>
<tr>
<td>(T_{c+})</td>
<td>Recovery of superconducting critical temperature due to spin-orbit coupling</td>
</tr>
<tr>
<td>(T_{c0})</td>
<td>Superconducting critical temperature of a bare superconductor in Chapter 3, critical temperature in the absence of a field in Chapter 4 (see Chapter 5 for clarification)</td>
</tr>
<tr>
<td>(T_{c,d}, T_{c,p_x}, T_{c,p_y}, T_{c,s})</td>
<td>Superconducting critical temperature of the (d)-wave, (p_x)-wave, (p_y)-wave and (s)-wave pair correlations</td>
</tr>
<tr>
<td>(u_{ink})</td>
<td>Probability amplitude of electron-like spin-up state</td>
</tr>
<tr>
<td>(U)</td>
<td>Coulomb repulsion in Chapter 2, intervortex interaction in Chapter 3, or the superconducting on-site interaction in Chapter 6</td>
</tr>
<tr>
<td>(U_i, U_i)</td>
<td>Superconducting on-site interaction at lattice site (i, i_x)</td>
</tr>
<tr>
<td>(v_F, \tilde{v}_F)</td>
<td>Fermi velocity</td>
</tr>
<tr>
<td>(v_{ink})</td>
<td>Probability amplitude of electron-like spin-down state</td>
</tr>
<tr>
<td>(v_R)</td>
<td>Rashba velocity</td>
</tr>
<tr>
<td>(V)</td>
<td>Superconducting nearest-neighbour interaction</td>
</tr>
</tbody>
</table>
Nomenclature

\( V_{ij}, V_{ij} \) Superconducting nearest-neighbour interaction between lattice sites \( i \) and \( j \), \( i_x \) and \( j_x \)

\( w_{ink} \) Probability amplitude of hole-like spin-up state

\( W_{k}^{\dagger}, W_k \) Basis vectors stacking the basis vectors \( B_{ik}^{\dagger}, B_{jk} \)

\( \tilde{x} \) \( x \)-direction normalised by the coherence length

\( x_{ink} \) Probability amplitude of hole-like spin-down state

\( \tilde{y} \) \( y \)-direction normalised by the coherence length

\( Z \) Atomic number

**Greek**

\( \alpha \) Rashba spin-orbit coupling strength

\( \tilde{\alpha} \) Normalised Rashba spin-orbit coupling strength

\( \vec{\alpha} \) Rashba spin-orbit coupling vector, or field

\( \vec{\alpha}_q \) Fourier transform of the Rashba spin-orbit coupling vector

\( \gamma \) Dresselhaus parameter

\( \gamma_{ks}^{\dagger}, \gamma_{ks} \) Quasi-particle creation, annihilation operator in momentum space

\( \gamma_{inks}^{\dagger}, \gamma_{inks} \) Quasi-particle creation, annihilation operator in eigenvalue-momentum space

\( \Gamma \) Number of vortices in a chain

\( \delta E \) Splitting in the energy bands of a ferromagnet

\( \delta k \) Momentum mismatch

\( \Delta \) Superconducting energy gap (general)

\( \Delta \) \( s \)-wave superconducting order parameter

\( \tilde{\Delta} \) Normalised \( s \)-wave gap magnitude

\( \Delta_i \) Superconducting gap at lattice site \( i \)

\( \Delta_k \) Momentum-dependent superconducting energy gap

\( \Delta_{d,i}, \Delta_{p_x,i}, \Delta_{p_y,i} \) Order parameters with \( d \)-wave, \( p_x \)-wave, \( p_y \)-wave symmetry at lattice site \( i \)

\( \Delta_s \) \( s \)-wave gap magnitude

\( \varepsilon_k \) Single-particle energy

\( \theta \) In-plane applied magnetic field angle, or magnetisation angle

\( \Theta \) Heaviside step function

\( \kappa \) Ginzburg-Landau parameter

\( \tilde{\kappa} \) Cyclic permutations of the momentum \( \kappa_x = k_x (k_y^2 + k_z^2) \)

\( \lambda \) Superconducting penetration depth

\( \lambda_{\text{eff}} \) Effective superconducting penetration depth

\( \lambda_F \) Fermi wavelength

\( \mu \) Chemical potential

\( \mu_B \) Bohr magneton

\( \mu_i, \mu_i \) Chemical potential at lattice site \( i \), \( i_x \)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu_S, \mu_F, \mu_P$</td>
<td>Chemical potential in the S, F and P layers</td>
</tr>
<tr>
<td>$\xi, \xi_S$</td>
<td>Superconducting coherence length</td>
</tr>
<tr>
<td>$\xi_F, \xi_N$</td>
<td>Coherence length in a ferromagnet, normal metal</td>
</tr>
<tr>
<td>$\xi_p$</td>
<td>Single-particle kinetic energy</td>
</tr>
<tr>
<td>$\vec{\sigma}$</td>
<td>Pauli spin matrix vector in spin space</td>
</tr>
<tr>
<td>$\sigma_x, \sigma_y, \sigma_z$</td>
<td>Pauli spin matrices</td>
</tr>
<tr>
<td>$\hat{\Sigma}$</td>
<td>Total self-energy</td>
</tr>
<tr>
<td>$\hat{\Sigma}_{\text{ex}}$</td>
<td>Self-energy due to exchange field</td>
</tr>
<tr>
<td>$\hat{\Sigma}_{\text{imp}}$</td>
<td>Self-energy due to magnetic impurities</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Critical temperature recovery</td>
</tr>
<tr>
<td>$\vec{\tau}$</td>
<td>Pauli spin matrix vector in particle-hole space</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>Superconducting phase, or electrostatic potential</td>
</tr>
<tr>
<td>$\phi_0$</td>
<td>Flux quantum</td>
</tr>
<tr>
<td>$\Phi$</td>
<td>Magnetic flux</td>
</tr>
<tr>
<td>$\vec{\Phi}$</td>
<td>Vorticity</td>
</tr>
<tr>
<td>$\hat{\Phi}_q$</td>
<td>Fourier transform of the vorticity</td>
</tr>
<tr>
<td>$\chi$</td>
<td>Pauli spin susceptibility (general)</td>
</tr>
<tr>
<td>$\chi_N, \chi_S$</td>
<td>Pauli spin susceptibility of a normal metal, superconductor</td>
</tr>
<tr>
<td>$\psi$</td>
<td>Superconducting order parameter (general)</td>
</tr>
<tr>
<td>$\psi_e, \psi_h$</td>
<td>Electron-like, hole-like part of superconducting order parameter</td>
</tr>
<tr>
<td>$\psi_{\infty}$</td>
<td>Superconducting order parameter in the bulk</td>
</tr>
<tr>
<td>$\omega_D$</td>
<td>Debye frequency</td>
</tr>
<tr>
<td>$\omega_n$</td>
<td>Matsubara frequency</td>
</tr>
<tr>
<td>$\tilde{\omega}_n$</td>
<td>Normalised Matsubara frequency</td>
</tr>
</tbody>
</table>

**Calculus**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta$</td>
<td>Kronecker or Dirac $\delta$-function, or a fluctuation around an expectation value in Chapter 6</td>
</tr>
<tr>
<td>$\delta_k$</td>
<td>Type of derivative used in Section 4.3.2</td>
</tr>
<tr>
<td>$\nabla, \vec{\nabla}$</td>
<td>Del-operator</td>
</tr>
<tr>
<td>$\nabla, \vec{\nabla}$</td>
<td>Covariant derivative</td>
</tr>
<tr>
<td>$\partial$</td>
<td>Partial derivative</td>
</tr>
</tbody>
</table>
Chapter 1
Introduction

"Keep your head in the clouds and your hands on the keyboard"
— Marissa Meyer

1.1 Motivation

Cloud computing is the backbone of every digital service, including social media, streaming entertainment, online shopping, data storage and networking. Cloud computing is the delivery of computing services over the Internet (“the cloud”), such as data storage and processing. Rather than owning and maintaining their own complex computer infrastructure, businesses can instead rent these computer services and simply pay for what they use. In turn, cloud computing providers benefit from the scale of delivering the same services to a wide range of customers [1].

Cloud computing has become a popular option for businesses because it lowers operating costs, runs infrastructure more efficiently and is more secure [2]. As a result of the Covid-19 pandemic in 2020, work went virtual, businesses adapted to the global situation and cloud computing exploded. The global cloud computing market size is expected to grow 17.5% by 2025 compared to 2019 [3].

Sustainability is another major driver of cloud innovation. Nowadays, every responsible business understands they must play their part in the fight against climate change. In technology, this often means reducing energy usage of powerful computing engines and the energy cost of providing 24/7 digital services [4]. Due to the centralisation, cloud computing results in 77% fewer servers, uses 84% less power and reduces carbon emissions by 88% [5].

While cloud computing is a major leap forward in terms of sustainability, there is still a lot of room for improvement. Energy consumption is continuing to move from individual computers to the data centres where cloud computing is centralised. The next big improvement can be made by tackling the power consumption of data centres, which currently consume about 5% of the world’s total electricity [6, 7]. Our growing digital economy is increasingly dependent on data-intensive technologies – e.g. for artificial intelligence, smart and connected energy systems [8]. As a result, the data centres’ electricity consumption is predicted to increase 15-fold by 2030 [6].

This high power requires huge refrigeration capacity: the computer engines dissipate large amounts of heat due to Ohmic losses associated with charge flow in interconnects and read/write operations at
logic gates in complementary metal oxide semiconductor (CMOS) circuits. Consequently, 40% of the consumed energy in data centres is used for cooling computer engines [6]. Extensive research is ongoing to develop alternative technologies that can outperform our current semiconductor-based technology in terms of speed and stability, while simultaneously tackling the heat-dissipation issue. An upcoming technology driven by the increasing concerns over power consumption is superconducting spintronics [9], which combines superconductivity with ferromagnetism. Superconductors operate at low temperature, typically around 4 K. Since data centres already require substantial cooling, refrigeration is an acceptable requisite. Superconducting spintronics has a greater intrinsic efficiency than semiconductors, because superconductors allow for a charge current without Ohmic losses. Magnetic readout can be achieved with record low heat dissipation \((I_c \Delta t/e \ll 10^{-6} \text{ J})\), where \(I_c\) is the critical current, \(\Delta\) is the superconducting energy gap, \(t\) is an upper limit for the magnetisation reversal time (0.1 ns), and \(e\) is the electron charge) [9]. The resulting power savings can potentially exceed the additional cooling load required for operation at 4 K [10].

The concept of superconducting spintronics [9] is not trivial, since the combination of superconductivity and magnetism is counter-intuitive. In 1933, Meissner and Ochsenfeld [11] discovered that superconductors expel a magnetic field. The interplay between superconductivity and magnetisation has fascinated generations of condensed matter physicists ever since. The first macroscopic description of superconductivity by the London brothers [12] followed shortly after. In 1950, Ginzburg and Landau [13] developed a phenomenological theory on superconducting phase transitions, which draws a parallel with the magnetic phase transition in ferromagnets. A real understanding of the interaction between superconductivity and magnetism came in the late 1950s with the microscopic picture of superconductivity. The first description was given by Bardeen, Cooper and Schrieffer (collectively known as BCS) [14] and was extended by Bogoliubov [15, 16], de Gennes [17] and Gor’kov [18, 19]. In the BCS picture, electrons in a superconductor are bound by an attractive potential and form Cooper pairs consisting of two electrons with opposite spin and momentum \((|\uparrow\downarrow\rangle – |\downarrow\uparrow\rangle)\) [20].

Ferromagnets, on the other hand, have an intrinsic magnetisation that tends to align electron spins [21, 22]. Since superconductors and ferromagnets impose different requirements on the electron spin, interesting effects happen in hybrid structures of the two materials. Effects include the oscillating decay of superconductivity [23, 24], and the formation of triplet superconductivity in which the Cooper pair electrons have equal spin \((|\uparrow\downarrow\rangle\text{ and } |\downarrow\uparrow\rangle)\) [25, 26].

A different effect on spin is spin-orbit coupling, which has recently been introduced in superconducting spintronics. Spin-orbit coupling is a relativistic effect that couples the electron spin to its momentum. This occurs in heavy metals [27], non-centrosymmetric crystals [28–30], and at certain interfaces [31, 32]. Although spin-orbit coupling and ferromagnetism are vastly different phenomena, mathematically, they are remarkably similar. In superconducting spintronics, the combination of spin-orbit coupling and ferromagnetism gives additional ways to manipulate the spin. For this reason, heavy metal interlayers with strong spin-orbit coupling are commonly inserted in superconducting junctions [33].

This thesis theoretically explores several ideas to enhance the performance and functionality of superconductors in conjunction with ferromagnetism, spin-orbit coupling, or both. The basic science developed in this PhD explores fundamental interactions in hybrid superconducting systems with magnetic order. The aim is to develop strategies to enable active control of superconductivity, spin and magnetism, and so build a framework for experiments to build on; and in this way, contribute to the collective goal of establishing more energy efficient computing and quantum technologies.
1.2 About this PhD

I went into my PhD with two master’s degrees in Applied Physics and Applied Mathematics. As part of these degrees, I had the chance to do two internships: one with my current research group in Cambridge, where I assisted in several experimental projects (leading to Papers 1, 2 and 9 in the list below), as well as a theoretical physics internship with Prof. Yukio Tanaka in Japan (Paper 3). The plan for my PhD was to continue on the same foot, doing both experimental and theoretical work.

Doing theoretical work while being part of a predominantly experimental group gave me an interesting and exciting position. Being surrounded by experimentalists gives an appreciation for what is experimentally feasible and ensures that the theoretical work is always experimentally driven. This also gave me the opportunity to collaborate with group members by making models to explain their data or devise new experiments, leading to my co-authorship on Papers 4 and 8.

My primary PhD supervisor Prof. Jason Robinson is most proficient in experimental materials physics. Alongside him, I also had two theoretical co-supervisors, one external, Prof. Alexander Buzdin, and one internal, Dr. Xavier Montiel (a Senior Postdoctoral Scientist in Jason’s group). I also collaborated with Prof. Jacob Linder. Each of them has their own expertise and I feel very lucky to have learned from them, giving me a broad view of the field and teaching me a variety of modelling techniques. During the first year of my PhD, I was co-supervised by Prof. Alexander Buzdin, who was on sabbatical in Cambridge. Under his co-supervision, I worked on Paper 5. Later that year, Dr. Xavier Montiel joined our group and together we published Paper 7.

In the final year of my PhD I initiated a collaboration with Prof. Jacob Linder at the university of Trondheim, Norway, and spent several months in his group, working with his team on a project involving the coupling of conventional and unconventional superconductivity at magnetic interfaces. This collaboration resulted in Paper 10, published in Physical Review Letters.

Although the focus of my PhD was on the development of the theory models presented in this thesis, I also undertook collaborative experimental work in Jason’s group during my PhD. The initial plan was to have a larger experimental focus, but due to Covid-19 and various laboratory restrictions Jason and I decided it would be more strategic to focus on theory. Although I concentrated on theory I continued to support the team with experimental work and modelling of experimental results.

I started out by growing ferromagnet SrRuO$_3$ onto unconventional superconductor Sr$_2$RuO$_4$ single crystals using pulsed laser deposition. I characterised the samples (using atomic force microscopy and X-ray diffraction), patterned them (using photo- and electron-beam lithography) and performed low-temperature magnetic and transport measurements. I developed a framework for growing and measuring Sr$_2$RuO$_4$/SrRuO$_3$ samples and this project will be continued by other students in the lab. My experience with non-local measurements led to my contribution to Paper 6.

I also did experimental work on metallic systems. I investigated superconducting Nb proximity-coupled to Pt/Co multilayers with perpendicular ferromagnetic anisotropy grown by magnetron sputtering. I trained and supported an internship student who worked on the Pt/Co multilayers.

Through a collaboration with Prof. Yossi Paltiel at the Hebrew University of Jerusalem, Jason and I decided to add chiral molecules to the Nb/Pt/Co structures. This had not been done in Cambridge before and I developed a process to fabricate the structures. Experiments were halted by the Department closure due to the Covid-19 pandemic. When the Department reopened several months later with limited access, the time-sensitive nature of the chiral molecule structures made it difficult to efficiently do measurements. The project was thus passed on to a new student who I trained and helped in the lab.

Finally, I developed a project with collaborators at the University of Twente, which was initiated by my Master's work. This project resulted in Paper 11.
1.3 Publications

In chronological order,


Publications 5, 7, and 10 were the main focus of my PhD and are thus discussed in this thesis.
1.4 Outline

Chapter 2 introduces the physical concepts used throughout the thesis, focusing on superconductivity, ferromagnetism, and spin-orbit coupling. Chapter 2 provides an overview of the different mathematical formalisms used to describe superconductivity in this thesis.

Chapters 3, 4 and 6 are the main results chapters and have led to peer-reviewed publications. Each chapter starts with an illustration that summarises the key result of the chapter. The most important mathematical steps are covered in the chapters themselves, with further details covered in the appendices at the end of the thesis.

Chapter 3 considers a superconductor with intrinsic spin-orbit coupling in a heterostructure with a ferromagnet, described by Ginzburg-Landau theory. Abrikosov vortices naturally occur in some superconductors. The interaction between spin-orbit coupling and ferromagnetism pins the vortices along the ferromagnet edges and creates a spontaneous current. The vortex movement can be controlled by the magnetisation-orientation of the ferromagnet.

Chapter 4 investigates the magnetic field-temperature phase diagram of a thin film superconductor with strong spin-orbit coupling in the Usadel formalism. Spin-orbit coupling renormalises the applied magnetic field such that the superconductor’s critical field increases. Considering a finite-size superconductor, the phase transition is suppressed compared to an infinite film, but can be recovered using spin-orbit coupling. In geometrically anisotropic superconductors, the critical field can be controlled by rotating the applied field direction.

Chapter 5 makes a comparison between the models used in chapters 2 and 3, which both describe superconductors with spin-orbit coupling.

Chapter 6 describes a $p$-wave superconductor/ferromagnet/$s$-wave superconductor junction in the lattice Bogoliubov-de Gennes model. The ferromagnet converts the $s$-wave singlets to $p$-wave triplets, which enter the $p$-wave via the proximity effect and boost the $p$-wave critical temperature. By rotating the ferromagnet magnetisation, a different type of triplets is generated which is not native to the $p$-wave and does not affect its critical temperature. Hence, by rotating the magnetisation of the ferromagnet, the $p$-wave critical temperature can be controlled.
Chapter 2

Theoretical concepts

“Art is fire plus algebra.”
— Jorge Luis Borges

The quote above sums up what theoretical physics means to me. The fire is a spark of imagination, a great idea, perhaps considered absurd and controversial at first. The algebra proves or disproves it, makes it rigorous and communicates the idea in the universally understood language of mathematics. The combination of imagination and mathematical rigour, fire and algebra, is the art of theoretical physics.

This chapter introduces the theoretical concepts that are used throughout this thesis. It starts with an introduction to phase transitions, which lies at the core of superconductivity and ferromagnetism. This is followed by microscopic descriptions of superconductivity (Section 2.2) and magnetism (Section 2.3). Central to this thesis is the role of spin-orbit coupling in superconductors, which will be introduced in Section 2.4. In Section 2.5, we consider proximity effects that occur in superconducting junctions.

2.1 Phase transitions

We consider a system with two phases: an ordered and a disordered phase. Here we focus on phase transitions triggered by a change in temperature, but they can also result from e.g. pressure or magnetic field, as we will see later on.

Generally, the system is in an ordered, condensed phase at low temperature. Increasing the temperature introduces disorder in the system. When the temperature reaches a certain critical temperature $T_c$, the disordered phase becomes more energetically favourable and the system undergoes a phase transition.

Some examples are a solid (atoms ordered at fixed lattice positions) transitioning to a gas (atoms moving freely), a ferromagnet (magnetic moments pointing in the same direction) transitioning to a paramagnet (magnetic moments in all directions) and a superconductor in its superconducting state (electrons in Cooper pairs occupy the same ground state) to a normal metal (single electron motion). These examples are illustrated in Fig. 2.1.
2.1.1 Thermodynamics

To be more precise, a phase is energetically favourable when it has the lowest free energy. Any phase is associated with a free energy $F$ that varies as a smooth function of temperature. Whenever the free energy curves of two phases cross, the system will adapt the phase with the lowest free energy and undergo a phase transition. Generally, the nature of this transition is classified as first-order or second-order.∗

In the case of a first-order phase transition, the two free energies cross and result in a kink in the free energy of the system. In a second-order phase transition, the free energies of the two phases are identical over a small temperature range such that they have the same tangent at the transition point. As a result, the free energy of the system is a smooth function.

The entropy $S$ is the temperature derivative of the free energy $S = \frac{\partial F}{\partial T}$. Since the free energy of a first-order transition has a kink, the corresponding entropy has a jump $\Delta S$ at the transition. This jump manifests itself in the form of latent heat, i.e., the system releases or absorbs a fixed amount of energy during the transition. Second-order transitions have a continuous entropy and there is no latent heat associated with them.

2.1.2 Landau theory

Lev Landau developed a phenomenological theory to generally describe second-order phase transitions from various fields of physics. The main concept of Landau theory is the introduction of an order parameter $Q(T)$ as a function of temperature. The order parameter is normalised such that $Q(0) = 1$, it is nonzero in the low-temperature, ordered phase and is zero above the transition. In a second-order

∗We note that “order” describes two different concepts here. We consider the ordered (low-temperature) and disordered (high-temperature) phase, whereas “order” in first-order and second-order refers to the differentiability of the free energy.
transition, $Q$ changes gradually with temperature, whereas in first-order transitions $Q$ drops to zero instantly at the transition. Mathematically, we say that $Q(T_c) = 0$ for second-order transitions and $dQ/dT(T = T_c)$ is discontinuous for first-order transitions. This is shown in Fig. 2.3.

![Figure 2.3: (a) Order parameter $Q$ versus temperature $T$ and (b) corresponding free energy $F$ at the transition $T = T_c$, for a first-order (blue) and second-order (pink) phase transition. The abrupt first-order transition causes $Q(T_c)$ to have multiple values $A$ and $B$, which are represented by multiple minima in the free energy.](image)

### Second-order transitions

To phenomenologically describe second-order phase transitions, Landau introduced the free energy as a function of the temperature $T$ and the order parameter $Q$. Generally, there is no directional preference in the system, which implies that reversing the order parameter should give the same energy, i.e., $F$ has to be symmetric in $Q$. Therefore, Landau started from a Taylor expansion only including the even powers of $Q$, expressing the free energy as

$$F = \int f(\mathbf{r})d^3r$$

with

$$f(T, Q) = f(T, 0) + A(T)Q^2 + B(T)Q^4,$$

where $T$ is assumed to be small, such that we can neglect higher order terms.

Considering the physical behaviour of materials, we can make a couple of general statements about the $A$ and $B$ coefficients. The free energy needs to have a minimum at finite $Q$. Therefore, $B(T)$ has to be positive for all temperatures. We usually define $B(T) = b/2$ by convention. In the disordered phase ($T > T_c$), we need $A(T) > 0$ in order for $f$ to have a minimum at $Q = 0$, while in the ordered phase ($T < T_c$), we require $A(T) < 0$ for $f$ to have a minimum at finite $Q$. The simplest function to describe this behaviour is $A(T) = a(T - T_c)$. To find the minima in $Q(T)$ that describe a stable state, we set $\partial F/\partial Q = 0$ and obtain

$$Q(T) = \pm \sqrt{\frac{a(T_c - T)}{b}}, \quad \text{for } T \leq T_c.$$ 

As the system heats up ($T \to T_c$), the two minima gradually move towards $Q = 0$. The free energy of a second-order phase transition is illustrated in Fig. 2.4.

### First-order transitions

Landau theory was derived specifically for second-order transitions, but can be extended to describe first-order transitions as well.

For second-order transitions, $Q(T)$ is single-valued. In first-order transitions, the two phases coexist in equilibrium over a limited temperature range and $Q(T)$ drops vertically at $T = T_c$. This implies that $Q(T)$ is no longer single-valued and $f(T_c, Q)$ must have at least one additional minimum, as illustrated
Theoretical concepts

Figure 2.4: Free energy $F$ as a function of the order parameter $Q$ for a second-order phase transition. It has two minima for $T < T_c$ that merge together at the transition $T = T_c$.

in Fig. 2.3. To mathematically describe the navy curve in Fig. 2.3b, we include the next term in the Taylor expansion and use an alternating pattern of plus- and minus-signs, i.e.,

$$f(T, Q) = f(T, 0) + a(T - T_c)Q^2 - \frac{b}{2} Q^4 + c Q^6.$$.

Finding the minima of this equation yields three critical temperatures $T_1 > T_c > T_0$, corresponding to the coexistence of two different phases. For $T > T_1$, the disordered phase has the lowest energy. For $T_1 < T < T_c$, the disordered (high-temperature) phase is stable, while the ordered (low-temperature) phase coexists in a metastable form. At the transition temperature $T_c$, the free energy is $F = 0$ in both minima, meaning that the phases are in thermodynamic equilibrium. For $T_c > T > T_0$, the system adapts the ordered phase, while the disordered phase is metastable. Finally, for $T < T_0$, the ordered phase is favourable.

2.1.3 Ginzburg-Landau theory of superconductivity

In 1911, Kamerlingh Onnes [35] discovered that the electrical resistance of mercury disappears a few degrees above absolute zero. This phenomenon became known as superconductivity and the materials that have this property are called superconductors. In 1933, Meissner and Ochsenfeld [11] discovered that superconductors expel a magnetic field. The first macroscopic description of superconductivity by the London brothers [12] followed shortly after. In 1950, Ginzburg and Landau [13] developed a phenomenological theory on superconducting phase transitions, by applying Landau theory to superconductors. Microscopic theory of superconductivity followed a couple of years later and will be discussed in Section 2.2.

The charge carriers in a normal conductor are single electrons. When the material becomes superconducting the electrons pair up, forming Cooper pairs. Since Cooper pairs are bosons and they all go in the same ground state (more on that in Section 2.2.1), we consider the superconductor the condensed (ordered) phase of the normal conductor.

Ginzburg and Landau were not aware yet of the existence of Cooper pairs, and simply described the superconductor as a system with a disordered (normal) and ordered (superconducting) phase. To define the superconducting order parameter, Ginzburg and Landau [13] took a quantum mechanical approach, using the wave function $\psi = |\psi|e^{i\varphi}$, with $|\psi|^2 = \psi^*\psi = \frac{1}{2}n_S$, where $n_S$ is the density of superconducting electrons. This implies that $\psi = 0$ in the normal state ($T > T_c$). The phase factor $\varphi$ is related to the supercurrent flowing through the material below $T_c$.

Following the principles of Landau theory, Ginzburg-Landau theory starts with the free energy of a
superconductor. In cgs units, it is given by

\[ F = F_0 + \int a|\psi|^2 + \frac{b}{2}|\psi|^4 + \frac{1}{4m} |\tilde{D}\psi|^2 + \frac{\tilde{h}^2}{8\pi} d^3 \vec{r}, \]  

(2.1)

where \( F_0 \) is the normal state contribution, \( a = a_0(T - T_c)/T_c \) and \( b \) are the standard Ginzburg-Landau coefficients, \( m \) is the electron mass, \( \tilde{h} \) is an applied field, \( \tilde{D} = -i\vec{\nabla} + 2e\tilde{A} \) is the gauge-invariant momentum operator with \( e \) the electron charge and \( \tilde{A} \) the vector potential related to \( \tilde{h} \) via the Maxwell equation \( \vec{\nabla} \times \tilde{A} = 4\pi \vec{j} \).

Ginzburg and Landau use the free energy (2.1) to derive two characteristic equations. The first one is obtained by minimising the free energy \( F \) with respect to \( \psi^* \) using the Euler-Lagrange method. Using that \( |\psi|^2 = \psi^* \psi \), the first Ginzburg-Landau equation is

\[ \frac{\partial F}{\partial \psi^*} = a\psi + b|\psi|^2\psi - \frac{\tilde{D}^2\psi}{4m} = 0. \]  

(2.2)

This differential equation determines the order parameter \( \psi \) (similar to the time-independent Schrödinger equation).

The second Ginzburg-Landau equation describes the dissipation-less electric current density \( \vec{j} \) through the superconductor and is obtained from minimisation with respect to the vector potential (\( \vec{j} = -\partial F/\partial \tilde{A} \)), i.e.,

\[ \vec{\nabla} \times \tilde{h} = 4\pi \vec{j} \quad \text{with} \quad \vec{j} = -\frac{e}{2m} \left[ \psi^* \tilde{D}\psi - \psi(\tilde{D}\psi)^* \right] = -\frac{e}{m} \left( \tilde{h} \vec{\nabla} \varphi + 2e\tilde{A} \right) |\psi|^2. \]  

(2.3)

The equation for the electric current density was first derived by London in 1933 [12] to explain the expulsion of the magnetic field.

The Ginzburg-Landau equations go accompanied by two characteristic length scales: the London penetration depth and the coherence length. The penetration depth \( \lambda \) is the distance over which a magnetic field penetrates a superconductor, given by

\[ \lambda = \sqrt{\frac{m}{8\pi e^2 |\psi|^2}}. \]  

(2.4)

The temperature-dependent coherence length \( \xi(T) \) is the decay length at the edge of the superconductor, which is defined as

\[ \xi(T) = \sqrt{\frac{\hbar^2}{4m|a(T)|}}. \]  

(2.5)

The coherence length was later linked to the Cooper pair size (see Section 2.2.1) and is the length scale of which \( \psi \) can vary.

At the interface between a normal metal and superconductor, these two length scales compete with each other. The free energy balances the positive magnetisation contribution (associated with \( \lambda \)) and the negative superconducting ordering contribution (associated with \( \xi \)). The temperature-independent Ginzburg-Landau parameter \( \kappa \equiv \lambda/\xi \) can be defined from the surface energy. Depending on the value of \( \kappa \), two types of superconductivity exist which behave differently in the presence of a magnetic field \( h \).

In a type I superconductor, \( \kappa < 1/\sqrt{2} \), the magnetisation contribution outweighs the ordering contribution. The resulting surface energy is positive, see Fig. 2.5a-c. To minimise the free energy, the number of surfaces has to be minimised. Type I superconductors have one critical field \( h_c \). If the applied magnetic field is smaller than this value (\( h < h_c \)), the superconductor is able to screen the magnetic

---

*The \( F_0 \) term is equal in both the normal and superconducting state. It is therefore not relevant for the description of superconductivity and is summarised in a pre-factor \( F_0 \).
Theoretical concepts

Figure 2.5: Normal metal/superconductor interface for a (a) type I and (b) type II superconductor. The superconducting order parameter $|\psi|$ is characterised by the coherence length $\xi$, while the magnetic field $h$ extends over the penetration depth $\lambda$. The corresponding free energy $F$ is (c) positive for a type I and (d) negative for a type II superconductor.

field completely. This is called the Meissner state [11]. For fields larger than the critical field ($h > h_c$), superconductivity breaks down and the superconductor is in its normal state.

For a type II superconductor, $\kappa > 1/\sqrt{2}$ and the surface energy goes negative, see Fig. 2.5b-d. This implies the free energy is minimised by forming surfaces. As a result, type II superconductors have two critical fields $h_{c1}$ and $h_{c2}$. When $h < h_{c1}$, the superconductor is in the Meissner state, and when $h > h_{c2}$, the superconductor is in the normal state. But when $h_{c1} < h < h_{c2}$, the free energy is minimised by forming small non-superconducting regions in the superconductor through which the magnetic field can penetrate. The properties of these non-superconducting regions will be discussed in the next section.

Elementary superconductor Al has $\lambda = 16$ nm and $\xi = 1600$ nm [36], making it a type I superconductor, whereas Nb has $\lambda = 39$ nm and $\xi = 38$ nm [36], which makes it type II.

### 2.1.4 Superconducting vortices

Superconducting vortices are essentially tubes of magnetic flux. The magnetic field partially penetrates a type II superconductor through small non-superconducting cores with radius $\xi$. Due to the proximity effect, the magnetic field extends over a length scale $\lambda$ around the core. The magnetic field distribution of a single vortex is $h(r) \approx \sqrt{\lambda/r} \exp(-r/\lambda)$ with $r$ the distance from the core. The tubes of magnetic flux are encircled by a supercurrent that acts to screen the magnetic field for $r > \lambda$. A schematic illustration of superconducting vortices is shown in Fig. 2.6.

The magnetic flux of a superconducting vortex is quantised. To see this, we consider the magnetic flux $\Phi$ over an enclosed area $S$, which is given by the integral over the magnetic field $\vec{h}$ over $S$. Using $\vec{h} = \nabla \times \vec{A}$, with $\vec{A}$ the vector potential, we obtain

$$\Phi = \int_S \vec{h} \cdot d\vec{S} = \oint_{\partial S} \vec{A} \cdot d\vec{l}.$$  

Substituting (2.3), $\Phi$ is expressed in the electrical current $\vec{j}$ and the wave function phase $\nabla \varphi$. The area
2.2. Microscopic theory of superconductivity

$S$ is large enough such that the vortex is completely enclosed and $\vec{j} = 0$ along $\partial S$. What remains is

$$\Phi = \frac{\hbar}{2e} \oint_{\partial S} \nabla \varphi \cdot d\vec{l} = \frac{\hbar}{2e} (2\pi n) \equiv n\phi_0.$$ 

The integral represents the change of phase after one turn around $S$. The wave function $\psi = |\psi|e^{i\varphi}$ is single-valued, meaning that it is identical for $\varphi = 0$ and $2\pi$. Hence, the phase has to be cyclic and the integral is equal to $2\pi n$, where $n$ is an integer. We define $\phi_0 \equiv \hbar/2e$ as the flux quantum. To minimize the free energy, the flux quanta are distributed evenly over the vortices such that each vortex carries one flux quantum [37].

![Magnetic flux lines](a) Supercurrent loop

Figure 2.6: (a) Schematic illustration of superconducting vortices. (b) The superconducting order parameter $|\psi|$ and magnetic field $h$ at the centre of a vortex.

2.2 Microscopic theory of superconductivity

The macroscopic Ginzburg-Landau theory of superconductors describes the superconductor as a whole. This method works well to calculate thermodynamic properties (e.g. the phase transition), but it is not able to capture microscopic mechanisms, such as electron spin, the formation of Cooper pairs, triplet pairing and scattering.

The microscopic description of superconductivity postulated in 1957 by Bardeen, Cooper and Schrieffer [14] forms the foundation of modern theories of superconductivity. The key components of their so-called BCS theory is the formation of electron pairs with opposite spin and momentum, and the condensation of these pairs. BCS theory specifically deals with clean, homogeneous systems, described by a mean-field Hamiltonian in momentum $k$-space.

To describe inhomogeneous systems, such as junctions and multilayers, Bogoliubov [15, 16] and de Gennes [17] extended BCS theory and derived a set of equations of motion for electrons and holes, coupled by the superconducting energy gap $\Delta$. These are expressed in an effective mean-field Hamiltonian in real-space, from which the superconducting wave function is obtained.

The difficulty with the Bogoliubov-de Gennes formalism is that generally impurity positions in real-space are unknown, making it difficult to describe scattering processes. This led to the introduction of Green’s functions. Whereas wave functions describe a particle’s probability amplitude, Green’s functions describe the particle’s propagation through a system with different types of interactions. Green’s functions allow for an easier treatment of impurity scattering, nonlinearities and non-equilibrium systems.

Gor’kov [18] expressed the BCS Hamiltonian in terms of two Green’s functions: a single-electron Green’s function and an anomalous Green’s function to describe Cooper pair correlations, coupled by a many-body Hamiltonian. Gor’kov used the set of Green’s functions to demonstrate that Ginzburg-Landau theory (Section 2.1.3) can be microscopically derived from BCS theory close to $T_c$ [19], uniting microscopic and macroscopic theories of superconductivity.

The two coupled Gor’kov equations are a powerful but mathematically complex way to describe superconductivity. To simplify the mathematics and reduce the description to one equation, Eilenberger
applied the quasiclassical approximation. The Cooper pair size $\xi$ is much larger than the Fermi wavelength $\lambda_F$, such that Cooper pairs only feel the average of microscopic effects of length scale $\sim \lambda_F$. In the quasiclassical approximation, these fine-scale structures are filtered out and disregarded.

Subsequently, Usadel [39] considered a dirty superconductor, dominated by impurities. As a result, the Green’s functions become nearly isotropic in space. Usadel used this simplification to derive a diffusion equation valid in the dirty limit. The Usadel equation is mathematically tractable, allows for easy implementation of a large variety of physical effects and is therefore widely used.

An overview of the different theoretical frameworks is shown in Table 2.1. This section introduces their fundamentals and the most crucial steps in their derivations.

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<th>Quasiclassical approx.</th>
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<tr>
<td>Bogoliubov-de Gennes equations</td>
<td>Andreev equations</td>
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<tr>
<td>Green’s function methods</td>
<td></td>
</tr>
<tr>
<td>Gor’kov equations</td>
<td></td>
</tr>
<tr>
<td>Eilenberger equation, Usadel equation</td>
<td></td>
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</tbody>
</table>

**Table 2.1:** The equations of motion of inhomogeneous superconductivity.

### 2.2.1 The foundation: BCS theory

The original BCS formulation [14] considers a negatively charged electron travelling through an atomic lattice with positively charged ions. The passing electron slightly deforms the surrounding lattice by pulling on the ions. This lattice distortion is called a phonon. Since the electron velocity (given by the Fermi velocity) is much larger than the phonon velocity, a second electron is attracted to the positively polarised ions before the lattice can relax. This indirect attraction between electrons produces a pairing of electrons, i.e., a Cooper pair [20]. The size of a Cooper pair is the superconducting coherence length $\xi$ given in (2.5).

The formation of Cooper pairs only occurs when attractive phonon interactions dominate the Coulomb repulsion between two negatively charged electrons. The attractive interaction is maximal when the total momentum of the Cooper pair is zero (its center of mass is stationary), which requires pairing between $+k$ and $-k$ states. To see this, we consider a simplified picture of two plane wave electron states with opposite momentum, i.e., $\psi_1 \sim e^{ikx}$ and $\psi_2 \sim e^{-ikx}$. The paired superposition of these states $\psi_{\text{pair}} = (\psi_1 + \psi_2)/\sqrt{2}$ has probability distribution $|\psi_{\text{pair}}|^2 \sim \cos^2(kx)$, extending over the Cooper pair size $\xi$. This can be interpreted as the spatial pattern of the lattice distortion, which brings positively charged ions closer together and consequently lowers the Coulomb energy. This is illustrated in Fig. 2.7.

Since BCS theory is isotropic in $k$-space, the spatial wave function is symmetric. To satisfy the Pauli exclusion principle, the spin has to be anti-symmetric, which involves pairing of electrons with opposite

![Image](image.png)

**Figure 2.7:** A lattice distortion in the presence of Cooper pairs brings positively charged ions closer together to lower the Coulomb energy.
2.2. Microscopic theory of superconductivity

spin (↑ and ↓). Consequently, the total spin of the Cooper pair is zero, which implies Cooper pairs are bosons and they condensate into the same ground state [14].

Since all Cooper pairs occupy the same ground state, they are described by a single wave function. In the second quantisation formulation, \( c_{ks}^\dagger \) creates an electron in a state with momentum \( k \) and spin \( s \in \{↑, ↓\} \), whereas the annihilation operator \( c_{ks} \) removes it. Using these operators, the BCS Hamiltonian in \( k \)-space is [14]

\[
H_{\text{BCS}} = \sum_{k,s} \varepsilon_k n_{k,s} + \sum_{k,k'} V_{kk'} c_{k\uparrow}^\dagger c_{-k'\downarrow} c_{-k'\uparrow} c_{k\downarrow}^\dagger.
\] (2.6)

The first term is the standard kinetic energy term, consisting of the number operator \( n_{k,s} = c_{k,s}^\dagger c_{k,s} \), which counts the number of particles in state \( (k, s) \), and the corresponding single-particle energy \( \varepsilon_k = h^2 k^2 / 2m - \mu \), with \( h \) the reduced Planck constant, \( m \) the electron mass and \( \mu \) the chemical potential. The second term describes Cooper pair scattering from \( (k', \uparrow, -k' \downarrow) \) to \( (k \uparrow, -k \downarrow) \). The interaction \( V_{kk'} = V \) is assumed constant (since its length scale is much smaller than \( \xi \)) and negative (attractive).

In the condensed ground state, all Cooper pairs have the same energy. To excite one Cooper pair, we have to break it and excite both electrons (since an unpaired electron cannot occupy the ground state). The energy associated with this is

\[
\Delta_k = V \langle c_k \uparrow c_{-k} \downarrow \rangle,
\] (2.7)

where \( \langle c_k \uparrow c_{-k} \downarrow \rangle \) is the expectation value of annihilating a Cooper pair. From this, it follows that the excited states are separated from the ground state by an energy gap \( \Delta \).

The BCS Hamiltonian (2.6) is accompanied by a self-consistency equation for \( \Delta_k \). By deriving a BCS ground state wave function and applying the variational principle to it, one obtains a minimisation condition for the gap

\[
\Delta_k = \frac{V}{2} \sum_{k'} \frac{\Delta_{k'}}{\sqrt{\varepsilon_{k'}^2 + \Delta_{k'}^2}}.
\] (2.8)

Solving the Hamiltonian (2.6) gives the eigenstates and energy eigenvalues of the superconductor for a certain superconducting interaction \( V \). The optimal value of \( V \) is obtained by iteratively inserting the solution in (2.8). The set of equations (2.6) and (2.8) form the foundation of the modern description of superconductivity.

For elemental superconductors like Nb, Al, Hg and Sn, the pairing energy of two electrons (and correspondingly, the energy gap) is quite weak and ranges up to about 1 meV and so thermal energy can easily break the pairs. At the critical temperature \( T_c \), Cooper pairs break, the gap closes (\( \Delta \to 0 \)) and the superconductor transitions to a normal metal.

Other ways to break Cooper pairs involve mechanisms that affect the pairing itself. BCS theory describes electrons close to the Fermi level. The corresponding Fermi surfaces of two paired electrons with \( (k, \uparrow) \) and \( (-k, \downarrow) \) are identical. When the symmetry between those Fermi surfaces is broken, the Cooper pair experiences a pair breaking force. Symmetry breaking effects fall into two categories: orbital or paramagnetic. Orbital effects are associated with a shift between the Fermi surfaces, which occurs when one electron acquires net momentum with respect to the other. Paramagnetic effects are related to a mismatch in size of the Fermi surfaces, resulting from an exchange energy between the two spin states (see also Section 2.3.3). The transition from the superconducting to the normal state happens when the kinetic or exchange energy of the pairs exceeds the condensation energy.

### 2.2.2 Wave function methods

#### Particle-hole formalism

A hole is usually described as a missing electron. In terms of second quantisation operators, the electron creation operator \( c_k^\dagger \) creates an electron (removes a hole) in state \( k \), whereas the electron annihilation operator \( c_k \) removes the electron (creates a hole).
Electrons and holes satisfy certain symmetry relations, known as “electron-hole symmetry”. We consider the time-independent Schrödinger equation for a free electron in one dimension is

\[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - \mu = E \psi. \]  

(2.9)

Substituting a plane wave \( \psi_\ell(x) = e^{i k x} \), we obtain the momentum-dependent energy (the dispersion relation) \( E \sim k^2 \). The hole wave function is related to the electron wave function by complex conjugation: \( \psi_h(x) = \psi_\ell^*(x) = e^{-i k x} \). From this, we obtain the dispersion relation \( E \sim -k^2 \), i.e., a hole has opposite energy and momentum compared to an electron.

The classical picture to describe a system of electrons is considering filled electron states up to the Fermi level \( E = E_F \) and empty states above it (the ground state). Exciting an electron above \( E_F \) leaves an empty state behind. In particle-hole formalism, the electrons in the ground state are ignored. Consequently, rather than exciting an electron, we create an electron-hole pair, as is depicted in Fig. 2.8.

<table>
<thead>
<tr>
<th></th>
<th>electron</th>
<th>hole</th>
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</thead>
<tbody>
<tr>
<td>mass</td>
<td>( m )</td>
<td>( m )</td>
</tr>
<tr>
<td>charge</td>
<td>(-e)</td>
<td>(+e)</td>
</tr>
<tr>
<td>creation</td>
<td>( c_k )</td>
<td>( c_k )</td>
</tr>
<tr>
<td>annihilation</td>
<td>( c_k )</td>
<td>( c_k^\dagger )</td>
</tr>
<tr>
<td>energy</td>
<td>( E )</td>
<td>(-E)</td>
</tr>
<tr>
<td>momentum</td>
<td>( k )</td>
<td>(-k)</td>
</tr>
<tr>
<td>wave function</td>
<td>( \psi )</td>
<td>( \psi^* )</td>
</tr>
</tbody>
</table>

Table 2.2: Properties of electrons and holes.

The Bogoliubov-de Gennes equations

In a normal metal, electrons and holes have a parabolic dispersion relation \( E \sim \pm k^2 \). In a superconductor, a gap \( \Delta \) is introduced, which causes mixing of the electron and hole bands. This is illustrated in Fig. 2.9. Consequently, electrons and holes are no longer well-defined. Bogoliubov [15] introduced the concept of coherent mixtures of electrons and holes, so-called Bogoliubov quasi-particles, which are linear

![Figure 2.8](image1)

Figure 2.8: Two ways of describing a Fermi system.

![Figure 2.9](image2)

Figure 2.9: The dispersion relation of a normal metal has separated electron (solid) and hole (dashed) bands. The introduction of the superconducting gap \( \Delta \) causes mixing of the two bands.
combinations of electron and hole wave functions:

\[ \gamma_{k \uparrow} = u_k c_{k \uparrow} - v_k c_{-k \downarrow}, \]
\[ \gamma_{-k \downarrow} = u_k^\dagger c_{-k \downarrow} + v_k^\dagger c_{k \uparrow}, \]

where \( u_k \) and \( v_k \) are the amplitudes of the electron and hole wave functions, respectively, satisfying the normalisation condition \(|u_k|^2 + |v_k|^2 = 1\). Electron-hole symmetry can be expressed as \( u_k c_{k \uparrow} |i\rangle = v_k c_{-k \downarrow}^\dagger |i\rangle \), i.e., the annihilation of an electron is identical to the creation of a hole with opposite spin and momentum.

The equations of motion for electron-like and hole-like quasi-particles have been generalised by Bogoliubov [16] and de Gennes [17]. Rather than using momentum operators in \( k \)-space, this formalism uses field operators in real-space. This makes it possible to describe systems in which momentum is not conserved (\( k \) is not a good quantum number) and the eigenfunctions are no longer plane waves.

The Bogoliubov-de Gennes equation can be considered as two Schrödinger equations (similar to (2.9)), coupled by the superconducting gap \( \Delta \), i.e.

\[
\begin{bmatrix}
H_0 & \Delta \\
\Delta^* - H_0^* & 0
\end{bmatrix}
\begin{bmatrix}
\psi_e \\
\psi_h
\end{bmatrix} = E
\begin{bmatrix}
\psi_e \\
\psi_h
\end{bmatrix},
\]

(2.10)

where \( H_0 = -\hbar^2 \nabla^2 / 2m - \mu \) is the single-electron Hamiltonian and \( -H_0^* \) is the time-reversal symmetric counterpart for holes. The eigenfunctions have an electron-like part \( \psi_e \) and a hole-like part \( \psi_h \). The notation \( \psi_e \) and \( \psi_h \) is used to represent real-space, equivalent to \( u_k \) and \( v_k \) in \( k \)-space. During the superconducting transition, the gap gradually closes (\( \Delta \rightarrow 0 \)), such that electrons and holes uncouple in the normal state.

The Bogoliubov-de Gennes formalism only describes quasi-particle excitations. The Cooper pairs in the ground state simply form a “background” in the particle-hole formalism and are not taken into account explicitly. They are, however, represented in \( \Delta \), which originates from the existence of Cooper pairs, as seen in (2.7).

### 2.2.3 Green’s function methods

In quantum field theory, Green’s functions are correlation functions of quantum fields at different positions in space and time. Here we focus on single-particle Green’s functions, which contain the information of transport probabilities of single particles. They describe the propagation of particles through a system with different types of interactions (correlation effects). Calculating the Green’s functions of a physical system is enough to determine all single-particle properties, such as the density of states and electrical current and, in the case of superconductivity, Cooper pair correlation functions.

Green’s functions are particularly useful for describing interactions between different states. We consider two single-particle states with a single excited particle

\[ |\vec{r}_1, t_1\rangle_{\text{state}} \equiv \psi^\dagger(\vec{r}_1, t_1) |\text{state}\rangle, \]
\[ |\vec{r}_2, t_2\rangle_{\text{state}} \equiv \psi^\dagger(\vec{r}_2, t_2) |\text{state}\rangle, \]

where the field operator \( \psi^\dagger(\vec{r}_1, t_1) \) creates a particle at position \( \vec{r}_1 \) at time \( t_1 \). We note that this is the standard electron operator and not the quasiparticle operator (as in the Bogoliubov-de Gennes formalism). The Green’s function is introduced as the overlap between these states

\[ \text{Green’s function} \rightarrow \langle \text{state} | \psi(\vec{r}_2, t_2) \psi^\dagger(\vec{r}_1, t_1) |\text{state}\rangle. \]

To take the full system into account, we have to average this over the states of the many-body system on which the field operator acts. This is achieved by taking the statistical average over all possible paths.
from \((\vec{r}_1, t_1)\) to \((\vec{r}_2, t_2)\).

The above notation describes the following process: we have a system of \(N\) identical fermions and add one extra particle, let it propagate from \((\vec{r}_1, t_1)\) to \((\vec{r}_2, t_2)\) and take it away. We can also do it the other way around, by first taking the particle away and looking how the resulting hole propagates, and then putting the particle back. The single-particle Green’s function describing both processes is defined as

\[
G_{s_1s_2}(\vec{r}_1, t_1; \vec{r}_2, t_2) = -i\langle \psi_{s_2}(\vec{r}_2, t_2) \psi_{s_1}^\dagger(\vec{r}_1, t_1) \rangle \Theta(t_2 - t_1) + i\langle \psi_{s_2}(\vec{r}_2, t_2) \psi_{s_1}^\dagger(\vec{r}_1, t_1) \rangle \Theta(t_1 - t_2)
\]

\[
\equiv -i\langle \mathcal{T}\psi_{s_2}(\vec{r}_2, t_2) \psi_{s_1}^\dagger(\vec{r}_1, t_1) \rangle.
\]  

(2.11)

In this notation, \(s_1, s_2 \in \{\uparrow, \downarrow\}\) are the spin indices corresponding to the spin of the incoming and outgoing state, respectively. The angular brackets \(\langle \ldots \rangle\) denote the expectation value resulting from averaging. The step function \(\Theta\) distinguishes between \(t_1 > t_2\) and \(t_1 < t_2\). This equation can be interpreted as the Green’s function describing the transition from an incoming state to different outgoing states. We defined \(\mathcal{T}\) as the time-ordering operator which orders the operators logically in time. Different types of Green’s functions are defined based on the time-ordering operator. Here, we focus on the retarded Green’s function \(G^R\) which describes particles moving forward in time, i.e., how a particle at time \(t_1\) correlates with one at a later time \(t_2\),

\[
G^R_{s_1s_2}(\vec{r}_1, t_1; \vec{r}_2, t_2) = -i\langle \{\psi_{s_2}(\vec{r}_2, t_2), \psi_{s_1}^\dagger(\vec{r}_1, t_1)\} \rangle \Theta(t_2 - t_1),
\]

where \(\{A, B\} = AB + BA\) is the anti-commutation relation. The normal single-electron Green’s function (2.11) is complemented by a Green’s function that describes the opposite movement

\[
\hat{G}_{s_1s_2}(\vec{r}_1, t_1; \vec{r}_2, t_2) = -i\langle \mathcal{T}\psi_{s_2}(\vec{r}_2, t_2) \psi_{s_1}^\dagger(\vec{r}_1, t_1) \rangle,
\]  

(2.12)

which can be interpreted as the single-hole Green’s function. The two Green’s function are related through the particle-hole symmetry relation \(G^* = -\hat{G}\), where \(^*\) represents complex conjugation.

### The anomalous Green’s function

We have encountered normal single-particle Green’s functions (using single-particle electron states). To describe Cooper pairs, a second type of Green’s function is needed containing the interaction between particles and holes. These are the anomalous Green’s functions which are defined as

\[
F_{s_1s_2}(\vec{r}_1, t_1; \vec{r}_2, t_2) = -i\langle \mathcal{T}\psi_{s_2}(\vec{r}_2, t_2) \psi_{s_1}(\vec{r}_1, t_1) \rangle, \quad \text{ (2.13)}
\]

\[
\hat{F}_{s_1s_2}(\vec{r}_1, t_1; \vec{r}_2, t_2) = -i\langle \mathcal{T}\psi_{s_2}^\dagger(\vec{r}_2, t_2) \psi_{s_1}^\dagger(\vec{r}_1, t_1) \rangle.
\]

The anomalous Green’s function \(F\) annihilates a Cooper pair, while \(\hat{F}\) creates one. A schematic illustration of the Green’s function \(G\) and \(F\) is shown in Fig. 2.10. Since the anomalous Green’s functions describe the Cooper pairs in the system, they are related to the superconducting energy gap \(\Delta\). For a conventional BCS superconductor,

\[
\Delta_{s_1s_2}(\vec{r}_1) = -VF_{s_1s_2}(\vec{r}_1, \vec{r}_1), \quad \text{ (2.14)}
\]

where \(V\) is attractive interaction between the particles in a Cooper pair \((V < 0)\). This is equivalent to the BCS gap equation (2.7). Using the anti-commutation relations \(\{\psi_{s_2}(\vec{r}_2), \psi_{s_1}^\dagger(\vec{r}_2)\} = \delta(\vec{r}_1 - \vec{r}_2)\delta_{s_1s_2}\) and \(\{\psi_{s_2}(\vec{r}_1), \psi_{s_1}(\vec{r}_2)\} = \{\psi_{s_2}^\dagger(\vec{r}_1), \psi_{s_1}^\dagger(\vec{r}_2)\} = 0\), we find \(\Delta_{s_1s_2}(\vec{r}_1) = -\Delta_{s_1s_2}(\vec{r}_1)\), which implies that the order parameter of equal spin Cooper pairs in a BCS superconductor is zero.

The Green’s functions we have discussed above have spin indices \(G_{s_1s_2}\), which allows the Green’s functions to be conveniently written as \(2 \times 2\) matrices in spin space. Spin space is spanned by the Pauli spin
Figure 2.10: Left: A spin-up electron is created at \((r_1, t_1)\). \(G_{\uparrow\uparrow}\) describes the probability of its propagation to \((r_2, t_2)\) with \(t_2 > t_1\) via any arbitrary path. Right: The spin-up electron is taken out of the Cooper pair at \((r_1, t_1)\). \(F_{\downarrow\uparrow}\) describes the probability of finding the remaining spin-down electron at \((r_2, t_2)\).

matrices

\[
\sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},
\]

(2.15)

where \(\sigma_0\) is the unity matrix and \(\sigma_i \sigma_i = \sigma_0\), for \(i \in \{x, y, z\}\).

These 2 \(\times\) 2 matrix Green’s functions can be ordered further by introducing Nambu (particle-hole) space. This creates a 4 \(\times\) 4 matrix in Nambu \(\otimes\) spin space, where \(\otimes\) denotes the tensor product. In Nambu space, the Green’s functions are ordered based on different combinations of electron and hole operators \(\psi^\dagger\) and \(\psi\). The matrices that span Nambu space are the same Pauli spin matrices that span the spin space, but are now denoted by \(\tau_0, \tau_x, \tau_y\) and \(\tau_z\). In equation form,

\[
\hat{G} = \begin{bmatrix} G & F \\ \bar{F} & \bar{G} \end{bmatrix}, \quad G = \begin{bmatrix} G_{\uparrow\uparrow} & G_{\uparrow\downarrow} \\ G_{\downarrow\uparrow} & G_{\downarrow\downarrow} \end{bmatrix}, \quad \psi = \begin{bmatrix} \psi_+ \\ \psi_- \end{bmatrix}.
\]

(2.16)

The Gor’kov equations

In thermal equilibrium, the system is in a stationary state, meaning that it only depends on the time difference between two operations, rather than the explicit times themselves. The Green’s function is simplified as \(\hat{G}(r_1, t_1, r_2, t_2) = \hat{G}(r_1, r_2, t_1 - t_2)\). Taking a Fourier transform over the time difference gives the energy-dependent Green’s function

\[
G(r_1, r_2, E) = \int \hat{G}(r_1, r_2, t_1 - t_2)e^{-iE(t_1 - t_2)/\hbar} d(t_1 - t_2),
\]

where \(E\) is the single-particle energy.

Gor’kov expressed the original BCS Hamiltonian (2.6) in terms of energy-dependent Green’s functions [18],

\[
\begin{bmatrix} H_0 - E \\ -\Delta^* \end{bmatrix} \hat{G}(r_1, r_2, E) = \hbar \delta(r_1 - r_2) \tilde{1},
\]

(2.17)

where \(\tilde{1}\) is the 4 \(\times\) 4 unity matrix. We note the similarity with the Bogoliubov-de Gennes equation (2.10), the main difference being that the eigenstate is now the Green’s function instead of the wave function.

The quasiclassical approximation

In the quasiclassical approximation, the Fermi wavelength \(\lambda_F\) is assumed to be much smaller than length scales of relevance for superconductivity. Cooper pairs are non-local objects of order \(\xi\), which far exceeds \(\lambda_F\). This implies that their transport properties (described by the Green’s functions) do not vary
strongly on the scale of $\lambda_F$ and the Cooper pairs only feel the average of these fine-scale structures. In the quasiclassical approximation, we disregard the effects on the $\lambda_F$ scale, such that the Gor’kov equations reduce to Green’s functions that vary only on the $\xi$ scale.

The quasiclassical approximation gets its name from using a mixture of classical and quantum mechanics - it uses quantum mechanical field operators (to derive the Green’s functions), while describing motion of classical particles with Fermi momentum $\vec{p}_F$.

We consider a Cooper pair with electrons located at $\vec{r}_1$ and $\vec{r}_2$. We introduce two coordinates; the centre-of-mass coordinate $\vec{R} = (\vec{r}_1 + \vec{r}_2)/2$ describes the centre of the Cooper pair, which is related to slow oscillations in the system; the relative coordinate $\vec{r} = \vec{r}_1 - \vec{r}_2$ takes the coordinates of the individual electrons into account and is related to fast oscillations in the system, which generally is redundant information.* To lose this redundant information, we take the Fourier transform over the relative coordinate (to separate fast and slow oscillations) which results in the relative momentum $\vec{p}$, i.e.

$$G(\vec{R}, \vec{p}, E) = \int G(\vec{r}_1, \vec{r}_2, E) e^{-i\vec{p}\cdot\vec{r}} d\vec{r} = \int G \left( \vec{R} + \frac{\vec{r}}{2}, \vec{R} - \frac{\vec{r}}{2}, E \right) e^{-i\vec{p}\cdot\vec{r}} d\vec{r}. \quad (2.18)$$

The physical quantities of interest (e.g. the superconducting gap, the supercurrent) are derivable from the energy-integrated Green’s function. Therefore, we integrate (2.18) over the kinetic energy $\xi_p$, which is linear close to the Fermi level, i.e., $\xi_p = v_F (\vec{p} - \vec{p}_F)$ and $d\xi_p = \vec{v}_F d\vec{p}$, with $\vec{p}_F = m\vec{v}_F$ the Fermi momentum and $\vec{v}_F$ the Fermi velocity. The energy-integrated Green’s function is

$$g(\vec{R}, \vec{p}_F, E) = \frac{i}{\pi} \int G(\vec{R}, \vec{p}, E) d\xi_p, \quad (2.19)$$

where $\vec{p}_F = |\vec{p}_F|/|\vec{p}_F|$ is the unit vector in the direction of the Fermi momentum. By integrating over the kinetic energy, we have lost one degree of freedom (the momentum magnitude), although we still have to integrate over all directions in momentum space.

**The Eilenberger equation**

The only interaction term included in the Gor’kov equation (2.17) is the attractive interaction responsible for superconductivity. The Gor’kov Green’s functions are considered non-interacting Green’s functions and are generally complemented by the self-energy $\Sigma$, which contains all other interactions, including electron-electron interactions and impurity scattering.

Since $\Sigma$ describes changes of the single-electron state, it is related to the single-electron Green’s function as $\Sigma_{s_1,s_2}(\vec{r}) \sim G_{s_1,s_2}(\vec{r}, \vec{r})$. Comparing $\Sigma$ to $\Delta$ in (2.14), $\Delta$ can be interpreted as the anomalous equivalent of the self-energy.

The Eilenberger equation is obtained by applying the quasiclassical approximation to the Gor’kov equation (2.17) and including the self-energy $\Sigma$. We use that $\vec{v}_F \cdot \nabla \gg \nabla^2$ at the Fermi surface, such that we can neglect the second order derivatives. The Eilenberger equation is [38]

$$-i\hbar \vec{v}_F \partial_\vec{R} g + \begin{bmatrix} -E \\ -\Delta^* \end{bmatrix} \cdot \begin{bmatrix} \Delta \\ E \end{bmatrix}, g = [\Sigma, g], \quad (2.20)$$

with the commutation relation $[A, B] = AB - BA$ and the Fermi velocity is $\vec{v}_F = v_F \hat{p}_F$.

**The Usadel equation**

The Gor’kov Green’s function (2.18) depends on the momentum $\vec{p}$, whereas the Eilenberger Green’s function (2.19) only depends on its direction $\vec{p}_F$. In the Usadel Green’s function, the direction dependence is removed as well.

*Related to impurities and self-interference effects (e.g. weak localisation). Carrying out the Fourier transform can be seen as averaging over impurity positions.
Usadel considered dirty superconductors dominated by impurity scattering, i.e., an electron scatters many times before losing its phase coherence, resulting in the loss of its initial momentum direction. As a result, the Green’s function (2.19) becomes nearly isotropic in space and can be approximated as the sum of a dominant isotropic term \( g_0 \) and a first order linear correction \( g_1 \) [39],

\[
g(R, \hat{p}_F, E) = g_0(R, E) + \hat{p}_F \cdot g_1(R, E),
\]

(2.21)

with \( |g_1| \ll |g_0| \) and \( |g|^2 = 1 \). Substituting this into (2.20), averaging over the momentum direction and keeping the leading terms, Usadel transformed the Eilenberger equation into the diffusion equation [39]

\[
- i \hbar D \partial_R \left( g_0 \partial_R g_0 \right) + \left[ \begin{array}{c}
- \Delta \\
\Delta^* \\
E
\end{array} \right] \cdot g_0 = [\Sigma, g_0],
\]

(2.22)

where the diffusion constant \( D = v_F \tau / 3 \) is related to the Fermi velocity magnitude \( v_F \) and mean free path \( \tau \), where \( \tau \) is the mean free time.

### 2.2.4 Unconventional superconductivity

To understand unconventional superconductivity, we first briefly discuss the concept of spin in a Cooper pair.

**Spin: a recap**

In quantum mechanics, the spin projections \( S_x, S_y \) and \( S_z \) are incompatible observables, meaning that, if you measure one of them, it affects the others and they cannot be known simultaneously. In fact, they anticommute following the cyclic relation \( [S_x, S_y] = i\hbar S_z \), \( [S_y, S_z] = i\hbar S_x \) and \( [S_z, S_x] = i\hbar S_y \). By convention, the spin quantisation axis is chosen as the \( z \)-axis and we consider only \( S_z \). The total spin momentum \( S \), defined as \( S^2 = S_x^2 + S_y^2 + S_z^2 \) does commute with the individual spin projections, i.e., \( [S, S_z] = 0 \) and \( S \) and \( S_z \) can be known at the same time. Therefore, the spin-state is described by those two quantum numbers, and is written as \( |S, S_z\rangle \). Observables are associated with eigenvalues. The eigenvalue of \( S_z \) is \( m_s \hbar \), where \( m_s \) is the spin magnetic quantum number. The eigenvalue of \( S \) is \( \sqrt{s(s+1)} \hbar \) [40]. The electron is a spin-\( \frac{1}{2} \) particle, which means the maximum value of any spin projection is \( \pm \hbar / 2 \). An electron with \( m_s = +1/2 \) is called spin-up, written as \( \uparrow \). An electron with \( m_s = -1/2 \) is called spin-down, written as \( \downarrow \). The magnitude of the electron’s total spin is then \( \sqrt{s(s+1)} \hbar = \sqrt{3} \hbar / 2 \). From geometry, it follows that the total spin has a \( \approx 55^\circ \) angle with respect to the \( z \)-axis, see Fig. 2.11.

![Figure 2.11: Spin-vector representations of electron spin. (a) In spherical representation. The radius of the sphere is the total spin \( S \). The projection on the \( z \)-axis is \( S_z = \pm \hbar / 2 \). Adapted from [40]. (b) The equivalent conical representation, which will be used throughout this chapter.](image)
Spin of a Cooper pair

Both individual electrons in a Cooper pair have either spin-up (\(\uparrow\)) or spin-down (\(\downarrow\)), resulting in four possibilities: \(\uparrow\uparrow, \uparrow\downarrow, \downarrow\uparrow, \downarrow\downarrow\). The spin-state \(|S, S_z\rangle\) of a Cooper pair is obtained by adding the spins, so for \(\uparrow\uparrow, \uparrow\downarrow, \downarrow\uparrow, \downarrow\downarrow\), we obtain 1, 0, 0 and \(-1\), respectively. We note that \(\uparrow\downarrow\) and \(\downarrow\uparrow\) both yield 0. However, quantum mechanically, two electrons are indistinguishable, and therefore, we have to take a superposition of them to describe this state: \((|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle)/\sqrt{2}\). Taking the total spin of all possible states, there is one way to get \(S = 0\) (spin-singlet) and three ways to get \(S = 1\) (spin-triplet), they are

\[
\begin{align*}
\text{spin-singlet} & \quad S = 0 \\
0, 0 & = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}, \\
1, 1 & = |\uparrow\uparrow\rangle, \\
1, 0 & = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}, \\
1, -1 & = |\downarrow\downarrow\rangle.
\end{align*}
\]

The corresponding spin-vector representations are illustrated in Fig. 2.12. The \(S_z = \pm 1\) are called equal-spin triplets and the \(S_z = 0\) is the opposite-spin triplet (with respect to the \(z\)-axis). We note that the relative angle between two spins is always \(\pi/70\), even for equal-spin pairs.

![Figure 2.12: Spin-vector representations of Cooper pairs. The two spin-\(\frac{1}{2}\) electrons in the Cooper pair combine their individual spins \(s_1\) and \(s_2\) such that the total spin of the pair is either \(S = 0\) or \(S = 1\). The \(S = 0\) case is the spin-singlet (left). The \(S = 1\) can be formed in three possible spin-triplet states with \(S_z = 0, \pm 1\). The \(S_z = \pm 1\) are equal-spin triplets and the \(S_z = 0\) is the opposite-spin triplet. Adapted from [41].](image)

Unconventional superconductivity

We recall the anomalous Green’s function \(F_{s_1 s_2}(\vec{r}_1, t, \vec{r}_2, t)\) defined in (2.13), which describes the Cooper pairs in terms of a spin, parity (related to position) and time component. Based on these components, superconductors can be divided into different classes of superconductivity.

To satisfy the Pauli-exclusion principle, the anomalous Green’s function has to be anti-symmetric under exchange of two electrons at equal times \(t_1 = t_2 \equiv t\), that is

\[F_{s_1 s_2}(\vec{r}_1, t, \vec{r}_2, t) = -F_{s_2 s_1}(\vec{r}_2, t, \vec{r}_1, t).\]

We first consider the spin component. Interchanging the two spins \(s_1\) and \(s_2\) of a spin-singlet results in a minus sign, i.e., \(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle = -(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\), whereas the sign stays the same for the spin-triplet. We say that spin-singlet pairs obey anti-symmetric exchange, while spin-triplet pairs are symmetric.

The parity is related to the orbital angular momentum \(l\) via the Fourier transform, which in turn is associated with the spherical harmonics, i.e., \(l = 0\) (s), \(l = 1\) (p), \(l = 2\) (d), \(l = 3\) (f), etc. The even numbers (s and d orbitals) are symmetric, while the odd numbers (p and f orbitals) are anti-symmetric.

The Cooper pairs in BCS theory (see Section 2.2.1) are in a singlet state with s-wave orbital state and are referred to as conventional superconductors. The superconducting energy gap \(\Delta\) (related to \(F\)
2.2. Microscopic theory of superconductivity

via (2.14)) is isotropic for s-wave orbital states. It does not depend on momentum $\vec{p}$ and there are no single particle states inside the gap. In unconventional \(p\)- and \(d\)-wave orbital states, the energy gap is no longer isotropic. Depending on the momentum $\vec{p}$, the gap can be full, reduced, or there can be no gap at all. Consequently, the density of single particle states inside the gap becomes nonzero.

To complete the possible superconducting symmetries, we consider interchanging the time coordinates. There is no (anti)commutation relation for operators at different times, but there is a constraint due to the time ordering inherent to $F$ [42]. Since the majority of literature works with Fourier-transformed Green’s functions in the frequency domain, symmetry with respect to the time coordinate is defined as

\[
\begin{aligned}
\text{even-frequency} & \quad F_{s_1s_2}(\vec{r}_1,t_1,\vec{r}_2,t_2) = F_{s_1s_2}(\vec{r}_1,t_2,\vec{r}_2,t_1), \\
\text{odd-frequency} & \quad F_{s_1s_2}(\vec{r}_1,t_1,\vec{r}_2,t_2) = -F_{s_1s_2}(\vec{r}_1,t_2,\vec{r}_2,t_1).
\end{aligned}
\]

To envision this, we consider Cooper pairs with \(p\)-wave pairing. Since the electrons have nonzero relative angular momentum ($l = 1$), they avoid each other more effectively in space, which lowers the Coulomb repulsion. Similarly, in an odd-frequency superconductor, the electrons avoid each other in time [42]. This may seem odd at first, but a similar retardation effect is, in fact, also present in BCS theory, i.e., electron-phonon interaction. Two electrons attract each other by interacting with the lattice and avoiding each other in time.

Odd-frequency superconductivity in bulk systems has only been reported once to date [43], but it can also be engineered by spin-rotation symmetry breaking (e.g. by magnetism) or spatial inversion symmetry breaking (e.g. in junctions). The complete set of possible symmetries including some examples is given in Table 2.3.

<table>
<thead>
<tr>
<th>$\Delta$</th>
<th>Time</th>
<th>Spin</th>
<th>Orbital</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>Even-frequency spin-singlet</td>
<td>even</td>
<td>singlet</td>
<td>even</td>
<td>BCS superconductors [14]</td>
</tr>
<tr>
<td>even-parity (ESE)</td>
<td></td>
<td></td>
<td></td>
<td>High-$T_c$ cuprates [44]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>S/N heterostructures [45]</td>
</tr>
<tr>
<td>Odd-frequency spin-triplet</td>
<td>even</td>
<td>triplet</td>
<td>odd</td>
<td>$^3$He [46]</td>
</tr>
<tr>
<td>odd-parity (ETO)</td>
<td></td>
<td></td>
<td></td>
<td>Sr$_2$RuO$_4$ [47]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>S/F heterostructures [48]</td>
</tr>
<tr>
<td>Odd-frequency spin-triplet</td>
<td>odd</td>
<td>triplet</td>
<td>even</td>
<td>MgB$_2$ [43]</td>
</tr>
<tr>
<td>even-parity (OTE)</td>
<td></td>
<td></td>
<td></td>
<td>S/F heterostructures [25]</td>
</tr>
<tr>
<td>Odd-frequency spin-singlet</td>
<td>odd</td>
<td>singlet</td>
<td>odd</td>
<td>S/N heterostructures [49]</td>
</tr>
<tr>
<td>odd-parity (OSO)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 2.3: Superconducting pairing symmetries. $S$ denotes a conventional BCS superconductor, $F$ refers to a ferromagnet and $N$ to a normal metal. We note that the pairing symmetry of Sr$_2$RuO$_4$ remains a point of discussion to date.

To describe mixed forms of superconductivity, the anomalous Green’s function is often decomposed in a singlet and triplet component as

\[
f = (f_s + \vec{f}_t \cdot \vec{\sigma})i\alpha^y = \begin{bmatrix} i f^y_t - f^x_t & f^z_t + f_s \\
 f^x_t & i f^y_t + f^z_t 
\end{bmatrix},
\]

where the scalar function $f_s$ is the singlet pair amplitudes and the vector $\vec{f}_t = (f^x_t, f^y_t, f^z_t)^T$ describes the triplets. We note that the spin-singlet carries no net spin ($S = 0$), whereas the spin-triplet does ($S = 1$). Therefore, only $\vec{f}_t$ interacts with the spin $\vec{\sigma}$. The multiplication with $i\alpha^y$ comes from the basis we use, introduced in (2.16).
2.3 Ferromagnetism

Just like superconductors, ferromagnetic materials can also be described using Landau theory (Section 2.1). The order parameter is the magnetisation $M$ and the critical temperature is called the Curie temperature $T_C$. The two states are illustrated in Fig. 2.1. The ordered, low-temperature phase is the ferromagnetic phase, in which all magnetic moments point in the same direction, resulting in a net magnetisation $M$. The value of $M$ is material-dependent and corresponds to the two non-zero minima in the free energy for $T < T_C$ in Fig. 2.4. The disordered phase above the Curie temperature is the paramagnetic phase, in which all magnetic moments point in random directions and cancel each other out. Accordingly, the free energy is minimised for $M = 0$.

In this thesis ferromagnets are used in superconducting heterostructures for their exchange field and magnetisation. This section gives a brief overview of the properties that are important in our devices. A more extensive treatment of ferromagnetism can be found in Refs. [21, 22].

2.3.1 Magnetic materials

The magnetic susceptibility of a material describes the way a material behaves in the presence of a magnetic field $h$. A general definition of the magnetic susceptibility for isotropic materials is [21]

$$\chi = \frac{\partial M}{\partial h},$$

with $M$ the magnetisation and $h$ the magnetic field. For anisotropic materials, a more complicated tensor form is required. The magnetic susceptibility is a dimensionless, temperature-dependent parameter.

Diamagnetic and paramagnetic materials do not generate a magnetic field by themselves. In the absence of an external field, the macroscopic magnetisation $\vec{M}$ is zero. This is the case either when the microscopic magnetic moments $\vec{m}$ of all electrons within one atom add up to zero (diamagnetism) or when the magnetic moments are randomly oriented, such that their sum is zero (paramagnetism).

Diamagnetism is present in every material (because it is related to the orbital degrees of freedom and is unrelated to the spin) and is characterised by a negative susceptibility, typically in the range $\chi \sim -10^{-8}$ to $-10^{-4}$. Diamagnetism is temperature independent.

When a paramagnetic material is placed in a magnetic field, the magnetic moments align, resulting in a finite net magnetisation (see Fig. 2.1). The paramagnetic susceptibility is positive and small, although still a couple of orders larger than the diamagnetic susceptibility, i.e., $\chi \sim 10^{-4}$ to $10^{-2}$. Paramagnetism is strongly temperature dependent, and the susceptibility follows the Curie-Weiss law $\chi = C/(T - \theta)$ for $T > \theta$, where $T$ is the temperature, $C$ is the Curie constant and $\theta$ is the Weiss constant.

Ferromagnetic materials have a nonzero macroscopic magnetisation $\vec{M}$, which implies that the microscopic moments $\vec{m}$ have a directional preference (we will see why in the following sections). No magnetic field is required to align the local spins. Hence, we speak of spontaneous magnetisation, which is the main characteristic of a ferromagnet. Ferromagnets have a large, positive susceptibility. Ferromagnets follow the Curie-Weiss law $\chi = C/(T - T_C)$, where $T_C$ is the Curie temperature. Well-known ferromagnets are the 3d-transition elements Fe, Co and Ni, which have Curie temperatures of 1043 K, 1388 K and 627 K, respectively [50].

2.3.2 Heisenberg model

Weiss [51] proposed the first microscopic theory of ferromagnetism in 1907. He came up with the idea that an effective molecular field inside the ferromagnet aligns the electron spins. The theory gave meaningful results and incorporated the temperature dependence according to the Curie-Weiss law. However, the field required was enormous (of the order of $10^9$ T) and nonphysical [22].

In 1928, Heisenberg [52] showed that the molecular field originates from the exchange interaction. He
assumed a fixed lattice of spins that each interact with their nearest neighbours according to

\[ E_{\text{ex}} = -J_{\text{ex}} \sum_{\langle i,j \rangle} \hat{s}_i \cdot \hat{s}_j, \]  

(2.26)

where \( E_{\text{ex}} \) is the total exchange energy of the system, \( J_{\text{ex}} \) is the exchange energy between two neighbouring spins, the sum is over all nearest neighbours given by \( \langle i,j \rangle \) and \( \hat{s}_i \) is the unit vector in the direction of the spin at lattice site \( i \). When \( J_{\text{ex}} < 0 \), the exchange energy is minimised for parallel alignment of the spins, which leads to ferromagnetism. When \( J_{\text{ex}} > 0 \), the exchange energy is minimised for antiparallel alignment, which is the case in anti-ferromagnetic or ferrimagnetic materials [22].

Since the exchange energy stems from nearest-neighbour interactions, it is short-ranged. At low temperatures, the nearest-neighbour interaction leads to the spin alignment of the entire system. When increasing the temperature and \( J_{\text{ex}} \sim k_B T \), only some nearest-neighbour spins tend to remain parallel, which forms spin clusters. This forms the basis of magnetic domains, which we will encounter in Section 2.3.4. When the Curie temperature is reached, all spin alignment is eventually lost.

### 2.3.3 Spin-split bands

The Heisenberg model describes a fixed lattice of interacting spins, which is appropriate for insulating ferromagnetic materials. However, in 3d-transition metals such as Fe, Co and Ni, delocalised electrons are responsible for the ferromagnetism. This type of ferromagnetism is called itinerant or band ferromagnetism and is described by spin-splitting of the band structure.

We have already encountered the parabolic density of states of a normal metal in Fig. 2.9. Normal metals have an equal amount of spin-up and spin-down electrons \( n \) at the Fermi level \( E_F \), corresponding to two degenerate spin bands. In a band ferromagnet, the exchange interaction offsets one spin band with respect to the other, resulting in different amounts of electrons \( n_\uparrow \) and \( n_\downarrow \) at the Fermi level, with \( n = n_\uparrow + n_\downarrow \). The band with the most (least) electrons is called the majority (minority) band and the energy difference between the two bands is the exchange energy \( E_{\text{ex}} \). Correspondingly, the magnetisation of the ferromagnet is given by the difference between the majority and minority spins, \( M = \mu_B (n_\uparrow - n_\downarrow) \) where \( \mu_B \) is the Bohr magneton.

To illustrate spin-splitting in a ferromagnet, we start from a normal metal with density of states \( N(E) \). Electrons in the spin-down band with energy \( E_F - \delta E \) move to the spin-up band with energy \( E_F + \delta E \), as illustrated in Fig. 2.13b. The number of spin-up and spin-down electrons in the system changes to \( n_{\uparrow\downarrow} = \frac{1}{2} (n \pm N(E_F) \delta E) \), respectively. This spin imbalance has two consequences for the energy of the ferromagnet.

Firstly, electrons originally occupying states with \( k < k_F \), now occupy states with \( k > k_F \), causing an increase in the kinetic energy \( \sim k^2 \). To be precise, \( \frac{1}{2} N(E_F) \delta E \) electrons increase their energy by \( \delta E \), resulting in a total kinetic energy increase

\[ \Delta E_K = \frac{1}{2} N(E_F) (\delta E)^2. \]

Secondly, the spin imbalance creates an effective magnetic field in the up-direction, shifting the up and down bands in energy, as shown in Fig. 2.13c. Since there are now less degenerate states doubly occupied, the spatial overlap between electron states decreases, which reduces the Coulomb repulsion \( U \). This leads to the decrease in potential energy

\[ \Delta E_P = -\frac{1}{2} U N(E_F) (\delta E)^2. \]

Spontaneous ferromagnetism is energetically favourable when the potential energy decrease \( \Delta E_P \) exceeds the kinetic energy increase \( \Delta E_K \), leading to the Stoner criterion for ferromagnetism

\[ U N(E_F) \geq 1. \]

The parabolic density of states in Fig. 2.13a-c allows for a simple mathematical description. The band
structure of real transition metals looks more complicated, as shown in Fig. 2.13d.

\[ E - E_F \]

\[ \delta E \]

\[ N(E) \]

\[ E_{ex} \]

Figure 2.13: Spin splitting of the density of states. (a) Normal metal: equal spin-up and spin-down at the Fermi level. (b) Moving electrons from the spin-down band to the spin-up band. (c) The resulting magnetic field shifts the energy bands to line up with the Fermi level. The energy difference is the exchange energy \( E_{ex} \). Diagrams adapted from [53]. (d) The spin-split density of states of Ni, adapted from [54].

2.3.4 Magnetic domains

The ferromagnet magnetisation is not necessarily homogeneous. It is energetically favourable to keep the magnetisation inside the material, resulting in the formation of magnetic domains. The magnetisation is homogeneous within a single domain. The domains are separated by domain walls in which the magnetisation vector continuously rotates from the orientation on one side to that on the other side.

The energy that is minimised consists of four different contributions. The exchange energy originates from the interaction between individual electrons and is minimised for parallel alignment of their magnetic moments. The Zeeman energy is associated with applied magnetic fields and is minimised when the magnetisation points along the field direction. The crystalline anisotropy energy results from the magnetisation with respect to the lattice orientation. It is minimised along the lattice easy axis. The magnetisation direction (in absence of an external field) is usually along the easy axis. But it’s possible to magnetise the material along a different direction.

Finally, the demagnetisation energy is determined by the shape of the ferromagnet. It is minimised by keeping the magnetic flux inside the ferromagnet and does this by forming magnetic domains. The width of the domain walls is determined by the competition between the exchange and crystalline anisotropy energies. The exchange energy favours broad walls such that adjacent magnetic moments can be as close to parallel as possible, whereas the crystalline anisotropy energy is in favour of narrow walls, such that the resulting domains are easier to align with the easy axis.

The typical domain size is in the \( \mu m \) range. When the sample dimensions becomes of this order, it is no longer possible to lower the energy by forming domains. Instead, the shape of the ferromagnet determines the magnetisation direction, e.g. in long, thin ferromagnetic wires the magnetisation aligns along the wire.

2.3.5 Hysteresis

A ferromagnet that has not been in the presence of an applied magnetic field is generally demagnetised and its net magnetisation is close to zero. Once the ferromagnet is magnetised, its magnetisation depends on previously applied magnetic fields, which is known as hysteresis. By measuring the magnetisation as a function of applied field, we obtain a hysteresis curve, as shown in Fig. 2.14.

The origin represents the initial, demagnetised, state of the ferromagnet in which the magnetic domains are oriented in random directions. Upon applying a positive magnetic field \( h \), we move over the

*The easy axis is the energetically favourable direction of the spontaneous magnetisation in a ferromagnetic material.
so-called virgin curve from point a to d. Domains that are already favourably aligned with respect to the field expand at the expense of domains that are not, known as domain wall motion (point b). At point c, all magnetic domains point along the easy axis, forming a single domain state. Increasing the field even further, this domain will align with the field and the ferromagnet saturates parallel to the applied field (point d).

Subsequently turning the field off, the magnetisation relaxes to point e. The main characteristic of the hysteresis curve is that it has a different path for going up and down in field. Points e and h are the remanent magnetisation points. After being magnetised once, the ferromagnet now has a net magnetisation in the absence of a field. Points f and i are the coercive field points, indicating the field required to return to a zero net magnetisation, at which the magnetisation changes direction.

The squareness of the curve is a measure for the magnetic “hardness” of the material. Materials with magnetic anisotropy have so-called easy and hard axes. Generally, only a small field is required to reach saturation magnetisation along the easy axis, whereas a large field is needed to do this along the hard axis. Hence, magnetic anisotropy results in differently shaped hysteresis curves depending on the field direction.

Figure 2.14: Left: The ferromagnet hysteresis curve shows the magnetisation $M$ as a function of applied field $h$. Points of interest are indicated. Right: Schematic illustrations of the behaviour of domain walls and the magnetisation at the points of interest.

2.4 Spin-orbit coupling

Spin-orbit coupling is a quantum-relativistic interaction that couples an electron’s spin and orbital angular momentum.

Perhaps the easiest way to envision spin-orbit coupling in analogy with the Lorentz force. We consider an electron with mass $m$, charge $e$ and momentum $\vec{p}$. When the electron moves through a magnetic field $\vec{B}$, it experiences a Lorentz force perpendicular to its motion $\vec{F} = -e(\vec{p} \times \vec{B})/m$. The electron obtains the Zeeman energy $H_Z = \mu_B \vec{\sigma} \cdot \vec{B}$, where $\mu_B$ is the Bohr magneton and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the Pauli matrix vector (see (2.15) for the definition) [31].

To consider spin-orbit coupling, we instead consider an electron moving through an electric field $\vec{E}$. In its own frame of motion, the electron experiences an effective magnetic field – the spin-orbit field – proportional to $\vec{B}_{\text{eff}} \sim (\vec{E} \times \vec{p})/mc^2$, with $c$ the speed of light [31]. This is illustrated in Fig. 2.15. The
spin-orbit field induces a momentum-dependent Zeeman energy, called the spin-orbit coupling (SOC). The general derivation of SOC from the Dirac equation gives

$$H_{SO} = -\frac{e\hbar}{4m^*c^2} \vec{\sigma} \cdot \left( \vec{E} \times \vec{p} \right).$$

(2.27)

This equation shows the coupling of the electron’s spin \( \vec{\sigma} \) to its momentum \( \vec{p} \) through the use of an electric field \( \vec{E} \). The electric field responsible for SOC can have different physical origins, resulting in different types of SOC.

![Figure 2.15: The relativistic transformation between the lab frame and electron’s frame of motion. A moving electron in an electric field \( \vec{E} \) in the lab frame is equivalent to a stationary electron in a magnetic field \( \vec{B} \) in the electron’s frame. This allows for spin-manipulation without a magnetic field.](image)

A crucial ingredient for SOC is symmetry, in particular, time-reversal and space-inversion symmetry. SOC preserves time-reversal symmetry, meaning that the system is symmetric under the transformation of time reversal \( t \mapsto -t \). Reversing the sign of time \( t \) does not affect the position \( x \), since time and space are independent. Linear momentum* picks up a minus sign, i.e., \( \vec{k} \mapsto -\vec{k} \), and so does half-integer spin, i.e., \( \uparrow \mapsto \downarrow \). This imposes a symmetry on the energy states, as shown in Table 2.4.

The presence of time-reversal symmetry is an important point for superconductors with SOC. Kramer’s Theorem states that, if a system with half-integer spin has time-reversal symmetry, then every energy eigenstate has at least one partner with the same energy. In a conventional superconductor, every spin-up electron \( |\psi_\uparrow(\vec{k})\rangle \) will have a time-reversal symmetric partner \( |\psi_\downarrow(\vec{k})\rangle \) to form a Cooper pair. Hence, Cooper pair formation is robust as long as time-reversal symmetry is conserved. This theory was used to explain the existence of dirty superconductors [56]. Similarly, superconductivity is robust to SOC. Because of this, SOC is a powerful mechanism for spin-manipulation without a magnetic field. Contrary to SOC, a magnetic field breaks time-reversal symmetry, it suppresses and eventually breaks down superconductivity (see Section 2.1.3).

Space-inversion symmetry is flipping the sign of the spatial coordinates, i.e., \( x \mapsto -x \). If the crystal lattice preserves this reflection symmetry, so does the reciprocal lattice and therefore, this is equivalent to \( \vec{k} \mapsto -\vec{k} \). Inversion symmetry does not affect spin.

Different types of SOC can be distinguished based on inversion symmetry. Atomic SOC is symmetry-independent. Anti-symmetric SOC, such as Dresselhaus and Rashba SOC, arises from the lack of space-inversion symmetry.

### 2.4.1 Atomic spin-orbit coupling

Atomic SOC is symmetry-independent and exists in every crystal, since it originates from SOC in atomic orbitals. The electric field giving rise to atomic SOC is the field the electron experiences by circling a nucleus. This electric field is given by \( \vec{E} = -\nabla \varphi = (d\varphi/dr)(\vec{r}/r) \), where \( \varphi \) is the electrostatic potential and \( \vec{r} \) is the distance between the electron and the nucleus [27]. We aim to express the SOC only in terms of operators of quantities characterising the atom as a whole, not its individual electrons. These

*Linear momentum is denoted by either \( \vec{p} \) and \( \vec{k} \). In our notation, \( \vec{p} \) is the relativistic momentum, whereas \( \vec{k} \) is the wave vector or crystal momentum. They are related to each other by \( \vec{p} = \hbar \vec{k} \).
2.4. Spin-orbit coupling

Symmetry Energy states

<table>
<thead>
<tr>
<th>Time-reversal symmetry</th>
<th>$E_\uparrow(\vec{k}) = E_\downarrow(-\vec{k})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Space-inversion symmetry</td>
<td>$E_\uparrow(\vec{k}) = E_\downarrow(-\vec{k})$</td>
</tr>
<tr>
<td>Both symmetries combined</td>
<td>$E_\uparrow(\vec{k}) = E_\downarrow(\vec{k})$ Two degenerate spin states</td>
</tr>
<tr>
<td>Broken inversion symmetry</td>
<td>$E_\uparrow(\vec{k}) \neq E_\downarrow(\vec{k})$ Spin degeneracy lifted</td>
</tr>
</tbody>
</table>

Table 2.4: The effect of time-reversal and space-inversion symmetry on the energy states.

operators are the orbital angular momentum operator $\hat{L}$ and the spin angular momentum operator $\hat{S}$. We replace $\vec{\sigma}$ by $2\hat{S}$. The cross product in (2.27) gives $\vec{r} \times \vec{p} = \hbar\vec{L}$. For hydrogen-like atoms, $\varphi = Ze/r$, where $Z$ is the atomic number. The SOC Hamiltonian becomes

$$H_{\text{SO}} = \frac{Ze^2\hbar^2}{2m^2c^2r^3} \hat{S} \cdot \vec{L}.$$  

(2.28)

The atomic SOC strength increases with increasing atomic number $Z$, meaning that heavy elements generally have strong SOC. The combination of time-reversal and inversion symmetry results in two degenerate spin states, as shown in Table 2.4.

A consequence of SOC is that the Hamiltonian no longer commutes with the operators $\hat{S}$ and $\hat{L}$, i.e., $[\hat{S} \cdot \hat{L}, \hat{L}] \neq 0$ and $[\hat{S} \cdot \hat{L}, \hat{S}] \neq 0$. This implies that spin and orbital angular momentum are not separately conserved. However, the total angular momentum $\hat{J} = \hat{L} + \hat{S}$ is still conserved.

2.4.2 Dresselhaus & Rashba spin-orbit coupling

Anti-symmetric SOC arises from the lack of space-inversion symmetry. Dresselhaus SOC occurs in crystals with bulk inversion asymmetry (intrinsic to the material), which means that there is a net electric field for certain crystal directions. Rashba SOC occurs in systems with structural inversion asymmetry (extrinsic, for example in heterostructures) which gives rise to a local net electric field.*

As a result of space-inversion asymmetry, an electron with momentum $\vec{k}$ has a different energy compared to an electron with $-\vec{k}$ (see Table 2.4). This means that the spin bands in the dispersion relation are shifted in $\vec{k}$, forming an $E_+$ and $E_-$ band.† Due to the spin-orbit interaction, the direction of the spin is coupled to the momentum, known as spin-momentum locking. Both are illustrated in Fig. 2.16.

Dresselhaus spin-orbit coupling

Dresselhaus SOC was first discovered in zinc-blende compounds such as GaAs and InSb and is commonly found in non-centrosymmetric materials. The Dresselhaus spin-orbit field is described by

$$H_D = \gamma \vec{\sigma} \cdot \vec{\kappa},$$  

(2.29)

where $\gamma$ is the Dresselhaus parameter and $\vec{\kappa}$ contains the cyclic permutations of $\kappa_x = k_x(k_y^2 - k_z^2)$. In thin films (where $z$ is finite), the Dresselhaus spin-orbit field (2.29) reduces to the more manageable form $H_D = \gamma (\sigma_x k_x - \sigma_y k_y)$. The spin polarisation is parallel to $\vec{k}$ for $k_x = 0$ and $k_y = 0$ and gradually changes for intermediate values of $\vec{k}$ [29]. This spin texture is illustrated in Fig. 2.16c.

*It is often said that Dresselhaus SOC occurs in bulk non-centrosymmetric crystals while Rashba SOC occurs at interfaces, but Rashba SOC can also occur in crystals with broken uniaxial inversion symmetry.

†Since spin is no longer conserved in the presence of SOC, these bands are called the $E_+$ and $E_-$ band, as opposed to spin-up and spin-down.
Rashba spin-orbit coupling

Rashba SOC takes place at interfaces as a result of structural inversion symmetry breaking. If two materials with different work functions are brought into contact, electrons travel from the material with the lower work function to that with the higher to make the Fermi level equal across the junction. This electron transfer results in an electric layer extending up to the electron screening length (of the order of the lattice constant) from the interface [57]. In solid-state physics, this electric layer is referred to as a two-dimensional electron gas (2DEG), because the electrons are free to move in two dimensions but are confined in the third (by the interface). The 2DEG is responsible for inversion symmetry breaking.

While in most cases the interfacial Rashba SOC is negligible, in some structures it can have a drastic effect. A famous example of a 2DEG is the LaAlO$_3$/SrTiO$_3$ interface [58], which becomes superconducting at low temperatures. It is possible to boost the interfacial Rashba SOC by introducing a thin heavy metal interlayer like Pt. The atomic SOC of the heavy metal enhances the interfacial Rashba SOC. The amount of SOC is tunable by changing the interlayer thickness.

Bychkov and Rashba [32] derived a phenomenological expression for the spin-orbit field

$$H_R = \alpha \left( \vec{\sigma} \times \vec{k} \right) \cdot \hat{n},$$

(2.30)

where $\alpha$ is the Rashba parameter and $\hat{n}$ is the axis of broken symmetry (e.g. the electric field direction). For an electric field $\vec{E} = E_z \hat{z}$, this reduces to $H_R = \alpha(\sigma_x k_y - \sigma_y k_x)$. The Hamiltonian of a 2DEG is $H = H_0 + H_R$, where $H_0$ describes the single-electron kinetic energy and $H_R$ can be considered as a perturbation [59]. This leads to the dispersion relation

$$E_{\pm}(k) = \frac{\hbar^2 k^2}{2m} \pm \alpha k.$$

(2.31)
In the absence of SOC \((\alpha = 0)\), the two spin bands are degenerate. Adding SOC splits the dispersion into two helical bands with spin helicity \(\pm\), meaning that the spin is tangential to \(\vec{k}\). To show this, we calculate the spin expectation values \(\hat{S} = \frac{1}{2} \psi^\dagger \vec{\sigma} \psi\). The eigenvector corresponding to the eigenvalue \((2.31)\) is \(\psi = \frac{1}{\sqrt{2}} \psi_n (1, \pm e^{i\theta})^T\), with \(\theta = \tan^{-1}\left(k_y/k_x\right)\). The spin expectation becomes \(\hat{S} = (\pm \frac{1}{2} \sin \theta, \mp \frac{1}{2} \cos \theta, 0)\). Consequently, \(\vec{k} \cdot \vec{S}_h = \vec{k} \cdot (S_x \pm iS_y) = 0\), meaning that the spin polarisation is locked perpendicular to the momentum, as shown in Fig. 2.16f.

### A note on notation

In the previous sections, the electron spin is written in terms of the \(2 \times 2\) Pauli matrices \(\sigma_x, \sigma_y\) and \(\sigma_z\), defined in (2.15). The Pauli matrices are derived from the spin-vector \(\vec{s} = (s_x, s_y, s_z)\) from a geometrical point of view by Cartan [60, 61] and applied to spin by Pauli [62].

The Pauli matrix notation and spin-vector notation are equivalent. Both will be used throughout this thesis. The Pauli matrices span the \(2 \times 2\) spin space, which makes it convenient to write Hamiltonians as \(4 \times 4\) matrices in spin \(\otimes\) particle-hole space. The spin-vector notation allows for insightful toy models to envision Rashba SOC. Using the spin-vector notation, the Rashba SOC Hamiltonian in (2.30) becomes the SOC vector

\[
\vec{a} = \alpha \left( \vec{s} \times \vec{k} \right) \cdot \hat{n}.
\]

(2.32)

For more details on notation of SOC in different spaces, see also Appendix B.4.

### 2.5 Proximity effects

The superconducting proximity effect is often thought of as superconductivity “leaking” into a neighbouring material. Cooper pairs are only formed in superconductors, but they can travel into adjacent materials and locally induce superconducting properties.

#### 2.5.1 S/N proximity effect

The charge carriers in a normal metal (N) are single electrons, whereas in a superconductor (S) they are pairs of electrons. Andreev reflection is the mechanism that converts single electron states in N to Cooper pairs in S.

We consider an incoming electron from N to S with subgap energy \((\varepsilon < \Delta)\). Since there are no available states inside the superconducting energy gap, it is not possible to enter as a single (quasi)particle. Instead, the incoming electron has to form a pair with another electron and drags along a second electron with energy \(-\varepsilon\), leaving behind a hole. This hole has opposite momentum and travels back along the path of the incoming electron [63].

This process goes accompanied by a charge transfer of \(2e\) from N to S, since it involves two electrons. Andreev reflection does not cost or yield energy, since the excited electron in N is replaced by a hole excitation and the newly formed Cooper pair in S is added to the condensate ground state [63].

The incoming electron and Andreev reflected hole in N form a correlated electron-hole pair that can be considered as a Cooper pair no longer bound by attractive interaction. This Cooper pair locally turns the N superconducting, but only over a short length scale. When the single-electron energy is above the Fermi energy, the incoming electron \((E_F + \varepsilon, k_F + \frac{1}{2} \delta k)\) and Andreev reflected hole \((E_F - \varepsilon, -k_F + \frac{1}{2} \delta k)\) have momentum mismatch \(\delta k = 2\varepsilon/hv_F\), with \(\delta k \ll k_F\) [64]. Even in a ballistic system, this mismatch results in resonance effects which eventually result in dephasing of the Cooper pair. The superconducting order parameter decays exponentially inside N. The dephasing in diffusive systems corresponds to the coherence length \(\xi_N = \sqrt{\hbar D_N/2k_BT}\), where \(D_N\) is the normal metal diffusion constant. The temperature \(T\) is the main cause of dephasing. Adding other dephasing effects such as magnetic fields shorten \(\xi_N\) further.
On the S side, the two electrons originating from N are converted into a Cooper pair over a distance $\xi_S = \sqrt{\hbar D_S/k_B T_c}$, where $D_S$ is the superconducting diffusion constant. Consequently, the superconductivity is weakened close to the interface, which is known as the inverse proximity effect.

- **Figure 2.17**: The proximity effect in a normal metal/superconductor junction. (a) An incoming electron at energy $\varepsilon < \Delta$ needs to form a Cooper pair to enter the superconductor. To do that, it drags along an electron with energy $-\varepsilon$, leaving behind a hole with opposite momentum. The pair of electrons is converted into a Cooper pair in the superconductor. The correlated electron-hole pair in the normal metal carries superconducting properties. (b) The normalised superconducting order parameter $|\psi|$. In the superconductor, it is suppressed over $\xi_S$ from the interface due to Cooper pair conversion (the inverse proximity effect). The electron-hole pair dephases over a distance $\xi_N$ in the normal metal.

### 2.5.2 S/F proximity effect

When replacing the normal metal by a ferromagnet (F), the proximity effect is modified. Conventional spin-singlet superconductors favour Cooper pairs with opposite spins, whereas ferromagnets tend to align the spins along their magnetisation. In a S/F junction the F’s exchange field breaks the Cooper pairs in order to align the spins along the exchange field direction (pair breaking), causing superconductivity to break down. The stronger the F, the faster this occurs.

The Cooper pair has two options for “survival”. A stubborn Cooper pair that keeps its spins in opposite directions attains some additional momentum, known as the Larkin-Ovchinnikov-Fulde-Ferrell (LOFF) state. Alternatively, one of the electrons performs a spin flip, changing the opposite-spin pair into an equal-spin pair, aligned with the ferromagnet magnetisation. To do this, a spin-active interface is needed, which will be discussed in the next section.

#### The LOFF state

In a conventional superconductor in the absence of magnetism, a Cooper pair is formed by two electrons with opposite spin $\uparrow$ and $\downarrow$ and opposite momenta $+k_F$ and $-k_F$, with $k_F$ the Fermi momentum. The total Cooper pair momentum is $k_F + (-k_F) = 0$. 
In a ferromagnet, there are unequal amounts of spin-up and spin-down electrons at the Fermi level (see Fig. 2.13). Consequently, momenta shift to \( k_\uparrow = k_F + R/2 \) and \( k_\downarrow = -k_F + R/2 \), where \( R \) is the centre-of-mass momentum of the Cooper pair. The total Cooper pair momentum is \( k_\uparrow + k_\downarrow = R \neq 0 \), which implies that the superconducting order parameter is spatially modulated and is proportional to \( \exp(\pm iRx) \) [26, 65].

Applying this to the singlet state \(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\), we find

\[
|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle = e^{iRx} |\uparrow\downarrow\rangle - e^{-iRx} |\downarrow\uparrow\rangle = \cos(Rx) (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) + i \sin(Rx) (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle),
\]

which is a mixture of the \(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\) singlet state and the \(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\) triplet state (triplets are introduced in Section 2.2.4). The two states are oscillating out-of-phase with a period \( Rx \). Since this particular spin-triplet state has opposite spin, the ferromagnet will break it down just as easy as a conventional spin-singlet pair.

The proximity effect in a S/F junction has an oscillation on top of exponential decay, as illustrated in Fig. 2.18. This state is known as the LOFF state [23, 24] and describes the modulation of the superconducting order parameter related to Zeeman splitting of electrons. The corresponding length scale is the ferromagnetic coherence length \( \xi_F = \sqrt{\hbar D_F/E_{ex}} \). Even for weak ferromagnets, \( \xi_F \) is no more than a few nanometers. Because of this, the triplets generated in the LOFF state are also referred to as short-range triplets.

**Figure 2.18:** The superconducting order parameter \(|\psi\rangle\) across a superconductor/ferromagnet junction. (a) The LOFF state. Since the spin-up and spin-down band are shifted with respect to each other in a ferromagnet, the different spins have different momenta. This causes the Cooper pair to pick up net momentum, causing an oscillating, short-ranged proximity effect of both singlets and triplets. (b) The long-range proximity effect. A spin-active interface rotates the spin quantisation axis. A \((\uparrow\downarrow - \downarrow\uparrow)_y\) pair in the \(y\)-basis is equivalent to a \((\uparrow\uparrow + \downarrow\downarrow)_z\) pair in the \(z\)-basis and can survive over a longer distance in a ferromagnet magnetised along \(z\).
2.5.3 Spin-active interfaces

Spin-active interfaces are not well defined. Generally, they are characterised by the transmission at an interface having some sort of spin-dependence.

In Section 2.2.4, we introduced the spin-state $|S, S_z\rangle$ with $S$ the total spin and $S_z$ the projection onto the quantisation axis; here, the $z$-axis. In a S/F junction, the ferromagnet exchange field $\vec{h}$ fixes the spin quantisation axis along the field direction $\hat{h}$.

If we consider a junction S/F$_1$/F$_2$ where the ferromagnets F$_1$ and F$_2$ have different exchange field directions, the two layers have different quantisation axes. The Cooper pair is magnetised along the direction of the F$_1$ exchange field, forming an opposite-spin triplet with respect to F$_1$’s quantisation axis. Once it enters F$_2$, it’s viewed from F$_2$’s quantisation axis along which it appears as an equal-spin triplet (see Fig. 2.19). This equal-spin triplet aligns with the F$_2$ exchange field and can survive over a much longer distance. This is known as the long-range proximity effect (see Fig. 2.18b). We note that the spin-singlet is rotationally invariant and behaves the same regardless of the quantisation axis [26].

Generally, short-range opposite-spin triplets (the LOFF-state) are generated in homogeneous ferromagnets. Long-range equal-spin triplets are generated when the Cooper pair experiences multiple directions of the exchange field, i.e., inhomogeneous magnetism. Using the notation introduced in (2.24), short-range triplets are described by the projection along the exchange field, i.e., $f_{SR} = \vec{f}_i \cdot \hat{h}$ [33], while long-range triplets are described by the perpendicular projection $f_{LR} = |\vec{f}_i \times \hat{h}|$ [33].

The middle layer is usually thin and is called a spin-active interface. Adding a spin-active interface rotates the spin quantisation axis, allowing the spin-triplet states to mix. Examples of spin-active interfaces include ferromagnetic heterostructures with noncollinear magnetisation [26, 66], an antiferromagnetic interlayer of Ho [67] or Cr [68] and interfacial SOC [33, 69]. As we will see in the following chapters, ferromagnets and SOC are modelled in the same way – they appear in the same matrix elements in the Hamiltonian. The main difference (mathematically) is that the ferromagnet has a constant exchange field, while effective spin-orbit field is momentum-dependent.
Chapter 3

Generating superconducting vortices via spin-orbit coupling

“You must plan to be spontaneous.”
— David Hockney

Spin-orbit coupling (SOC) plays an important role at superconductor/ferromagnet interfaces. By using the generalised London and Ginzburg-Landau theories, we demonstrate that SOC induces spontaneous vortices in zero applied magnetic field in an s-wave superconductor (S) placed below a ferromagnetic (F) metal with intrinsic or interfacial SOC. Even for small SOC strength, the interaction between SOC and vortices is attractive, pinning vortices along the S/F interface with the SOC reinforcing the superconducting state.

The results discussed in this chapter are published in

Superconducting vortices generated via spin-orbit coupling at superconductor/ferromagnet interfaces.


Author contributions: I performed the calculations, wrote the paper and contributed equally to devising the project with my supervisors Jason Robinson and Alexander Buzdin. Xavier Montiel helped fill out some important details in the calculations and came up with the interpretation of the criterion for vortex generation. Jason Robinson was of great help putting the results in perspective and discussing the experimental feasibility of our theoretical predictions. Alexander Buzdin provided overall theory support.
3.1 Chapter in an image

Figure 3.1: (a) Ferromagnetic strip (F) on a superconducting thin film (S) with interface normal $\hat{n}$. The F has an in-plane magnetisation $\vec{M}$. The system is considered to have interfacial Rashba spin-orbit coupling (SOC), which couples the electron spin $\vec{s}$, the electron momentum $\vec{p}$ and normal vector $\hat{n}$ as $(\vec{s} \times \vec{p}) \cdot \hat{n}$. The electron spin $\vec{s}$ tends to align along $\vec{M}$. The interface normal is along $\hat{z}$. As a result of SOC, the momentum $\vec{p}_{\text{max}}$ along $\hat{y}$ gives the largest contribution to the energy of the system. Hence, the electrons will flow in this direction, creating a spontaneous current at the F edges. (b) The phase diagram of a type II superconductor. In the presence of SOC, the critical field $h_{c1}$ has two contributions: a positive contribution from the vortex energy and a negative contribution from the interaction between the vortices and SOC. Since the latter is negative, the SOC acts to lower $h_{c1}$. When the SOC is strong enough, $h_{c1}$ reaches zero and vortices are generated in the absence of an external magnetic field.

3.2 Rashba spin-orbit coupling in S/F systems

As introduced in Section 2.4, SOC occurs as a result of broken inversion symmetry. Rashba SOC is naturally present at S/F interfaces [57, 69–73] and can be enhanced by introducing a material with strong SOC between the S and F layers. Spin is not conserved in the presence of SOC and the interfacial SOC acts as a spin-active interface (see Section 2.5.3). The SOC locally disrupts the singlet pairs, meaning that it rotates the spin quantisation axis. In the reference frame of the F, the singlet pairs are now spin-aligned triplet pairs whose net spin is aligned along the F magnetisation. The generation of spin-aligned triplet pairs in systems combining a single F layer with SOC is discussed in detail in Refs. [69, 74, 75].

Here we study another effect of the interaction between SOC and the F. The interfacial Rashba SOC vector is given by [76]

$$\vec{\alpha} = \frac{\alpha}{\hbar} (\vec{s} \times \vec{p}) \cdot \hat{n},$$

(3.1)

where $\alpha$ is the Rashba SOC strength, $\vec{s}$ is the electron spin, $\vec{p}$ is the orientation of the momentum and $\hat{n}$ is the unit vector along the broken inversion symmetry axis. In this work, we consider a F strip on top of an infinite S thin film. The interface normal is along the $z$-axis such that $\hat{n} = \hat{z}$.

The F tends to align the spins along its magnetisation $\vec{M}$, meaning that $\vec{s} \parallel \vec{M}$. Here, we consider $\vec{M} = M\hat{x}$, such that the spins point along $\hat{x}$ too. The presence of SOC given in (3.1) results in a preferred direction for the electron momentum $\vec{p}$. If $\vec{p} \parallel \hat{x}$, then $\vec{\alpha} \sim (\hat{x} \times \vec{x}) \cdot \hat{z} = 0$. Similarly, if $\vec{p} \parallel \hat{z}$, then $\vec{\alpha} \sim (\hat{z} \times \hat{z}) \cdot \hat{x} = 0$. $\vec{\alpha}$ non-zero for any other direction and reaches its maximum when $\vec{p} \parallel \hat{y}$. This is illustrated in Fig. 3.1a. In general, the momentum along $\vec{s} \times \hat{n}$ becomes energetically favourable. As a result, the electrons move in the $\hat{y}$-direction. This creates a spontaneous current originating from the interaction between the F and SOC. In turn, this current induces a local magnetic field within the London penetration depth form the interface [76]. This phenomenon has been studied theoretically in a variety of S/F interfaces with SOC, including an infinite S/F bilayer, a S/F/S junctions and a bulk S with a cylindrical F core [76].
The role of the F is to polarise the electron spin. This effect is not unique to ferromagnetism and can be achieved by any kind of magnetic ordering. In fact, the generation of spontaneous currents has been predicted in a variety of systems with magnetic order and SOC. For instance, Pershoguba et al [77] reported superconducting currents induced by F islands and magnetic impurities in a S with SOC. They show that SOC adds a spin-dependent term to the velocity operator which induces a current through the magnetoelectric effect. Robinson et al [78] studied a closed S loop partially covered by a ferromagnetic insulator. They show that the combination of SOC with an exchange field generates a nondissipative current in the S loop, with a chirality determined by the magnetisation alignment. Baumard et al [79] have shown that a Néel skyrmion in a thin-film S induces a spontaneous current, which gives rise to a perpendicular magnetic field. Additionally, in the presence of SOC, the skyrmion is able to nucleate a superconducting vortex via a magnetoelectric proximity effect.

Mathematically, these systems [76–79] all have a similar, unusual term in the free energy. The phenomenological Landau theory of phase transitions (see Section 2.1.2) is based on the assumption that the free energy is an even function of the order parameter. This means that the system has no directional preference, i.e., when the order parameter is reversed, the system has the same energy. However, in the presence of both SOC and magnetic ordering, an extra linear term appears in the free energy, meaning that the inversion symmetry with respect to the order parameter is broken. As we will see in the derivations below, this linear term is responsible for the spontaneous currents.

Considering different mechanisms to polarise spin, an external magnetic field is perhaps the most obvious one. However, Mironov and Buzdin [76] point out that this does not work. The current density \( \vec{j} \) is calculated as the derivative of the free energy \( f \) over the vector potential \( \vec{A} \) (i.e., \( \vec{j} = -\delta f / \delta \vec{A} \)) and an external magnetic field depends on \( \vec{A} \). Hence, an external magnetic field gives an additional term in the current density. This term is equal in magnitude and opposite in sign to the linear term contribution. Consequently, the two terms cancel each other and no spontaneous currents occur.

In the following, we consider a type II S, characterised by two critical fields \( h_c1 \) and \( h_c2 \). The S is in the Meissner state below \( h_c1 \) and Abrikosov vortices appear when \( h_c1 \) is exceeded. We will show that \( h_c1 \) can be expressed as the sum of two energies, i.e., \( h_c1 \sim E^{\text{vor}} + E^{\text{int}} \), with \( E^{\text{vor}} \) the vortex energy and \( E^{\text{int}} \) the interaction energy between the vortices and SOC. The two energies have the opposite effect on \( h_c1 \), that is, \( E^{\text{vor}} \) increases \( h_c1 \) (\( E^{\text{vor}} > 0 \)), whereas \( E^{\text{int}} \) decreases \( h_c1 \) (\( E^{\text{int}} < 0 \)). When \( E^{\text{int}} \) is strong enough, it cancels the effect of \( E^{\text{vor}} \), such that \( h_c1 = 0 \) and the vortices occur spontaneously (in the absence of an external field). This situation is illustrated in Fig. 3.1b. Since both energies depend on the SOC strength \( \alpha \), we will calculate a minimum value \( \alpha \) to observe spontaneous vortices.

Finally, since \( E^{\text{int}} \) is negative, the interaction between the vortices and SOC is attractive, meaning that the vortices are pinned along the F edges. Our theory predicts vortex pinning and guiding using only SOC without the requirement of stray fields. The vortex motion is reversible with current or magnetisation direction. This provides the basis for Abrikosov vortex memory.

### 3.3 Spontaneous currents and vortices

#### 3.3.1 The free energy

We model a type-II S of thickness \( d_S \) (with \( d_S < \xi \)) that is partially covered by a thin-film metallic F of thickness \( d_F \), as shown in Fig. 3.2a-b. We use the general Ginzburg-Landau (GL) approach introduced in Section 2.1.3 to describe the system where the density of the free energy \( F = \int f(\vec{r})d^3\vec{r} \) is

\[
f = a|\psi|^2 + \frac{b}{2} |\psi|^4 + \frac{1}{4m} |D\psi|^2 + \frac{\hbar^2}{8\pi} + \frac{2}{4m} \left( \psi^* \hat{D} \psi + \psi (\hat{D} \psi)^* \right).
\]  

(3.2)

The free energy density \( f \) is expressed in terms of the superconducting order parameter \( \psi \). The first four terms are the standard terms in GL theory and are explained in more detail in Section 2.1.3. To

*We note that the spontaneous current discussed here is a charge current. It is still possible to have a spin current in the presence of an external magnetic field, as we will see in the next chapter.
recapitulate, the first two terms come from Landau theory for phase transitions, in which the free energy is expressed as an even function of $\psi$ (see Section 2.1.2) and $a = a_0 (T - T_c)/T_c$ and $b$ are the standard coefficients. The third and fourth term are specific to superconductors, where $\vec{D} = -i\nabla + 2e\vec{A}$ is the gauge-invariant momentum operator with $\hbar = c = 1$ and $\vec{A}$ the vector potential and $\vec{h}$ is an applied magnetic field. These magnetic terms are introduced in GL theory to study the properties of a $S$ in a magnetic field.

In general, magnetism has three effects on superconductivity: 1. overall suppression, 2. an orbital effect (on the orbital angular momentum) and 3. a paramagnetic effect (on the spin angular momentum). Here, we do not consider spin and neglect the paramagnetic effect on superconductivity. Therefore, the magnetic field term is considered the same in the superconducting and normal state, and will be contained in the $F_0$ term (see Section 2.1.3 for the introduction of $F_0$). The vector potential $\vec{A}$ corresponding to $\vec{h}$ is therefore also negligible. However, the $F$ in our system gives exactly the same contribution to $\vec{A}$, i.e., the $F$ introduces vortices in the system ($\vec{A}^{\text{rot}}$ term in the next section), which is why a $\vec{A}$ term remains.

The fifth term is the unusual linear term in $\psi$ originating from the interaction between SOC and the $F$. We consider the $F/S$ heterostructure in the London framework, which describes field variations over distances $\lambda \gg \xi$. The length scales related to vortices are illustrated in Fig. 2.6. The assumption $\lambda \gg \xi$ implies that the generated current does not modify the modulus of the superconducting order parameter [79]. The spatial dependence of the order parameter will be considered separately in Section 3.4.1. Furthermore, the $\vec{a}$ term varies over the length scale $\xi$. The magnetisation of $F$ is in-plane along $x$ such that $\vec{a}$ points along $y$ (see Fig. 3.1a). Under the assumption $\lambda \gg \xi$, $\vec{a}$ can be modelled as a step function, i.e., $\vec{a} = \frac{\phi}{|\phi|} \Theta (x - L/2) \Theta (L/2 - x) \vec{y}$, where $\Theta(x)$ is the Heaviside step function and the magnitude $\alpha$ is [80]

$$\alpha \approx \frac{v_R}{v_F} \frac{c}{d_S} \frac{h_{\text{ex}}}{T_c \xi}.$$  

(3.3)

where $\phi_0/2\pi = 1/2e$ is the flux quantum, $c$ is the atomic lattice parameter, $v_R$ the Rashba velocity and $v_F$ the Fermi velocity. We emphasise that $\vec{a}$ results from the interaction between the SOC and magnetic ordering from the $F$ [81, 82]. This becomes evident by looking at (3.3) which incorporates both the Rashba velocity $v_R$ (originating from Rashba SOC) and the exchange field $h_{\text{ex}}$ (originating from the $F$).

Before working with this model, a few things need to be clarified. Firstly, it may seem strange that the SOC is included in (3.2) based on its interaction with the $F$. However, we will see in the derivations below that having this interaction term results in an extra contribution from the SOC to the vector potential $\vec{A}$ and in turn, to the locally induced magnetic field $\vec{h}$. Secondly, in the introduction of this chapter, we mentioned spin-aligned triplet pairs as a result of a $F$ combined with SOC. Triplet correlations affect sample properties such as the density of states and transport. Nevertheless, thermodynamic properties (such as $h_c$ and $T_c$) are governed by singlet correlations. The GL model describes the superconducting order parameter of the singlet correlations, which makes it suitable to study $h_c$ and $T_c$. In the next chapter, we will use a quasiclassical model to study the presence of triplets.

For $T \ll T_c$, superconductivity is well-developed, such that the GL order parameter is $\psi = |\psi|e^{i\varphi}$, where $|\psi|$ is constant and $\varphi$ is the phase of the superconducting order parameter. Following Ref. [83], we introduce the vorticity

$$\Phi = \phi_0 \hat{n} \times (\vec{r} - \vec{r}_0) / (r - r_0)^2$$

(3.4)

to describe the phase singularity related to a vortex at $\vec{r} = \vec{r}_0$ with normal vector $\hat{n}$. Appendix A.1 shows how the individual terms of (3.2) are rewritten in terms of $\Phi$.

Assuming a thin $S$ film with $d_S \ll \lambda$, superconductivity along $z$ can be taken to be constant. The $z$-integral in $F = \int f(\vec{r})d^5r$ then yields a factor $d_S$ which is used to renormalise the London penetration depth to the effective penetration depth $\lambda_{\text{eff}} = \lambda^2/d_S$ [83]. The free energy becomes

$$F = F_0 + \frac{1}{8\pi \lambda_{\text{eff}}} \int (\Phi - \vec{A} + \frac{\vec{a} \phi_0}{2\pi})^2 d^2\vec{r},$$

(3.5)
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where \( F_0 \) is the free energy in the normal state (above \( T_c \)).

### 3.3.2 Physical quantities

The GL free energy can be related to physical quantities. We start by evaluating the vector potential \( \vec{A} \), which is related to the current density and locally induced magnetic field via the Maxwell equations.

The current density in the plane \( z = 0 \) is given by \( \vec{j} = -\partial \vec{f} / \partial \vec{A} \delta (z) \). From the Maxwell-Ampere equation \( 4\pi \vec{j} = \nabla \times \vec{h} = \nabla \times (\nabla \times \vec{A}) = -\Delta \vec{A} \), we obtain the differential equation for \( \vec{A} \),

\[
-\Delta \vec{A} = \frac{1}{\lambda_{\text{eff}}} \left( \vec{\phi} - \vec{A} + \frac{\vec{\alpha} \phi_0}{2\pi} \right) \delta (z).
\]  

(3.6)

Appendix A.2 shows how (3.6) is solved in Fourier space. The solution \( \vec{A}_q \) (the two-dimensional Fourier transform of \( \vec{A}(z = 0) \)) is

\[
\vec{A}_q = \frac{\vec{\Phi}_q + \vec{\alpha}_q \phi_0 / 2\pi}{1 + 2 |q| \lambda_{\text{eff}}}
\]  

(3.7)

\( \vec{A}_q \) consists of two contributions \( \vec{\Phi}_q \) and \( \vec{\alpha}_q \), which are terms that describe the two-dimensional Fourier transforms of the vortices \( \vec{\Phi} \) and SOC \( \vec{\alpha} \), respectively. We write \( \vec{A}_q = \vec{A}_q^{\text{vor}} + \vec{A}_q^{\text{soc}} \). In the absence of vorticity \( (\vec{A}_q^{\text{vor}} = 0) \), the remaining term \( \vec{A}_q^{\text{soc}} \) is the anomalous phase \( \varphi = \vec{\alpha} \cdot \vec{r} \). This shows the equivalence between a superconductor with a phase and a superconductor with a vector potential.

Following [83], we use \( \vec{A}_q \) to derive several physical quantities. The current density \( \vec{j} \) is related to \( \vec{A} \) via the Maxwell equation \( \vec{j} = -\Delta \vec{A} / 4\pi \). Since \( \vec{A}_q \) consists of two contributions, \( \vec{j} \) can be expressed in the same contributions as well, i.e., \( \vec{j} = \vec{j}^{\text{vor}} + \vec{j}^{\text{soc}} \). These two contributions are evaluated in Appendix A.3.

We find that the current generated due to SOC is

\[
\vec{j}^{\text{soc}}(x) = j_0^{\text{soc}} \hat{y} \int_0^\infty \sin \left( \frac{p(x-z)}{\lambda_{\text{eff}}} \right) + \sin \left( \frac{p(x+z)}{\lambda_{\text{eff}}} \right) dp
\]  

(3.8)

with \( j_0^{\text{soc}} = \alpha \phi_0 / 4\pi \lambda_{\text{eff}} \) and \( p = q_x \lambda_{\text{eff}} \).

The locally induced magnetic field (as a result of the spontaneous currents) at the surface of the superconductor is obtained by transforming the Maxwell equation \( \vec{h} = \nabla \times \vec{A} \) into Fourier space. The magnetic field consists of two contributions \( \vec{h} = \vec{h}^{\text{vor}} + \vec{h}^{\text{soc}} \) which are assessed in Appendix A.4. The magnetic field induced by the SOC is

\[
\vec{h}^{\text{soc}}(x) = h_0^{\text{soc}} \hat{z} \int_0^\infty \cos \left( \frac{p(x-z)}{\lambda_{\text{eff}}} \right) + \cos \left( \frac{p(x+z)}{\lambda_{\text{eff}}} \right) dp
\]  

(3.9)

with \( h_0^{\text{soc}} = \alpha \phi_0 / 2\pi^2 \lambda_{\text{eff}} \).

The interaction between the vortexes and SOC is described by the cross terms \( (\sim \vec{\alpha}_q \cdot \vec{\Phi}_q^* + \vec{\alpha}_q^* \cdot \vec{\Phi}_q) \) in the total free energy (3.5). The interaction energy has contributions the combined superconductivity and SOC term [first integral in (3.5)] and from the magnetic field [second integral in (3.5)]. Both contributions are evaluated in Appendix A.5. The combined effect is expressed as

\[
E^{\text{int}}(x) = -E_0^{\text{int}} \int_0^\infty \frac{\sin \left( \frac{pL}{2\lambda_{\text{eff}}} \right) \sin \left( \frac{px}{\lambda_{\text{eff}}} \right)}{p(1 + 2p)} dp
\]  

(3.10)

with \( E_0^{\text{int}} = \alpha \phi_0^2 / 2\pi^3 \).

The current density (3.8), magnetic field (3.9) and interaction energy (3.10) are plotted in Fig. 3.2c-e. These quantities are proportional to the SOC strength \( \alpha \) and depend on the F strip’s width \( L \). The current density shows maxima at the F/S interfaces and decays into the superconductor, as was predicted
Figure 3.2: A ferromagnetic strip F on a superconductor S at $T \ll T_c$. (a) A perspective and (b) top view schematic illustration of the S/F heterostructure with magnetization $\vec{M}$ and SOC $\vec{\alpha}$. Vortices and antivortices are represented by circular currents at the F edges. (c) The current $j_y^{\text{soc}} / j_0^{\text{soc}}$ and (d) the magnetic field $h_z^{\text{soc}} / h_0^{\text{soc}}$ due to SOC. (e) The interaction energy between the vortices and SOC $E_{\text{int}} / E_0^{\text{int}}$. 
from the toy model in Section 3.2. Since the SOC is an edge effect located inside the F, the current exhibits a discontinuity at the F strip’s edges.

The SOC causes local spikes in the magnetic field at the edges, which are positive and negative, corresponding to the in-plane magnetisation direction. That is, the spikes shown in Fig. 3.2d correspond to the magnetisation direction $\hat{x}$. Reversing the magnetisation to $-\hat{x}$ flips the sign of the spikes. The importance of these spikes is that they are experimentally observable with, for instance, magnetic force microscopy.

The interaction energy is attractive at one edge of the ferromagnet and repulsive at the other, with a gradual continuous profile across the heterostructure. In the next section, we will see the consequences this has on vortices.

### 3.3.3 Spontaneous vortex generation

We use the interaction energy (3.10) to derive the criterion for spontaneous generation of vortices without applied magnetic field. The expression for the lower critical field $h_{c1}$ is modified by the presence of SOC.

The modified $h_{c1}$ is derived in Appendix A.6 and is equal to

$$h_{c1} = \frac{4\pi}{\phi_0} (E^{\text{vor}} + E^{\text{int}}),$$

where $E^{\text{vor}}$ is the energy of the vortices and $E^{\text{int}}$ is the interaction energy between the vortices and SOC. The vortex energy is [83]

$$E^{\text{vor}} = \left(\frac{\phi_0}{4\pi}\right)^2 1 \frac{1}{\lambda_{\text{eff}}} \ln \left(\frac{\lambda_{\text{eff}}}{\xi}\right).$$

The interaction energy $E^{\text{int}}$ in (3.10) depends on $x$. To obtain an expression for $h_{c1}$, we estimate $E^{\text{int}}$ in the limit $L \gg \lambda_{\text{eff}}$ in Appendix A.5. We obtain

$$E^{\text{int}} \approx -\frac{\alpha\phi_0^2}{4\pi^2} \ln \left(\frac{L}{\lambda_{\text{eff}}}\right).$$

This interaction is negative, implying that $h_{c1}$ decreases in the presence of SOC. The spontaneous generation of vortices occurs when $h_{c1}$ becomes negative - i.e., when the positive energy of the vortices is balanced by the negative interaction (this is illustrated in Fig. 3.1b). Solving $h_{c1} < 0$, we find that the SOC strength required for the formation of vortices is

$$\alpha > \frac{\pi}{4\lambda_{\text{eff}}} \ln \left(\frac{\lambda_{\text{eff}}}{\xi}\right).$$

Condition (3.14) shows that an increase in $L$ or a reduction in $d_S$ favours vortex creation. Typical ratios in (3.3) are $v_R/v_F \sim 0.1$ [31, 84] and $c_{\text{ex}}/d_ST_c \sim 0.1$ [78], giving $\alpha \approx 0.01/\xi$. By assuming $\xi/\lambda_{\text{eff}} \sim 10^{-3}$ and $\xi \ll L$, (3.14) is satisfied and spontaneous vortices are generated.

The interaction energy profile in Fig. 3.2e has a minimum at $L/2\lambda_{\text{eff}}$, meaning that vortices are attracted and stabilised at this F edge. The maximum at $-L/2\lambda_{\text{eff}}$ repels vortices, which is also known as an antivortex and can be pictured as a vortex with the opposite chirality (see Fig. 3.2a-b). Due to the symmetry of the system, the vortices come in vortex-antivortex pairs.

### 3.3.4 Comparison with stray fields

The spatial profiles of $j_y^{\text{soc}}$ and $E^{\text{int}}$ in Fig. 3.2 follow the same trend as Vlasko-Vlasov et al [85], even though their system is slightly different. Vlasko-Vlasov et al [85] consider multiple parallel F strips on a S thin-film. The distance between the strips is much smaller than the strip width, such that the vortex-antivortex pair is located on the edges of two adjacent strips (rather than on two sides of a single strip). Each F edge forms a linear magnetic monopole with radially diverging magnetic stray fields. They use
a small out-of-plane applied field to introduce vortices. The vortices accumulate at the strip edges due to the stray fields. There is no SOC in their system.

Using their setup, Vlasko-Vlasov et al [85] obtain a magnetic potential identical to our interaction energy $E^{\text{int}}$, and a magnetic pinning force which is exactly opposite to our current density $j_y^{\text{soc}}$. This sign difference is not an actual discrepancy as it stems from the definition of the exchange integral determining $h_{\text{ex}}$. Moreover, the same sign can be obtained in our system with SOC by simply inverting the magnetisation or current direction.

Since the two systems are similar, the question arises whether we have the same stray fields in our system and whether we need the SOC at all. The answer is that we probably do have small stray fields, but we will now show that the SOC dominates.

Vlasko-Vlasov et al [85] argue that when the F film thickness is much smaller than all other dimensions, the magnetic field can be modelled as a long thin linear magnetic monopole. The monopole has radially diverging magnetic stray fields that decay with radius $r$, i.e., $B = b/r$, where $b$ is the magnetic charge per unit length given by $b = 2M_d d_F$, where $M_s$ is the saturation magnetisation and $d_F$ the F thickness [85]. The stray field penetrates the S by $r = \lambda_{\text{eff}}$, such that $B = 2M_d d_F/\lambda_{\text{eff}}$.

The magnetic field induced by the SOC is calculated in (3.9). Its magnitude is the prefactor $h_{\text{soc}}^{\text{mag}} = \alpha \phi_0 / 2\pi^2 \lambda_{\text{eff}}$. Comparing the two magnetic field contributions, the SOC dominates when $h_{\text{soc}}^{\text{mag}} > B$. Substituting the expressions gives the condition $\alpha > 4\pi^2 M_s d_F/\phi_0$.

To write this condition in the parameters of our calculations, we introduce the magnetic induction in F, given by $B(0) = 4\pi M_s$. The lower critical field of a general S is $h_{\text{c1}} = (\phi_0 / 4\pi^2 \lambda_{\text{eff}}) \ln(\lambda/\xi)$ [37]. Using that $\lambda^2 = \lambda_{\text{eff}} d_S$ (see page 54), the magnitude is $h_{\text{c1}} \approx \phi_0 / 4\pi \lambda_{\text{eff}} d_S$. Substituting this in the condition for $\alpha$ gives

$$\alpha > \frac{B(0)d_F}{4\lambda_{\text{eff}} d_S h_{\text{c1}}}.$$

We estimate that $B(0) \sim h_{\text{c1}}$ and $d_F \sim d_S \sim \xi$. What remains is $\alpha > 1/4\lambda_{\text{eff}}$. We recall that the condition for vortex generation in (3.14) is $\alpha > \pi/4\lambda_{\text{eff}}$. Hence, if $\alpha$ is strong enough to generate vortices, the SOC will also dominate the stray field contribution.

The setup relying on stray fields [85] is harder to fabricate and control than the setup with SOC. The stray fields depend on the microscopic structure of the F and its applied magnetic field history (see Sections 2.3.4 and 2.3.5 for details). This makes it hard to control the stray fields independently of the F. The current density (3.8), magnetic field (3.9) and interaction energy related to the pinning force (3.10) all scale with $\alpha$. This implies that, to increase these physical properties in a system with stray fields, one needs to increase the stray field itself. This in turn suppresses the superconductivity, making it more difficult to deconvolute the role of SOC from stray fields.

In the setup with SOC, the SOC and F are independent, which means the vortices can be controlled by rotating the F magnetisation. The SOC does not suppress the superconductivity.*

### 3.3.5 Vortex density

We have established that chains of vortices and antivortices are generated at the F strip’s edges in the presence of SOC. In this section, we will estimate the intervortex distance $d$. The current through a vortex is given on page 62 of Ref. [83] as $J(r) = \phi_0 / 4\pi^2 r^2$, for $r > \lambda_{\text{eff}}$. The corresponding intervortex interaction writes

$$U(r) = -\int \phi_0 \cdot J(r) \, dr = \frac{\phi_0^2}{4\pi^2 r}.$$

The energy density consists of the vortex energy $E^{\text{vor}}$ [defined in (3.12)], the interaction between vortices and SOC $E^{\text{int}}$ [defined in (3.13)] and the intervortex energy between one vortex and the other vortices

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*Unlike magnetism, SOC preserves time-reversal symmetry, which is crucial for the existence of superconductivity. This is explained in Section 2.4. In a similar setup to the one described in this chapter, SOC even acts to stabilise and enhance the superconductivity. This is the main topic of Chapter 4.
3.3. Spontaneous currents and vortices

in the chain [83]. The latter is a sum over all $N$ vortices, such that the linear energy density is

$$E = \frac{E^{\text{vor}} + E^{\text{int}}}{d} + U(d) \sum_{n=1}^{N} \frac{1}{nd}.$$ 

Since the vortices are close together, we approximate the sum by an integral, which gives

$$\sum_{n=1}^{N} (nd)^{-1} = \ln(N)/d.$$ 

To prevent divergence of the interacting term, we consider a cut-off $\Gamma = \min(L, L_y)$, where $L$ and $L_y$ are the lengths of the F strip in the x- and y-direction, respectively. We consider two scenarios.

**Figure 3.3:** A schematic illustration of a ferromagnetic strip with dimensions $L \times L_y$ on a superconducting thin film. A chain of antivortices (vortices) forms under the left (right) F edge. For $L_y \gg L$, the vortex and antivortex chains interact.

When $L_y \gg L$, the intervortex interaction in the vortex chain has to be compared to the interaction between the vortex chain on one F strip’s edge and the antivortex chain on the other strip’s edge (which are separated by $L$), as illustrated in Fig. 3.3. In the case $L_y \ll L$, the cut-off comes from the size of the F layer in the y-direction. Hence, the cut-off $\Gamma = \min(L, L_y)$ takes both scenarios into account and the number of vortices in a chain $N$ is $Nd = \Gamma$. The energy density becomes

$$E = \frac{E^{\text{vor}} + E^{\text{int}}}{d} + \frac{\phi_0^2}{4\pi^2d^2} \ln \left( \frac{\Gamma}{d} \right).$$

The expression for $d$ is obtained from $\partial E/\partial d = 0$. For $\Gamma \gg d$,

$$d \approx \frac{\phi_0^2}{2\pi^2} E^{\text{vor}} + E^{\text{int}} = \frac{\ln \left( \frac{\Gamma}{d} \right)}{\alpha \ln \left( \frac{L}{\lambda_{\text{eff}}} \right) - \frac{1}{8\lambda_{\text{eff}}} \ln \left( \frac{\lambda_{\text{eff}}}{\xi} \right)}.$$ 

Assuming that $E^{\text{vor}} + E^{\text{int}} < 0$ (the requirement for vortex generation), this expression holds for $d \gg \lambda_{\text{eff}}$. It shows that an increase in $\alpha$ results in a decrease in $d$, meaning that strong SOC can stabilise the vortices closer together.

When $d$ approaches $\lambda_{\text{eff}}$, a second row of vortices may appear, giving rise to a dense vortex structure. Determining this structure is beyond the scope of our calculations.
3.4 Limiting cases

3.4.1 Limit I: at the critical temperature

So far, we have considered the case where the superconductivity is well-developed such that the order parameter could be written as $\psi = |\psi|e^{i\phi}$. For $T < T_c$, superconductivity is weak and this assumption no longer holds. We calculate the order parameter’s spatial dependency explicitly. We use this to calculate the current density for $T \to T_c$ to show that our previous calculation for $T \ll T_c$ is consistent with the limit $T \to T_c$.

The GL equation is obtained by minimising the free energy $F = \int f \, d^2r$ where $f$ is given by (3.2), which is done in Appendix A.7. The GL equation in the absence of a magnetic field is

$$a\psi + b|\psi|^2\psi - \frac{1}{4m} \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) - \frac{ie}{2m} \frac{\partial \psi}{\partial y} = 0.$$  \hspace{1cm} (3.15)

At $T_c$, the order parameter magnitude vanishes ($|\psi|^2 \to 0$) and the GL equation is linearised. We solve (3.15) for $\psi$ in Appendix A.7. The current density is obtained from $\bar{j} = -\partial f/\partial A$ and equal to

$$\bar{j} = \frac{ie}{2m} \left[ \psi^* \nabla \psi - \psi \nabla \psi^* \right] - \frac{e\alpha}{m}|\psi|^2.$$  \hspace{1cm} (3.16)

The first term is the supercurrent, which is present in every $S$. The second term results from the SOC and is specific for this system. Considering the regions with and without SOC, we rewrite $\bar{j}$ as

$$\bar{j}(x) = \begin{cases} j_0 |\psi(x)|^2 \hat{y} & \text{for } |x| > L/2, \\ -\varepsilon j_0 |\psi(x)|^2 \hat{y} & \text{for } |x| < L/2, \end{cases}$$  \hspace{1cm} (3.17)

where $j_0 = e\alpha/m$ and $\varepsilon$ is a small difference between the modulation vector and $\alpha$, that is found self-consistently.

The wave function $\psi(x)$ and current density $j_0(x)$ from (3.17) are shown in Fig. 3.4. The wave function is enhanced inside the F and gradually decays towards the edges. The significance of this result is that at $T = T_c$, superconductivity normally breaks down ($\psi \to 0$), and outside of the F strip, it does. However, the order parameter is still non-zero underneath the F strip, meaning that the combined effect of the SOC and F locally enhances $T_c$. We will discuss this in more detail in the next section.

The current density $j_0(x)$ exhibits large peaks at the edges, similar to the $T \lesssim T_c$ case in Fig. 3.2b. The profile inside the F is different. At $T = T_c$, $j_0(x)$ is slightly suppressed inside the F and goes up near the F edges. This is a result of the suppression of the order parameter shown in Fig. 3.4a.

![Figure 3.4: Limit I: A ferromagnetic strip on a superconducting film at $T = T_c$. Spatial dependence of (a) the normalised wave function $\psi(x)$ and (b) the current density $j_0(x)$ for different (labelled) lengths $L/\xi$.](image-url)
3.4. Limiting cases

3.4.2 Modulated critical temperature

We use the GL equation (3.15) to investigate the critical temperature $T_c$. We do this in two steps. We first assume that superconductivity is uniform in $x$ such that $\psi(x, y) = \psi_0 e^{i q_y y}$, with $\psi_0$ a constant. By optimising the GL equation for this wave function, we find that $T - T_c$ is maximised for $q_y = -\alpha$. The value $q_y = -\alpha$ is exact in infinite samples and is an estimate in finite size samples.

Subsequently, we use the wave function $\psi(x, y) = \psi(x) e^{-i q_y y}$ and use separation of variables to evaluate the $x$- and $y$-dependence separately. The normalised wave function $\psi(x)$ is plotted in Fig. 3.4a. Underneath the F, superconductivity is locally enhanced as a result of the interaction between the F and the SOC.

Since the $y$-direction has already been optimised, the $y$-derivatives in the GL equation can be considered a constant offset to $T_c$ that results in local modulations in $T_c$. Since the $y$-terms are constant, they can be absorbed into $T_c$, which gives a new $T_{c+}$ in the presence of SOC. The details are shown in Appendix A.8. In the presence of SOC, $T_c$ increases according to

$$T_{c+} = T_c \left(1 + \frac{\alpha^2}{4m a_0} \right).$$  \hfill (3.18)

We are now dealing with three different critical temperatures: $T_{c0}$ is the critical temperature of the bare superconductor. $T_c$ relates to the F/S bilayer without SOC and $T_{c+}$ corresponds to the F/S bilayer with SOC. Hence, $T_{c0} \geq T_{c+} \geq T_c$, meaning that $T_{c+} - T_c$ represents a recovery of the critical temperature of the bilayer due to SOC. This can be interpreted as a stabilisation of superconductivity via SOC.

This is a slightly counter-intuitive result considering that $\alpha$ scales linearly with $h_{ex}$ [see the definition in (3.3)]. We note that the effect we describe here should lead to a $T_c$-dependence on the orientation of $h_{ex}$: for an out-of-plane orientation, no modulation occurs and $T_c$ is smaller than the case in which $h_{ex}$ is in-plane (recall Fig. 3.1a). The decrease of $T_c$ due to the presence of ferromagnetism (meaning, compared to $T_{c0}$) does not depend on the orientation of $h_{ex}$. The exact dependence of the critical temperature on $h_{ex}$, including the dependence via SOC, is studied in Section 5.4.

3.4.3 Limit II: ferromagnetic half-plane

Another consistency check for our model is to consider an F covering the half-plane $x \in [0, \infty)$, with $T \lesssim T_c$. Rather than taking the SOC into account explicitly using the $y$-derivatives, we take the SOC into account implicitly by substituting $T_{c+}$ (3.18) into the GL equation (3.15). This gives a GL equation that only depends on $x$ and allows us to derive an expression for the temperature-dependent coherence length $\xi(T)$, as shown in Appendix A.9. The coherence length is equal to

$$\xi^2(T) = \frac{1}{4m a_0 |T - T_{c+}|}. \hfill (3.19)$$

An important property of $\xi(T)$ is that it diverges as $T \to T_{c+}$. We write the wave function as $\psi(x) = \psi_\infty f(x)$, where $\psi_\infty$ is a constant and $0 \leq f(x) \leq 1$ describes the spatial variation. The GL equation becomes

$$\begin{cases}
\xi^2(T) (f')^2 = \frac{1}{2} (1 - f^2)^2 & \text{for } x > 0, \\
\xi^2(T) (f')^2 = \tau f^2 + \frac{1}{2} f^4 & \text{for } x < 0,
\end{cases} \hfill (3.20)$$

with $f' = df/dx$ and $\tau \equiv (T - T_c)/|T - T_{c+}|$. We solve these differential equations in Appendix A.10, assuming continuity of $f$ and $f'$ at $x = 0$. The resulting wave function is plotted in Fig. 3.5a. It has a gradual shape going from no enhancement in the bare S to an enhanced state underneath the F, following the same trend as in Fig. 3.4a.

The total current consists of a current along the F edge (originating from the SOC) and the supercurrent, equivalent to (3.16). In the half-plane limit, we consider $\lambda \gg \xi$ such that the edge current can
Generating superconducting vortices via spin-orbit coupling

Figure 3.5: Limit II: A superconducting film half covered by ferromagnetic metal with \( T \leq T_c \). Inset: Schematic illustration of the S/F heterostructure with magnetisation \( \vec{M} \) and edge current \( \vec{j} \). Spatial dependence of (a) the normalised wave function \( \psi(x) \) and (b) the current density \( j_y(x) \).

The current density can be modelled as a Dirac \( \delta \)-function, i.e., \( j_y = j_0 \delta(x) \). The total current is

\[
\vec{j}(x) = j_0 \delta(x) \hat{y} - \frac{1}{4\pi \lambda_{\text{eff}}} \vec{A}(x). \tag{3.21}
\]

We use Biot-Savart’s law \( \vec{A} = \int \frac{\vec{j}/\sqrt{x^2 + y^2} \, dx}{x^2 + y^2} \), which results in an implicit equation for \( A_y(x, z) \). The derivation is shown in Appendix A.11. In the \( z = 0 \) plane, we have

\[
A_y(x, z = 0) = \ln |x - L| - \ln |x| + \frac{1}{2\pi} \int_0^L A_y(x') \ln |x - x'| dx'. \tag{3.22}
\]

We solve the above for \( A_y(x) \) iteratively, letting \( L \to \infty \) and obtain the current density from (3.21). The current density is shown in Fig. 3.5b. It is zero outside the F and has a \( \delta \)-peak resulting from the edge current, then drops and gradually recovers inside the F. We note that the horizontal axis of Fig. 3.5b is scaled versus \( x/\lambda \) and \( \lambda \gg \xi \). If it was plotted as a function of \( x/\xi \), the \( \delta \)-peak would look more gradual like the peaks in Fig. 3.4b. The gradual recovery inside F is consistent with the behaviour seen in Fig. 3.2c.

In the case of a F covering the half-plane, vortices exist at the F edge. However, since there is only one edge, no antivortices are generated.

### 3.5 Conclusions & Outlook

In summary, we have theoretically investigated the role of SOC in F/S bilayers in the superconducting state. Studying the effect of different energies on the critical field \( h_{c1} \), we found that SOC lowers \( h_{c1} \). Even weak SOC (\( \alpha \approx 0.01/\xi \)) can bring \( h_{c1} \) down to zero which enables spontaneous vortex generation. Due to the geometry of the system, the vortices appear in pairs of a vortex and antivortex (interpreted as a vortex with opposite chirality). The interaction between vortices and SOC is attractive, such that the vortices are pinned along one F edge and the antivortices along the other.

Contrary to previous experiments \([76, 77, 79, 85]\), this effect solely relies on the SOC. Therefore, an important aspect of our theory is that it raises the prospect for vortex guiding without the usual requirement of stray magnetic fields to generate vortex-antivortex pairs. Using SOC instead of stray fields allows for independent control of the SOC and F, whereas the stray fields depend on the F. The vortex motion is reversible with current or magnetisation direction. These are key requirements for Abrikosov memory.

We have calculated the current density in two limiting cases – at the critical temperature and for a F half-plane – and found that our theory is consistent in these limits.

We have also calculated the superconducting order parameter and critical temperature of the system.
A bare S has critical temperature $T_{c0}$, which is suppressed in the F/S bilayer to $T_c$. We have found that SOC partially recovers the critical temperature of the bilayer to a new critical temperature $T_{c+}$, with $T_{c0} \geq T_{c+} \geq T_c$. Finally, we have shown that the superconducting order parameter $\psi$ is spatially modulated due to SOC in conjunction with a magnetic exchange field.

### 3.5.1 Possible experiments

To utilise the effects of rotating the magnetisation, a F with an in-plane magnetisation is required. Rashba SOC is naturally present at the S/F interface and can be enhanced by depositing a very thin layer (1-3 nm) of a heavy normal metal in between the S and F [33], as shown in Fig. 3.6. Good candidate materials for SOC/F bilayers are Pt/Co, Pd/Co, Pt/Pt and Pd/Pt, which have high interfacial transparency with Nb [86, 87].

![Figure 3.6: Schematic illustration of a setup for enhancing the interfacial SOC: a thin heavy metal such is inserted between the superconductor and ferromagnet. Materials suggestions are included in the figure.](image)

Using these materials, we discuss two different experiments that would be suitable to observe the effects predicted by our theory. We note that the theory considers an infinitely long strip. For practical purposes, this means that the length of the strip $L_y$ is much longer than the relevant length scales $\xi, \lambda$. A safe estimate is $L_y > 100\xi, 100\lambda$.

The first experiment aims to visualise the vortices. Spontaneous vortex generation and pinning would manifest experimentally as peaks in magnetic field profile at the F edges below $T_c$, see Fig. 3.2d. These could be visualised by magneto-optical techniques such as low temperature magnetic force microscopy [88] or polarised light microscopy [85]. However, magneto-optical techniques also pick up stray fields from out-of-plane domain walls [85]. Measuring through $T_c$ makes it possible to distinguish the two effects, i.e., the stray fields appear at all $T$, whereas the SOC effect only appears below $T_c$.

![Figure 3.7: (a) Schematic illustration of SOC/F strips on a S thin-film. (b) In the case of a magnetisation perpendicular to the strips, a magneto-optical technique would show the vortices as a positive and a negative signal on opposite sides of the strip. (c) When rotating the magnetisation along the strip, this signal should disappear.](image)
Vortex generation and pinning are most prominent when the magnetisation is perpendicular to the F edge, as explained in Section 3.2. The expected SOC effect is sketched in Fig. 3.7b: a positive and negative signal on opposite sides of the strip. Vortex generation diminishes as the magnetisation rotates in-plane and vanishes when the magnetisation is parallel to the F edge. Or equally, when rotating the magnetisation out-of-plane. The magnetisation direction can be changed using an external magnetic field. When the magnetisation points along the strip or out-of-plane, the signal should disappear, as shown in Fig. 3.7c. By inverting the magnetisation direction (i.e., from $x$ to $-x$) the positive and negative signals should switch places.

The second experiment is to study the effect on the critical current. The critical current is measured using a four point setup similar to the one in Fig. 3.8a. This setup is created as follows: first the thin-film S is patterned according to the blue shape. This can be done by either patterning first, depositing second and performing lift-off, or by depositing first, patterning second and etching. The shape does not have to be precise and can be patterned using electron beam lithography or optical lithography. Next, the SOC/F strip is put on top according to the pink rectangle in Fig. 3.8a. Depending on the desired width of the strip, optical lithography is used for wider strips and electron beam lithography for narrower ones (exact numbers depend on the resolution of the equipment used). The lift-off method is recommended for the second step to prevent damage to the underlying S. The structure illustrated in Fig. 3.8a is designed to leave room for misalignment between the first and second round of patterning: if the SOC/F strip is shifted slightly horizontally and/or vertically, the setup is still usable.

The area underneath the SOC/F strip is the weak link in the structure and will be the first area to become resistive, while the rest of the S remains superconducting. This means that the Josephson critical current of this region is being measured. The critical current measurement is illustrated in Fig. 3.8b. Measuring the critical current through the S for different magnetisation directions should give different values.

\[ \begin{align*}
V_+ & \quad V_- \\
I_+ & \quad I_-
\end{align*} \]

(a) schematic illustration of a four point measurement setup to measure the critical current of the SOC/F strip on a S thin-film. (b) A voltage $V$ is applied while the current $I$ is being measured. For voltages $V < V_c$, the structure remains superconducting. At the critical voltage $V_c$, corresponding to the critical current $I_c$, the region under the SOC/F strip becomes resistive and the $I(V)$ exhibits a jump.

A limitation of the model is that it assumes an infinitely long F strip with a uniform, perpendicular magnetisation. The magnetisation in real materials is made up of magnetic domains that result from the competition of different effects, as introduced in Section 2.3.4. Most likely, the shape anisotropy of the F strip will align the magnetisation along the strip, in which case the vortices disappear. In the next chapter, we build onto this model using quasiclassical theory, to study more realistic, finite-size samples.
Chapter 4

The phase diagram of superconductors with spin-orbit coupling

"After all, computers crash, people die, relationships fall apart. The best we can do is breathe and reboot."
— Carrie Bradshaw about computational physics and the Covid-19 pandemic

Strong intrinsic or interfacial spin-orbit coupling (SOC) can enable a thin-film superconductor to exceed the paramagnetic limit. For Rashba-type SOC, we show that the superconducting thermodynamic properties of a finite-size thin film are strongly sample-size dependent due to the creation of edge states; for example, in the case of geometrically anisotropic thin films, the critical field is found to be tunable through the direction of an externally applied in-plane magnetic field. These findings open perspectives for the development of superconducting spin-orbitronic devices.

The results in this chapter are published in

Tunable critical field in Rashba superconductor thin films.

Author contributions: This project was developed as a continuation of the previous chapter. I initiated studying finite samples in the Ginzburg-Landau framework. Initially, I supervised visiting master student Jordi Weggemans to build the model together. We found that the lack of a microscopic description was too limiting and collaborated with Xavier Montiel who suggested the Usadel framework and helped apply this to the system. Building on that, I had the idea to calculate the phase diagrams that now play the central role of this project. Xavier suggested which limits and details to check. Graham Kimbell helped me optimise the numerical method when we were stuck together during the first lockdown in March 2020. Jason Robinson gave overall guidance and advice and helped with the experimental context. The project was supervised by Jason and Xavier.
4.1 Chapter in an image

![Image of phase diagram](image_url)

Figure 4.1: The magnetic field versus temperature phase diagram of a thin-film type II superconductor. The red graph represents the superconductor-to-normal metal transition of an infinite film without spin-orbit coupling (SOC). Adding intrinsic Rashba SOC to the infinite film effectively renormalises the magnetic field, resulting in an upward shift of the transition (green). In a finite $L \times L$ superconductor with SOC (blue), the edges cause singlet-to-triplet conversion which, in turn, induces an out-of-plane spin magnetisation at the edges. This effect suppresses the transition. Decreasing the sample size lowers the transition until it coincides with the red graph in very small samples ($L \sim \xi$). Due to the size-dependence, the transition can be controlled in shape-anisotropic samples by rotating the applied magnetic field direction.

4.2 Phase diagram of type II superconductor thin-films

The original phase diagram for a type II superconductors was postulated by Abrikosov [89] and describes two critical fields $h_{c1}$ and $h_{c2}$. For applied magnetic fields $h < h_{c1}$, the superconductor completely screens the magnetic field (Meissner screening). For fields $h_{c1} < h < h_{c2}$, type II superconductors allow partial flux penetration by forming Abrikosov vortices, i.e., normal core filaments of the order of the penetration depth $\lambda$ with circulating currents around them (see Section 2.1.4).

Abrikosov’s phase diagram is based on Ginzburg-Landau theory, which is a phenomenological model that does not include corrections due to microscopic mechanisms. Generally, in spin-singlet $s$-wave superconductors, an applied field exceeding the upper critical field $h_{c2}$ destroys superconductivity by means of both orbital [83] and Pauli paramagnetic effects [90, 91].

In thin-film superconductors, the orbital contribution is negligible for in-plane magnetic fields [92] and depairing results from aligning spin-singlet pairs with the magnetic field. A Cooper pair breaks when its binding energy is surpassed by the Zeeman splitting energy, as described by the Clogston-Chandrasekhar or Pauli paramagnetic limit [90, 91]. The corresponding critical field $h_p$ is typically higher than the bulk $h_{c2}$, but goes accompanied with a first-order rather than second-order transition from the superconducting to the normal state [93–95].

4.2.1 Second-order transition from self-consistency

We start by analytically calculating a standard phase diagram $h(T)$ for a type II superconductor. We will do this by deriving the self-consistency equation in the presence of an applied in-plane magnetic
field $h$, which gives the relation between $h_{c2}$ and $T_c$. The Hamiltonian of a BCS superconductor with an in-plane field $h$ is

$$H = \begin{bmatrix} \varepsilon_k - h & 0 & 0 & -\Delta \\ 0 & \varepsilon_k + h & \Delta & 0 \\ 0 & \Delta & -\varepsilon_k + h & 0 \\ -\Delta & 0 & 0 & -\varepsilon_k - h \end{bmatrix}$$

where $\varepsilon_k = \frac{h^2}{2m}(k^2 - k^2_F)$ is the single-particle energy, with $h$ the reduced Planck constant, $m$ the electron mass, $k$ the momentum, $k_F$ the Fermi momentum, and $\Delta$ the superconducting energy gap. The Green’s functions are obtained from $G = [i\omega_n \mathbb{1} - H]^{-1}$, with $\omega_n$ the Matsubara frequency. Due to the presence of the magnetic field, the Green’s function becomes spin dependent. The ordinary and anomalous Green’s functions are

$$G_{1\uparrow}(\omega_n, \varepsilon_k) = \frac{i\omega_n + h + \varepsilon_k}{(\omega_n + ih)^2 + \varepsilon_k^2 + \Delta^2}, \quad F_{1\uparrow}(\omega_n, \varepsilon_k) = \frac{\Delta}{(\omega_n + ih)^2 + \varepsilon_k^2 + \Delta^2}.$$  

The general self-consistent gap equation is defined as [41]

$$\Delta = VT \sum_n \int_0^{\infty} F_{1\uparrow}(\omega_n, \varepsilon_k) d\varepsilon_k,$$

where $V$ is the attractive Cooper pair interaction. The integral is evaluated using the Residual Theorem, as shown in Appendix B.1, such that the self-consistency equation becomes

$$\Delta = \pi VT \sum_n \frac{\Delta}{\sqrt{(\omega_n + ih)^2 + \Delta^2}}. \quad (4.1)$$

The kernel is a mathematical object that allows us to study physical properties at the transition. It is obtained by dividing (4.1) by $\Delta$. This is only allowed if $\Delta$ is single-valued, i.e., the phase transition is second-order. The kernel is

$$K(T, \Delta, h) = \pi VT \sum_n \frac{1}{\sqrt{(\omega_n + ih)^2 + \Delta^2}} = 1. \quad (4.2)$$

In the presence of a magnetic field, we define two critical temperatures: $T_{c0} \equiv T_c(0)$ and $T_c \equiv T_c(h)$. At both transitions, the kernel is equal to 1, i.e., $K(T_{c0}, 0, h) = 1$ and $K(T_c, 0, 0) = 1$ and therefore, $K(T_{c0}, 0, 0) = K(T_c, 0, h)$. This relation is evaluated in Appendix B.2 and leads to the self-consistency equation

$$\ln \left(\frac{T_{c0}}{T_c}\right) = 2\pi T_c \sum_n \left(\frac{1}{|\omega_n|} - \frac{1}{|\omega_n + ih|}\right). \quad (4.3)$$

Plotting this equation gives the solid line connecting $T_c$ and $h_{c2}$ in Fig. 4.2. Assuming a second-order phase transition from the superconducting to the normal state (i.e., the gap closes at the transition, $\Delta \to 0$), causes a suppression of $h_{c2}$ at low $T$ [93].

This assumption was made to do the calculation analytically. If we do a numerical calculation of the phase diagram instead (with a first-order transition), we find the familiar phase diagram where $h(T)$ has a maximum at $T = 0$. This effect can be recovered by including the paramagnetic limit.

### 4.2.2 First order paramagnetic limit

The Ginzburg-Landau model does not describe the effect of the magnetic field on the electron spins, which is a reasonable approximation if the field is small. However, for type II superconductor thin-films, the upper critical field $h_{c2}$ becomes significant (see Fig. 4.2) and the effect is no longer negligible.

The Pauli spin susceptibility $\chi$ is a measure of how easy it is to rotate electron spin using a magnetic
The phase diagram of superconductors with spin-orbit coupling

field (see Section 2.3.1 for an introduction). In a normal metal, the spin susceptibility $\chi_N$ is a small finite number. In a superconductor, the existence of Cooper pairs reduces the spin susceptibility, i.e., to polarise an electron spin, one must break a Cooper pair. Therefore, in the ground state at $T = 0$, all electrons form pairs and $\chi_S = 0$.

However, at high magnetic fields, the polarised normal state could have a lower free energy than the superconducting state. This is the case when the polarisation energy (associated with the spin susceptibility) is smaller than the condensation energy (associated with the phase transition from the normal to superconducting state). This happens when

$$\frac{1}{2}(\chi_N - \chi_S)h_p^2 > \frac{h_{c2}^2}{8\pi}.$$  \hspace{1cm} (4.4)

We use that $\chi_S = 0$, $\chi_N = \frac{1}{2}(g\mu_B)^2N(E_F)$ and $h_{c2}^2 = 4\pi N(E_F)\Delta_0^2$, with $g$ the spectroscopic splitting factor of electrons ($g = 2$), $\mu_B$ the Bohr magneton, $N(E_F)$ the density of states at the Fermi level and $\Delta_0$ the gap at $T = 0$ [37]. We find the paramagnetic limit $h_p$ at zero temperature [90, 91]

$$h_p(0) = \frac{\sqrt{7}\Delta_0}{g\mu_B},$$

which is exactly the formation energy of a Cooper pair (i.e., to polarise the superconductor, one must break a Cooper pair). The paramagnetic limit is an increase in the upper critical field ($h_p > h_{c2}$) resulting from spin paramagnetism. Since the magnetic field can penetrate type II superconductors, the paramagnetic effect can be substantial. A superconductor with a high magnetic field is a metastable system and the corresponding transition from the superconducting to the normal state becomes of the first order [93, 94]. The transition in the temperature regime $T_c > T > T^*$ remains second order [95].

![Figure 4.2: Magnetic field vs. temperature phase diagram of a type II superconductor. Solid and dashed lines represent second and first order transitions, respectively. $h_{c1}$ and $h_{c2}$ are the lower and upper critical field and the $h_p$ is the paramagnetic limit. $T_c$ is the critical temperature and $T^*$ the tricritical point. Adapted from [37].](image)
4.3. Spin-orbit coupling

4.2.3 Overcoming the paramagnetic limit

During the past decades, several ways have been explored to overcome \( h_p \). In the Larkin-Ovchinnikov-Fulde-Ferrell (LOFF) state, Cooper pairs acquire a finite momentum and the pair wave function periodically oscillates in space (see Section 2.5.2). This state is stable in the clean limit \([23, 24, 96]\). In spin-triplet superconductors, spin-aligned Cooper pairs are unaffected by paramagnetism \([97–99]\) (see Section 2.5.3). The idea to use SOC to overcome \( h_p \) is not new. Here, we briefly review two methods to do this.

Spin-orbit scattering

Theoretically, the spin susceptibility in superconductors \( \chi_S \) is zero. However, a nonzero Knight shift was found in measurements performed on superconductors at zero temperature \([100, 101]\) which is directly related to \( \chi_S \) \([102]\). This discrepancy between theory and experiments was resolved by including spin-orbit interaction of scattering electrons in the models \([103–105]\). Due to spin-orbit interaction, scattering events can be accompanied by a spin-flip (spin-orbit scattering). This occurs in small superconductors (dimensions smaller than the coherence length) at the boundaries \([103]\) and in dirty superconductors in the form of impurity scattering \([104–109]\). Hence, spin-orbit scattering destroys Cooper pair correlations and \( \chi_S \) becomes a function of the spin flip length \( \ell_{so} \), such that \( \chi_S > 0 \). Considering (4.4), this results in a larger value of \( h_p \).

Spin paramagnetism and spin-orbit scattering have to be taken into account simultaneously to obtain a realistic \( h_{c2} \) that can be compared with experiments. Since spin-orbit scattering weakens the spin pairing, it increases the amount of spin paramagnetism needed to convert the transition from second order to first. Hence, in the presence of strong spin-orbit interaction, the value of \( h_{c2} \) increases and the transition is of second order \([110, 111]\).

Ising superconductivity

More recently, Ising superconductivity has been of great interest. In an Ising superconductor, SOC induces an effective Zeeman-like field that pins the Cooper pair spins out-of-plane, making them insensitive to in-plane applied magnetic fields, such that \( h_{c2} \) is enhanced \([112]\). Ising SOC in conjunction with an applied in-plane magnetic field causes conversion of singlet to equal-spin triplet pairs \([112]\). One specific \( d \)-vector triplet component is coupled to the singlet state. This coupling makes it robust against disorder and controls \( h_{c2} \) \([112, 113]\). Type I Ising superconductivity relies on in-plane inversion symmetry breaking to generate SOC and is most well-understood in noncentrosymmetric transition metal dichalcogenides \([114–119]\), whereas type II Ising superconductivity is a result of spin-momentum locking in two-dimensional materials with multiple degenerate orbitals \([120–122]\).

The above methods to surpass \( h_p \) require exotic materials and/or specific inversion asymmetries. In our work, we predict a similar effect that may be engineered in conventional thin film superconductors with intrinsic or proximity induced Rashba SOC (e.g. by putting a thin heavy metal layer on top).

4.3 Spin-orbit coupling

As seen in Section 2.4.2, Rashba SOC splits the usual quadratic dispersion into two helicity bands with energies \( E_{\pm} = \hbar k^2/2m \pm \alpha |k| \), where \( \alpha \) is the SOC strength and \( k \) the single-particle momentum \([30]\). The spins are polarised tangential to their momentum as illustrated in Fig. 4.3a. For each direction in momentum space, there are two zero-momentum opposite-spin pairs on the Fermi surface. With an in-plane magnetic field \( \mathbf{h} = (h_x, h_y, 0) \), the dispersion becomes \([30]\)

\[
E_{\pm} = \frac{\hbar k^2}{2m} \pm \sqrt{(\alpha k_y + h_x)^2 + (\alpha k_x - h_y)^2}.
\] (4.5)
The Fermi surfaces shift in the direction perpendicular to the magnetic field, producing an intrinsic spatial anisotropy (see Fig. 4.3b). Consequently, the singlet pairs acquire a net momentum and a LOFF-like state forms in the clean limit [123–125]. The critical field experiences a sharp incline at low temperatures, surpassing the paramagnetic limit [80, 124]. In the diffusive regime, the LOFF-like state disappears and a spatially modulated helical state remains [80, 126, 127]. Disordered Rashba superconductors with strong SOC in an in-plane magnetic field thus have an enhanced critical field [80, 126] and critical temperature [128].

\[
\begin{align*}
\text{(a)} & \quad k_y \quad \text{and} \quad h = 0 \\
\text{(b)} & \quad k_y \quad \text{and} \quad h
\end{align*}
\]

**Figure 4.3:** (a) Fermi surface of a Rashba superconductor with spins locked to the momentum, forming two helicity bands \( E_+ \) and \( E_- \). (b) The magnetic field \( \vec{h} = (h_x, 0, 0) \) shifts the helicity bands vertically (the dots represent their new centres). In a magnetic field, the Rashba superconductor has intrinsic spatial anisotropy.

### 4.3.1 The Usadel equations

We investigate superconducting thin-films with in-plane magnetic field \( \vec{h} \) (externally applied or via an induced exchange field). We model superconductivity in the diffusive limit via the Usadel formalism, which is formulated in terms of Green’s functions [129]. The Green’s functions \( \hat{g}(\vec{R}, \omega_n) \) depend on the spatial centre-of-mass coordinate \( \vec{R} \) and the Matsubara frequencies \( \omega_n = (2n + 1)\pi T \) (\( T \) is the temperature and \( n \in \mathbb{Z} \)); in \( 4 \otimes 4 \) spin \( \otimes \) particle-hole space, \( \hat{g}(\vec{R}, \omega_n) \) is expressed as [129]

\[
\hat{g} = \begin{pmatrix} g & f \\ \bar{f} & \bar{g} \end{pmatrix},
\]

(4.6)

where \( g \) and \( f \) are the normal and anomalous Green’s functions, respectively, and \( \bar{g} \) and \( \bar{f} \) are their particle-hole conjugates [129]. By convention, we choose the z-axis as the spin-quantisation axis. We write the single-particle Green’s function \( g \) as

\[
g = g_0 + \tilde{g} \cdot \vec{\sigma} = \begin{pmatrix} g_{\uparrow \uparrow} & g_{\uparrow \downarrow} \\ g_{\downarrow \uparrow} & g_{\downarrow \downarrow} \end{pmatrix} = \begin{pmatrix} g_0 + g^z & g^x - ig^y \\ g^x + ig^y & g_0 - g^z \end{pmatrix},
\]

(4.7)

where \( g_0 \) is the bare Green’s function, \( \tilde{g} = (g_x, g_y, g_z)^T \) is the magnetic contribution and \( \vec{\sigma} \) contains the Pauli spin matrices \( \vec{\sigma} \equiv (\sigma^x, \sigma^y, \sigma^z)^T \). In this notation, the \( g^z \) term is the magnetic (Zeeman) contribution to the system. In-plane magnetic effects are contained in \( g^x \) and \( g^y \).

The anomalous Green’s function \( f \) contains the pair amplitudes \( f_s \) for singlets and \( f_t = (f_t^x, f_t^y, f_t^z)^T \) for triplets and is defined as

\[
f = \begin{pmatrix} f_s + f_t \cdot \vec{\sigma} \end{pmatrix} i\sigma^y = \begin{pmatrix} f_t^x - f_t^y \\ f_t^y - f_t^x \\ f_s \end{pmatrix} f_s + f_t^z + f_s \]

(4.8)

In the diffusive limit, the Green’s functions satisfy the Usadel transport equation [129]

\[
\frac{D}{\pi} \nabla (\hat{g} \nabla \hat{g}) + \left[ i\omega_n \hat{\tau}_z - \hat{\Sigma} \hat{g} \right] = 0.
\]

(4.9)
with the commutation relation $[A,B] = AB - BA$, satisfying the normalisation condition $\hat{\gamma}^2 = -\pi^2 \hat{1}$. Here, $\hat{\sigma}$ and $\hat{\tau}$ are the Pauli matrices in spin and particle-hole space, respectively. $D$ is the diffusion coefficient and $\Sigma$ is the self-energy. The self-energy consists of three contributions $\Sigma = \Sigma^{\text{imp}} + \Sigma^{\text{exx}} + \Delta$ [130]. The term $\Sigma^{\text{imp}}$ is the self-energy produced by spin-flips in the presence of magnetic impurities. We assume there are no impurities and hence $\Sigma^{\text{imp}} = 0$. The second term describes the exchange field from a ferromagnet or applied field and is given by $\hat{\Sigma}^{\text{exx}} = \hat{h} \cdot \hat{\sigma}$. Finally, $\Delta = \Delta_0 \sigma^y$ is the s-wave superconducting order parameter. We substitute (4.6), (4.7) and (4.8) into the Usadel equation (4.9) and focus the upper-right component of the matrix, which describes superconductivity. The transport equation in terms of $f$ and $g$ is

$$\frac{D}{\pi} \nabla (g \nabla f + f \nabla \tilde{g}) + 2i \omega_n f = \tilde{\Delta} \tilde{g} - g \tilde{\Delta} + \tilde{h} \cdot \tilde{\sigma} f - f \tilde{h} \cdot \tilde{\sigma}^*.$$

(4.10)

As $T \to T_c$, $\Delta_0 \to 0$ and we keep only the first order terms in $\Delta_0$. The simplification of (4.9) close to the transition is shown in Appendix B.3. We obtain the equilibrium Usadel equations near $T_c$ [120]

$$\begin{cases}
(D \nabla^2 - 2|\omega_n|) f_s = -2\pi \Delta_0 + 2i \sgn(\omega_n) \tilde{h} \cdot \tilde{f}_t, \\
(D \nabla^2 - 2|\omega_n|) \tilde{f}_t = 2i \sgn(\omega_n) \tilde{h} f_s.
\end{cases}$$

(4.11)

The system is now described by two coupled transport equations: a scalar equation for the singlet pair amplitude $f_s$ and a vector equation for the triplet pair amplitude $\tilde{f}_t$.

### 4.3.2 Spin-orbit coupling in the Usadel equations

SOC gives rise to an effective momentum-dependent exchange field, i.e. the spin-orbit field. In our system, we consider the Rashba spin-orbit field $\vec{\alpha} = \alpha (\vec{s} \times \vec{p}) \cdot \hat{n}$ (see Section 2.4.2), where $\alpha$ is the SOC strength. The spin aligns with the in-plane field, meaning that the spin is in-plane as well and written as $\vec{s} = (s_x, s_y, 0)^T$. The momentum in a thin-film is confined in the in-plane directions, i.e. $\vec{p} = (p_x, p_y, 0)^T$. The axis of broken symmetry is $\hat{n} = \hat{z}$. Hence, the spin-orbit field becomes $\vec{\alpha} = \alpha (s_x p_y - s_y p_x) \hat{z}$. The corresponding spin-orbit field coefficients in spin-space are $A_x = -\alpha \sigma^y$, $A_y = \alpha \sigma^x$ and $A_z = 0$ (see Appendix B.4 for details).

The spin-orbit field in the Usadel equations, we introduce the covariant derivative $\nabla \mapsto \nabla - i [\vec{\alpha}, \cdot]$, where $\nabla$ is the standard derivative, the square brackets represent the commutator and $\vec{\alpha}$ the spin-orbit field matrix [33, 69, 130]. The covariant derivatives of the anomalous Green’s function $\tilde{f}$ are of particular interest. They are derived in Appendix B.4. Introducing the notation $\delta_k \circ \tilde{a} = \partial_k \tilde{a} + 2 A_k \times \tilde{a}$, the first and second covariant derivative of $f$ are, respectively,

$$\partial_k f \mapsto \left[ \partial_k f_s + \left( \delta_k \circ \tilde{f}_t \right) \vec{\sigma} \right] i \sigma^y,$$

(4.12)

$$\partial_k^2 f \mapsto \left[ \partial_k^2 f_s + \left( \delta_k \circ \left( \delta_k \circ \tilde{f}_t \right) \right) \vec{\sigma} \right] i \sigma^y.$$

(4.13)

To include SOC in the Usadel equations (4.11), we replace the standard derivative $\nabla$ by the covariant derivative $\nabla = (\partial_x, \partial_y, \partial_z)$, as shown in Appendix B.5.

Next, the Usadel equations are normalised by the coherence length $\xi = \sqrt{D/2\pi T_{c0}}$, where $T_{c0}$ is the critical temperature of a bare superconductor without SOC (we will see later that the critical temperature becomes modified in the presence of SOC). In a dirty superconductor, $\xi$ depends on disorder, e.g., in Nb, $\xi$ ranges from 10 nm (very dirty) to 40 nm (clean). By normalising with respect to $\xi$, we do not have
to consider the actual values of the quantities. The normalised Usadel equations are

$$\begin{align}  
\partial_x^2 f_x + \partial_y^2 f_x - 2|\tilde{\omega}_n|f_x - 2i \text{ sgn}(\tilde{\omega}_n) \left( \hat{h}_x f_x^x + \hat{h}_y f_x^y \right) &= -\Delta, \\
\partial_x^2 f_t^x + \partial_y^2 f_t^x + 4\alpha \partial_x f_t^x - 4\alpha^2 f_t^x - 2|\tilde{\omega}_n|f_t^x - 2i \text{ sgn}(\tilde{\omega}_n)\hat{h}_x f_x &= 0, \\
\partial_x^2 f_t^y + \partial_y^2 f_t^y + 4\alpha \partial_y f_t^y - 4\alpha^2 f_t^y - 2|\tilde{\omega}_n|f_t^y - 2i \text{ sgn}(\tilde{\omega}_n)\hat{h}_y f_x &= 0, \\
\partial_x^2 f_t^z + \partial_y^2 f_t^z - 4\alpha \left[ \partial_x f_t^x + \partial_y f_t^y \right] - 8\alpha^2 f_t^z - 2|\tilde{\omega}_n|f_t^z &= 0, 
\end{align}$$

(4.14)

with normalised quantities $\tilde{x} = x/\xi$, $\tilde{y} = y/\xi$, $\alpha = \alpha \xi$, $\tilde{\omega}_n = (2n + 1)T/2T_c$, $\tilde{h}_{x,y} = h_{x,y}/2\pi T_c$ and $\tilde{\Delta} = \Delta_0/T_c$.

### 4.4 Numerical method

There are two ways to calculate the $(h, T)$ phase diagram: we could either fix $h$ and compute $T_c$ (horizontal) or fix $T$ and compute $h_c$ (vertical), see Fig. 4.4. Some values of $h$ have two values of $T_c$, and $h$ becomes very flat around $T/T_{c0} \sim 0.6$, which make the computation numerically demanding. Therefore, it is easier to fix $T$ and find the corresponding $h_c$. This does result in everything being normalised by $T_{c0}$.

![Figure 4.4](image)

**Figure 4.4:** Two ways to calculate the $(h, T)$ phase diagram.

1. **Parameters.** We define the parameters of the system: the dimensions $L_x$ and $L_y$ (normalised by the coherence length), the spin-orbit coupling strength $\alpha$ and the angle $\theta$ between the spin-orbit coupling and the magnetisation.

2. **The grid.** We discretise two-dimensional real space with coordinates $(x, y)$ onto a grid by defining indices $i$ and $j$ corresponding to the $x$- and $y$-coordinate, respectively. Hence, the function $f(x, y)$ maps to the gridpoint $f_{i,j}$. We define the number of desired gridpoints in the system in the $x$- and $y$-direction as $N_x$ and $N_y$, respectively, such that we obtain a $N_x \times N_y$ grid. The calculation works with a ghost cell for the boundary conditions on either side of the grid. Hence, the number of internal points is $(N_x - 2)(N_y - 2)$. The grid is illustrated in Fig. 4.5.
3. Discretisation. To discretise the derivatives in the Usadel equations (4.14) and boundary conditions (4.19) we use a central difference scheme. The discretised derivatives of $f(x,y)$ on the two-dimensional grid are defined as

$$\frac{\partial f}{\partial x}_{i,j} = \frac{f_{i-1,j} - f_{i+1,j}}{2d_x}, \quad \frac{\partial f}{\partial y}_{i,j} = \frac{f_{i,j-1} - f_{i,j+1}}{2d_y},$$

$$\frac{\partial^2 f}{\partial x^2}_{i,j} = \frac{f_{i-1,j} - 2f_{i,j} + f_{i+1,j}}{d_x^2}, \quad \frac{\partial^2 f}{\partial y^2}_{i,j} = \frac{f_{i,j-1} - 2f_{i,j} + f_{i,j+1}}{d_y^2}.$$

We apply this to the Usadel equations on the $(N_x - 2) \times (N_y - 2)$ interior points. The boundary conditions contain the first derivatives, which require the use of ghost cells. The discretised Usadel equations and corresponding boundary conditions are stored in an $N_x \times N_y$ matrix.

4. Vectorisation. Vectorisation is the process of transforming the 2D grid into 1D vector, which can be solved numerically more easily. Essentially, the columns of the grid are stuck underneath each other into one long vector. Rather than working with two indices $i$ and $j$, we now define the vector index $k$. The gridpoint $f_{i,j}$ is mapped onto the vector element $f_k$ via $k = (i - 1)N_y + j$.

In the case of the Usadel equations, we have to take this one step further since we are dealing with a nested vector of four of $f_{i,j}$'s. We transform the nested vector $\vec{f} = [f_s(x,y), f_t(x,y)] \in \mathbb{C}^2 \times \mathbb{C}^2 \times \mathbb{C}^2 \times \mathbb{C}^2$ into one long vector $\vec{f} = (f_s, f_t^x, f_t^y, f_t^z)^T \in \mathbb{C}$ by defining the transformation

$$k = l(N_xN_y) + (i - 1)N_y + j,$$

where $l \in \{0, 1, 2, 3\}$ corresponds to $f_s, f_t^x, f_t^y$ and $f_t^z$, respectively. We now have a linear equation $A\vec{f} = \vec{b}$, where $A$ is a $4N_xN_y \times 4N_xN_y$ matrix and $\vec{f}$ and $\vec{b}$ are $4N_xN_y \times 1$ vectors. The matrix $A$ contains the coefficients originating from the Usadel equations and boundary conditions. The vector $\vec{b}$ describes the right hand side of the Usadel equation and $\vec{f}$ contains the singlet and triplet pair amplitudes. The corner points in the ghost cell have to be equal to zero. If we do not give them any conditions, the matrix $A$ becomes singular. Hence, we simply set a 1 on the diagonal of $A$ and a 0 on the corresponding spots in $\vec{b}$.
5. **Solving the linear system.** The linear equation \( A\hat{f} = \hat{b} \) can be solved using any linear solver. We use the Matlab backslash operator \( \hat{f} = A \backslash \hat{b} \), which is a solver that first tests whether the matrix satisfies certain properties (e.g. triangular, Hermitian, Cholesky) and utilises these properties to solve the equation more efficiently [131]. To reduce the computation time further, we store the matrices and vectors as sparse matrices, which reduces the computation order from \( O(n^2) \) to \( O(n) \).

6. **Matsubara frequencies.** The above is all for one Matsubara frequency, whereas the self-consistency equation (4.18) contains an infinite sum of \( f_x \) over the Matsubara frequencies. For the purpose of the numerical calculation, we have to introduce a cut-off to this sum. We recall that the normalised Matsubara frequency that we use here is \( \omega_n = (2n + 1)T/2T_c \). Hence, at lower temperatures, the frequencies are closer together, which requires us to include more frequencies. To test this, we fixed \( T/T_{c0} = 0.05 \) and computed \( h_c \) for different cut-offs. Comparing 10 and 20 frequencies results in a 10% divergence in \( h_c \). Comparing 20 and 40 frequencies gives the same \( h_c \) up to five decimals. To include sufficient frequencies (but not a redundant amount that slows the calculation down), we scale the cut-off linearly with temperature as 

\[
\text{cut-off} = \text{round} \left( -\frac{10T}{T_c} + 20 \right).
\]

When \( T \to 0 \), the number of frequencies required diverges, therefore, we use a fixed cut-off of 100 for \( T < 0.17T_c \). We repeat steps 3-5 for the Matsubara frequencies ranging from 0 to the cut-off. Note that we have already used in the self-consistency equation that the sum is even in \( x \), i.e., \( \sum_{n=-\infty}^{\infty} = 2 \sum_{n=0}^{\infty} \).

7. **Self-consistency equation.** We started the calculation by using an initial value for the kernel \( \Delta_0 = 1 \) everywhere on the grid. After going through steps 3-6, we use the self-consistency equation (4.18) to obtain a new set of values \( \Delta_i \) for all \( i \). We repeat the whole process iteratively 10 times to find \( \Delta_{10} \) for all \( i \). For the phase diagram, we are not interested in the spatial dependence and we only store the maximum value, i.e., \( \Delta_{10} = \max_{i,j} \Delta_{10} \).

8. **Finding \( h_c \).** The above calculation gives the value of \( \Delta_{10} \) for one value of \( h \) and one \( T_c \). For \( h > h_c \), we expect the kernel to diverge, for \( h < h_c \) the kernel falls to 0, and at \( h = h_c \) it is stable at 1. We repeat steps 3-7 to find the value of \( h \) for which \( \Delta_{10} = 1 \) using Brent’s method of root finding [132]. Within our tolerance, this is the field where the kernel neither diverges nor falls to zero. We call this the critical field \( h_c \).

9. **Phase diagram.** The above process yields \( h_c \) corresponding to one fixed value of temperature \( T/T_{c0} \). We then repeat the full calculation 3-8 for the temperature range \( T/T_{c0} \in [0, 1] \) to obtain the full \((h, T)\) phase diagram.

10. **Pair amplitudes.** Once the optimal value for \( h_c \) has been found, the corresponding solution of the system (step 5) gives the pair amplitudes \( f_x, f_x^+, f_y^+ \) and \( f_y^+ \) at the transition. These can be used to calculate properties of the superconducting film, such as the spin magnetisation.

### 4.5 Phase diagrams

In this section, we will study superconducting thin-films in the \( xy \)-plane with thickness \( d \) smaller than the superconducting coherence length, i.e., \( d \leq \xi \). We assume that the superconductivity is uniform in \( z \), such that the Green’s functions only depend on the \( x \) and \( y \) coordinates, i.e., \( \tilde{G}(\vec{R}, \omega_n) = \tilde{g}(x, y, \omega_n) \). We map out the \((h, T)\) phase diagram for an in-plane field similar to Fig. 4.2 and study the effect of Rashba SOC on this diagram.
4.5. Phase diagrams

4.5.1 Infinite films

Figure 4.6: Schematic illustration of a thin-film superconductor with thickness $d$ and out-of-plane spin-orbit coupling field $\vec{\alpha}$ in an externally applied in-plane magnetic field $\vec{h} = (h_x, h_y, 0) = (|\vec{h}| \cos \theta, |\vec{h}| \sin \theta, 0)$.

We start with infinite thin-films in $(x, y)$. The system is shown in Fig. 4.6. Superconductivity is homogeneous, such that $f$ is constant and its derivatives are zero. Since we consider a thin film, we also set $f_z = 0$. The Usadel equations (4.14) become

\[
\begin{aligned}
-2|\tilde{\omega}_n| f_s - 2i \text{sgn}(\tilde{\omega}_n) \left( \tilde{h}_x f_x^s + \tilde{h}_y f_y^s \right) &= -\Delta, \\
-4\tilde{\alpha}^2 f_t^x - 2|\tilde{\omega}_n| f_t^x - 2i \text{sgn}(\tilde{\omega}_n) \tilde{h}_x f_s &= 0, \\
-4\tilde{\alpha}^2 f_t^y - 2|\tilde{\omega}_n| f_t^y - 2i \text{sgn}(\tilde{\omega}_n) \tilde{h}_y f_s &= 0.
\end{aligned}
\]  

(4.16)

From the bottom two equations, we obtain expressions for $f_t^x$ and $f_t^y$ in terms of $f_s$, which are substituted in the top equation (details in Appendix B.6), which gives

\[
f_s = \frac{1}{2} \frac{\tilde{\Delta}}{|\tilde{\omega}_n| + \frac{|\tilde{h}|^2}{2\tilde{\alpha}^2 + |\tilde{\omega}_n|}}.
\]  

(4.17)

We note that (4.17) only depends on $|\tilde{h}|$ and no longer on $\tilde{h}_x$ and $\tilde{h}_y$, meaning that the infinite film is isotropic. Furthermore, upon increasing $\tilde{\alpha}$, the effective $\tilde{h}$ decreases, i.e., $\tilde{\alpha}$ renormalises the magnetic field. At zero magnetic field, SOC does not affect $T_c$, showing that SOC does not affect the superconductivity, but screens the applied magnetic field. A similar screening effect is observed in the presence of spin-orbit scattering in disordered superconductors [105, 107], as discussed in Section 4.2.3. We note that this only applies since SOC in our model is weak ($\tilde{\alpha} \ll 1$). Therefore, we do not take the modulated order parameter into account, which is valid for strong SOC [80, 126, 128].

We use $f_s$ in (4.17) to derive a self-consistency equation, similar to Section 4.2.1. The normalised self-consistency equation is

\[
\tilde{\Delta} \ln \left( \frac{T_{c0}}{T_c} \right) = \frac{2T_c}{T_{c0}} \sum_{n=0}^{\infty} \left( \frac{\tilde{\Delta}}{2\tilde{\omega}_n} - f_s(\tilde{\omega}_n) \right).
\]  

(4.18)

We solve (4.18) analytically in Appendix B.6 to map the phase diagram in Fig. 4.7a. SOC increases the critical field, as shown at zero temperature in Fig. 4.7b. The magnitude of $\Delta T_c$ at finite magnetic field, seen in Fig. 4.7c, is similar to the temperature recovery predicted in superconductor/ferromagnet bilayers [133] (we will return to this point in the next chapter). We note that the largest change in $h_{c2}$ is two orders of magnitude higher than the change in $T_c$, implying that the effect of SOC on magnetic field is more easily observable.
The phase diagram of superconductors with spin-orbit coupling

\[ T = T_c(\alpha = 0) \]

\[ \alpha = 0 \]

\[ \alpha = 0.5 \]

\[ \alpha = 1 \]

\[ \alpha = 2 \]

\[ \alpha = 3 \]

\[ \Delta_0/2 \]

\[ \Delta_0/\sqrt{2} \]

\[ \Delta_0/2 \]

\[ T \]

\[ T^* \]

\[ h \]

\[ h_{c0} \]

\[ \Delta h_{c0} \]

\[ \Delta T_c \]

**Figure 4.7:** Properties of an infinite thin-film Rashba superconductor. (a) Phase diagram for different values of Rashba spin-orbit coupling strength \( \alpha \). Solid lines are second-order self-consistent transitions, meaning that the order parameter vanishes at \( \Delta(T = T_c) = 0 \). The dashed line is the first-order paramagnetic limit at \( \alpha = 0 \). Both phase transition lines meet at the tricritical point at \( T = T^* \). For \( T < T^* \), the second order phase transition defines the supercooling magnetic field. (b) The increase in critical field at zero temperature \( \Delta h_{c0} = |h_{c0}(\alpha) - h_{c0}(\alpha = 0)|/T_{c0} \) with \( \alpha \). (c) The increase in critical temperature \( \Delta T_c = |T_c(\alpha) - T_c(\alpha = 0)|/T_{c0} \) with \( \alpha \), for fixed applied field \( h/T_{c0} = 0.5 \).

### 4.5.2 Finite films

While the SOC screens the magnetic field in infinite thin-films, an additional effect appears at the edge of finite samples. Edge states with distinct physical properties from the infinite film superconductors may appear similar to topological superconductors [134, 135].

**Figure 4.8:** Geometrically constrained \( L \times L \) thin-film superconductor with thickness \( d \) and out-of-plane spin-orbit coupling field \( \vec{a} \) in an applied magnetic field \( \vec{h} = (h_x, 0, 0) \).

We now consider a finite square superconductor thin-film located at \([0, L] \times [0, L] \), where \( L \) is in units of \( \xi \), see Fig. 4.8. Having a finite film implies we have to impose boundary conditions. We assume the spin current cannot leave the sample, meaning that its component perpendicular to the edges is zero [69, 135]. Since the spin current is proportional to the covariant derivative \( j_{x,y} = \partial_{x,y} \), the latter is also zero at the edges \( \partial_x = 0 \) at \( x = 0, L \) and \( \partial_y = 0 \) at \( y = 0, L \). Following the steps in Appendix B.7,
we obtain the boundary conditions

\[
\begin{align*}
\text{at } x = 0, L : & \quad \partial_x f_x = 0, \\
& \quad \partial_x f^x + 2\tilde{\alpha} f^z = 0, \\
& \quad \partial_x f^y = 0, \\
& \quad \partial_x f^z - 2\tilde{\alpha} f^x = 0; \\
\text{at } y = 0, L : & \quad \partial_y f_y = 0, \\
& \quad \partial_y f^y + 2\tilde{\alpha} f^z = 0, \\
& \quad \partial_y f^z - 2\tilde{\alpha} f^x = 0.
\end{align*}
\] (4.19)

Using these boundary conditions, we calculate the phase diagram iteratively, starting from the analytical infinite film solution as an Ansatz. The numerical method is described in Section 4.4. The numerical phase diagram for a \( L \times L \) superconductor is shown in Fig. 4.9a. Since \( L \) is in units of \( \xi \), \( L = 20 \) converges to the analytical infinite film solution. Decreasing \( L \) reduces \( h_{c2} \) compared to the corresponding infinite film value.

The presence of triplet correlations \( \tilde{f}_t \) induces a spin magnetisation in the superconducting film defined as [26]

\[
\tilde{M}(x, y) = (M_x, M_y, M_z) = M_0 \frac{T_c}{T_{c0}} \sum f_x \tilde{f}_t,
\] (4.20)

with \( M_0 = 2N(E_F)\mu_{\text{eff}}k_B T_{c0} \), where \( N(E_F) \) is the density of states at the Fermi level, \( \mu_{\text{eff}} \) is the effective quasiparticle magnetic moment and \( k_B \) is the Boltzmann constant [26] and the summation is over the Matsubara frequencies.

It follows from the boundary conditions (4.19) that the in-plane triplet correlations \( f^x_t \) and \( f^y_t \) couple to the out-of-plane triplet \( f^z_t \) at the edges. Under an applied field \( \vec{h} = (h, 0, 0) \), this results in an out-of-plane magnetisation \( M_z \) at the edges transverse to \( \vec{h} \) [135]. The resulting magnetisation profile is positive on one side of the sample, zero in the middle and negative on the other side [135], as shown in Fig. 4.9b-c. The magnetisation acquires this profile in the field direction (along \( x \)), whilst remaining nearly constant in the perpendicular direction (along \( y \)). For small \( L \), a magnetisation gradient spans the whole sample. Upon increasing \( L \), the magnetisation becomes concentrated at the edges. A similar effect is seen when increasing \( \alpha \). The profile resembles that of the spin-orbit induced local magnetic field in a superconductor/ferromagnet bilayer (see Fig. 3.2d) and could therefore lead to the formation of vortices [133].

In very small samples (\( L \sim \xi \))" the boundary conditions (4.19) dominate the sample properties. This means that the covariant derivative is zero everywhere and the Usadel equations (4.14) simplify to

\[
\begin{align*}
-2|\tilde{\omega}_n| f_s - 2i \text{ sgn}(\tilde{\omega}_n)\tilde{h}_x f^x &= -\Delta, \\
-2|\tilde{\omega}_n| f^y - 2i \text{ sgn}(\tilde{\omega}_n)\tilde{h}_x f^z &= 0,
\end{align*}
\] (4.21)

and \( f^y = f^z = 0 \). We recover the equations (4.11) for an infinite film in the absence of SOC, as seen in Fig. 4.9a. We thus conclude that the SOC gives rise to two competing effects: the infinite film screening effect (increasing \( h_{c2} \)) and the edge effect (suppressing \( h_{c2} \)).

The critical field at zero temperature \( h_{c0} \) and magnetisation \( M_z \) are shown as a function of \( L \) for different values of \( \alpha \) in Fig. 4.9d-e. We first look at \( h_{c0} \). For \( L \sim \xi \), the edge effect dominates and \( h_{c0} \) rapidly increase with \( L \) until it saturates. The dependence of \( M_z \) on \( L \) and \( \alpha \) is more complicated and is the result of an optimisation of different competing effects. For small \( \alpha \) (\( \alpha = 0.5 \)), the triplet effect is not very strong so \( M_z \) is small. \( M_z \) gradually increases with increasing \( L \), similar to \( h_{c0} \). For strong \( \alpha \) but small \( L \), everything is dominated by the sample edges; the triplet correlations at the edges interfere and \( M_z \) is strong. The interference disappears when \( L \) increases and \( M_z \) gradually drops off to a lower value.

*We consider films with lateral dimensions down to \( L \sim \xi \), while the thickness is \( d \sim \xi \). We expect all modifications to the superconducting order to take place in-plane, since there is no inhomogeneity in the system along \( z \). This is valid when neglecting orbital effects and proximity effects.
The phase diagram of superconductors with spin-orbit coupling

The remaining $M_z$ in the film when $L$ is large can be interpreted as a residual magnetisation in the film. We note that this residual magnetisation is not present in infinite films (in which $M_z = 0$). However, the residual magnetisation no longer affects the thermodynamic properties which become similar to the infinite film (see Fig. 4.9a).

### 4.5.3 Geometric anisotropy

To investigate further the edge effect, we calculate the phase diagram of a rectangular superconductor with $L_x > L_y$. The shape anisotropy introduces an in-plane angle $\theta$ between $\vec{h}$ and the $x$-axis (see Fig. 4.3a). When $\vec{h}$ points along the larger dimension ($\theta = 0$), the edge magnetisation $M_z$ is concentrated along the shorter dimension (see Fig. 4.10b). It covers only a small part of the sample resulting in a slight suppression of $h_{c2}$. Upon rotating $\theta$, $M_z$ becomes more widely distributed over the sample, resulting in further suppression of $h_{c2}$. Finally, when $\vec{h}$ is along the short dimension ($\theta = \pi/2$), $M_z$ affects most of the film and $h_{c2}$ reaches a minimum, approaching again the infinite film in the absence of SOC (see Fig. 4.10a). This shows that, in a shape-anisotropic sample, $h_{c2}$ is controllable by changing the applied field direction.

The quantitative effect of the field direction on a superconductor with constant $L_x$ and increasing $L_y$ is shown in Fig. 4.10c. When the field is along $L_x$ ($\theta = 0$), $h_{c0}$ is nearly constant, except for a slight decrease for small $L_y$ corresponding to the overall size suppression. The $\theta = 0$ and $\theta = \pm \pi/2$ graphs intersect for $L_x = L_y$. Upon increasing $L_y > L_x$, the $\theta = \pm \pi/2$ direction becomes favourable (because it’s favourable to align the field along the longer direction, which is now the $y$-direction). In this regime, the difference between the angles is less severe, since the size suppression is small.

### The one-dimensional limit

In narrow superconducting strips with $L_x \gg L_y$, the system becomes effectively one-dimensional. We consider a shape-anisotropic sample with $L_x \gg L_y$. The length $L_x$ can be considered infinite, such that the superconductivity in the $x$-direction can be considered constant, the derivatives vanish and the

---

**Figure 4.9:** The effect of finite size. (a) Phase diagram of a $L \times L$ superconductor with $\alpha = 2$ (coloured), along with the analytical infinite film solutions for $\alpha = 2$ (black) and $\alpha = 0$ (grey). (b) The profile of the induced out-of-plane spin magnetisation $M_z$ in the field direction (along $x$) in the middle of the sample ($y = L/2$), for fixed $\alpha = 2$ and different values of $L$. (c) The same profile for fixed $L = 10$ and different values of $\alpha$. (d) The critical field at zero temperature $h_{c0}$ and (e) the maximum of $M_z$ as a function of $L$, for different values of $\alpha$. 

---

**Notes:**

- The shape anisotropy introduces an in-plane angle $\theta$ between the angles.
- The critical field at zero temperature $h_{c0}$ and the maximum of $M_z$ as a function of $L$, for different values of $\alpha$.
- The remaining $M_z$ in the film when $L$ is large can be interpreted as a residual magnetisation in the film.
boundary conditions for \( x = 0, L_x \) in (4.19) no longer hold. The Usadel equations (4.14) reduce to

\[
\begin{align*}
\partial_y^2 f_s - 2 |\tilde{\omega}_n| f_s - 2i \text{sgn}(\tilde{\omega}_n) \left( \tilde{h}_x f_t^x + \tilde{h}_y f_t^y \right) &= -\tilde{\Delta}, \\
\partial_y^2 f_t^x - 4(\tilde{\alpha}^2 + 2|\tilde{\omega}_n|) f_t^x - 2i \text{sgn}(\tilde{\omega}_n) \tilde{h}_x f_s &= 0, \\
\partial_y^2 f_t^y + 4\tilde{\alpha} \partial_y f_t^x - 4(\tilde{\alpha}^2 + 2|\tilde{\omega}_n|) f_t^y - 2i \text{sgn}(\tilde{\omega}_n) \tilde{h}_y f_s &= 0, \\
\partial_y^2 f_t^z - 4\tilde{\alpha} \partial_y f_t^z - (8\tilde{\alpha}^2 + 2|\tilde{\omega}_n|) f_t^z &= 0.
\end{align*}
\]

This limit is shown in Fig. 4.10d. When the field is along the infinite direction, \( h_{c0} \) equals the infinite film limit, which confirms that any suppression of \( h_{c0} \) (compared to the infinite film) is a result of finite size. This implies that, experimentally, the effect of SOC can be turned on and off in a narrow strip by rotating the in-plane field. Since our calculation is in the diffusive limit (i.e., mean free path \( \lambda \ll \xi \)), we expect our results to be valid when \( L, L_x, L_y \gg \xi \).

Subsequently, we consider this limiting case \( L_x \gg L_y \) and \( L_y \sim \xi \), such that the boundary conditions for \( y \) are valid everywhere (the covariant derivative vanishes everywhere). The resulting Usadel equations are

\[
\begin{align*}
-2|\tilde{\omega}_n| f_s - 2i \text{sgn}(\tilde{\omega}_n) \left( \tilde{h}_x f_t^x + \tilde{h}_y f_t^y \right) &= -\tilde{\Delta}, \\
-4(\tilde{\alpha}^2 + 2|\tilde{\omega}_n|) f_t^x - 2i \text{sgn}(\tilde{\omega}_n) \tilde{h}_x f_s &= 0, \\
-2|\tilde{\omega}_n| f_t^y - 2i \text{sgn}(\tilde{\omega}_n) \tilde{h}_y f_s &= 0,
\end{align*}
\]

and \( f_t^z = 0 \). If \( \tilde{h} \parallel \hat{y} (h_x = 0) \), it follows that \( f_t^z = 0 \) and we find the same equations as those without SOC in (4.11). This means that the effect of the SOC is not observable and \( h_c \) remains the same. This can be interpreted as the sample being so small in the \( y \)-direction, that there is “no physical space” for a modulation in this direction. However, if \( \tilde{h} \parallel \hat{x} (h_y = 0) \), the SOC effect is recovered and \( h_c \) is enhanced.
4.6 Conclusions & Outlook

We have shown that the paramagnetic limit $h_p$ of a thin-film superconductor is enhanced by Rashba SOC and that tunable superconductivity is achieved using three parameters: the SOC strength, the sample geometry and the applied field direction. In shape anisotropic samples, the critical field is changed by rotating the magnetic field for the entire temperature range up to $T_c$. The ability to control superconductivity using SOC opens possibilities for new superconducting spin-orbitronics devices.

4.6.1 Possible experiments

A possible experimental setup is a $s$-wave superconducting thin-film/heavy metal bilayer (with a bilayer thickness within $\xi$). The S should have low, intrinsic spin-orbit scattering to study spin-dependent properties [109]. Commonly used materials are Al/Pt [108, 109] and Nb/Pt [136, 137].

To study the infinite thin-film Rashba superconductor (as in Fig. 4.7), one can perform a van der Pauw measurement [138]. This involves growing the superconductor/heavy metal bilayer on a square isolating substrate and putting contacts at the four corners, as illustrated in Fig. 4.11.

![Figure 4.11: Schematic illustration of a van der Pauw setup to measure the phase diagram of an infinite thin-film Rashba superconductor in an applied magnetic field $h$.](image)

To study the finite size case and the effect of anisotropy on the phase diagram (as in Fig. 4.10), one would use electron beam lithography* to pattern a structure similar to the one shown in Fig. 4.12a and perform a four point resistivity measurement. The four squares are the contacts and the narrow rectangle in the middle is the rectangular finite-size sample. The narrow rectangle is the weakest link and will be the first part of the structure that becomes resistive, while the contacts and leads remain superconducting. Hence, the resistance of the rectangle is being measured in this setup.

In both the infinite and finite case, two types of measurements are possible, which correspond to the two ways of numerically calculating a phase diagram, indicated in Fig. 4.4. By measuring resistance versus temperature in a constant in-plane applied field, one obtains $T_c$. This is done for a range of applied fields to obtain the entire phase diagram. By measuring resistance versus field at a fixed temperature, one obtains $h_c$. This is done for a range of temperatures to obtain the entire phase diagram. Additionally, in the finite size case, the field can be rotated in-plane to study the anisotropy effect. Which of the two methods is preferable depends on the instruments used, e.g., it can be challenging to obtain good temperature stability at very low temperatures, whereas the applied field is stable. In this case, one would fix the field and sweep the temperature.

The model discussed in this chapter can be extended to heterostructures with ferromagnets (e.g. Nb/Pt/Co as suggested in Section 3.5.1) in which $h_{c2}$ is controlled by the ferromagnetic exchange field. To do this, one would use the setup sketched in Fig. 4.12b. An extra electron beam lithography step is required to grow a heavy metal/ferromagnet bilayer rectangle on top of the existing structure. The rectangle where all three layers overlap is the weakest link and this is the finite-size rectangle that is being measured. Note that the heavy metal/ferromagnet bilayer is purposefully drawn longer than it has to be. This is done to allow for slight misalignment between the two lithography steps. The field magnitude is fixed by the exchange field and it is not possible to obtain the entire phase diagram using

*Section 3.5.1 describes the lithography process in more detail.
this setup. However, it is possible to observe the anisotropy effect by rotating the magnetisation direction using an external magnetic field.

Another possibility is to control the SOC within a single sample, the superconductor can be coupled to a two-dimensional chalcogenide in which the SOC is tuned by gating [139, 140].

![Diagram of four point measurement setup](image)

**Figure 4.12:** (a) Schematic illustration of a four point measurement setup to measure the resistance of the narrow rectangle in the middle. This configuration requires an in-plane applied field \( h \). (b) Alternative setup where a ferromagnet replaces the applied field.
Chapter 5

Comparison between models for superconductors with spin-orbit coupling

“If you change the way you look at things, the things you look at change.”
— Wayne Dyer

The previous two chapters both model superconductors with spin-orbit coupling (SOC). This chapter briefly outlines the differences and similarities between the two models.

In Chapter 3, published in [133], we consider a ferromagnetic strip on an infinite superconducting film with interfacial Rashba SOC. The system is modelled using phenomenological Ginzburg-Landau (GL) theory. When we attempted to realise this setup experimentally, we noticed a flaw in the model. Due to the shape anisotropy of the ferromagnetic strip, the magnetisation aligns along the strip, whereas the theory requires a perpendicular magnetisation. The model still holds for sufficiently long strips, as experimentally realised in Vlaskov-Vlasov et al [85], but it was this realisation that motivated us to look into finite-size systems.

Initially, visiting student Jordi Weggemans and I extended the GL model to a finite-size superconductor. We found that the GL model was limited. It describes the superconducting order parameter phenomenologically and cannot take microscopic mechanisms, such as the co-existence of singlet and triplet superconductivity, into account. With the help of Xavier Montiel, we switched to quasiclassical theory (the Usadel equations) and replaced the ferromagnet by an external magnetic field to generalise our results to the magnetic field vs. temperature phase diagram. This formed the foundation of Chapter 4, published in [141].

In the following, we will refer to Chapter 3 as the GL model and to Chapter 4 as the quasiclassical model.
5.1 Chapter in an image

Figure 5.1: The two models side by side. Both models contain Rashba spin-orbit coupling (SOC) $\alpha$ and consider the critical temperature $T_c(h, \alpha)$ in the presence of both a magnetic field and SOC. (a) The GL model describes a ferromagnet with magnetisation along $\hat{x}$ on top of a thin-film superconductor. The vector $\vec{\alpha}$ implicitly contains the exchange field $h_{ex}$ and phenomenologically describes the interaction between the SOC and the exchange field, which points along $\hat{y}$. The critical temperature recovery compares $T_c(h, \alpha)$ to the case without SOC, $T_c(h, 0)$. The field (here, the magnetisation) is always present. (b) The quasiclassical model describes a thin-film superconductor in an external in-plane magnetic field $\vec{h}$. The Rashba SOC is the effective spin-orbit field along $\hat{z}$ which explicitly takes the microscopic interaction with $\vec{h}$ into account. The critical temperature increase compares $T_c(h, \alpha)$ to the system in the absence of a field, $T_c(0, \alpha)$. The SOC is always present.

5.2 Definitions

Before comparing the two models, we note a couple of differences. In the quasiclassical model, we consider the anomalous Green’s function $f = (f_s + \vec{f}_i \times \vec{\sigma})i\vec{\sigma}\gamma$, which contains both the singlets and triplets. The GL model works with the order parameter $\psi$, which only takes singlets into account.

The treatment of the SOC $\vec{\alpha}$ in the two models is different. Both models describe the same Rashba SOC given by

$$\vec{\alpha} = \alpha(\vec{s} \times \vec{p}) \cdot \hat{n},$$

with $\vec{s}$ the spin, $\vec{p}$ the momentum and $\hat{n}$ the axis of broken symmetry.

In the GL model, the exchange field $h_{ex}$ is contained in $\alpha$, such that $\vec{\alpha}$ effectively describes the interaction between the SOC and $\vec{h}$. Equation (5.1) is not implemented in the model directly. Instead, it is used to argue that the combination of SOC and the exchange field makes the momentum along the $\vec{s} \times \hat{n}$ direction most favourable. Based on this, we use the phenomenological expression $\vec{\alpha} = \alpha \vec{g}$.

In the quasiclassical model, we use that $\vec{s}$ and $\vec{p}$ are both in-plane, in the case of $\vec{s}$ because the magnetic field is in-plane and in the case of $\vec{p}$ because we consider a thin film. We write $\vec{s} = (h_x, h_y, 0)^T$ and $\vec{p} = (p_x, p_y, 0)^T$, and use definition (5.1) directly. The SOC becomes $\vec{\alpha} = \alpha(h_x p_y - h_y p_x) \hat{z}$. In the quasiclassical model, $\vec{\alpha}$ and $\vec{h}$ are considered separately.

The way $\vec{\alpha}$ and $\vec{h}$ are incorporated in the models results in a different definition of the critical temperature, making a direct comparison between the two models impossible.

To qualitatively compare the different critical temperatures, we introduce the notation $T_c(h, \alpha)$ for the critical temperature in the presence of a field $\vec{h}$ and SOC strength $\alpha$. In the presence of $\vec{h}$ (but absence of SOC), the critical temperature is suppressed, i.e. $T_c(h, 0) < T_c(0, 0)$. Using our GL model, we have shown a recovery of $T_c(h, 0)$ in the presence of SOC, given by

$$T_c(h, \alpha) = T_c(h, 0) \left(1 + \frac{\alpha^2}{4ma_0}\right),$$

(5.2)
such that $T_c(h, 0) < T_c(h, \alpha) < T_c(0, 0)$. In the quasiclassical model, we compare the ratio between the critical temperatures in the presence and absence of a magnetic field, i.e. $T_c(h, \alpha)/T_c(0, 0)$. This ratio always lies between 0 and 1.

On top of that, the GL model relies on a linearisation, which makes it valid for $T \lesssim T_c(h, 0)$ and $\alpha$ small, whereas we consider the full temperature range using the quasiclassical model.

### 5.3 Angular dependency of $T_c$ in the GL model

The GL model shows the $T_c$ recovery in the presence of SOC. The quasiclassical model shows the enhancement of the magnetic field vs. temperature phase diagram. To show the agreement between the two models, we make a qualitative comparison of the angle dependency of $T_c(h, \alpha)$ in the two models.

We start from the GL model for a superconducting thin film with an infinitely long ferromagnetic strip with width $L_x$, an in-plane exchange field $h_{ex}$ perpendicular to the strip edge and SOC $\vec{\alpha}$ along the strip. In the case of thin layers ($\sim \xi$) and transparent interfaces (continuity of the order parameter at the interface), this is equivalent to an infinitely long superconducting strip with an external field $\vec{h}$.

This setup can be compared to the quasiclassical model in the effective one-dimensional limit, presented in Fig. 4.10d.

To mimic the quasiclassical model, we extend the GL model by including the angle $\theta$ between $\vec{h}$ and the $x$-axis. We use that the Rashba SOC vector is $\vec{\alpha} = \alpha(\sin \theta \vec{e} - \cos \theta \vec{y})$ inside the ferromagnet (i.e. $-L_x/2 < x < L_x/2$) and zero outside of it. The GL free energy density $f$ is

$$f = a|\psi|^2 + \frac{b}{2}|\psi|^4 + \frac{1}{4m} |\hat{D}\psi|^2 + \frac{1}{4m} \vec{\alpha} \cdot (\psi^* \hat{D} \psi + \psi \hat{D}^* \psi),$$ (5.3)

with $a = a_0(T_c(h, 0))/T_c(0, 0)$. In the absence of the vector potential $\hat{A}$, the gauge-invariant momentum operator is $\hat{D} = -i\vec{\nabla}$ (in units where $\hbar = c = 1$). Applying the Euler-Lagrange equation to the free energy density (5.3), we obtain the GL equation

$$a\psi + b|\psi|^2 \psi - \frac{1}{4m} \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) + \frac{i\alpha}{2m} \left( \cos \theta \frac{\partial \psi}{\partial y} - \sin \theta \frac{\partial \psi}{\partial x} \right) = 0.$$ (5.4)

For $T \to T_c(h, 0)$ and $\alpha$ small, we linearise (5.4) by setting $b = 0$ [37].

Since there are no mixed terms in (5.4), we can apply separation of variables to the order parameter. Using that the sample is infinitely long in the $y$-direction, we assume the order parameter in that direction to be a plane wave, i.e. $\psi(x, y) = \psi(x)e^{iy\phi}$. Substituting the order parameter into (5.4), we find

$$a\psi + \frac{q^2}{4m} \alpha \psi = 0.$$ (5.5)

We normalise the lengths $\tilde{x} = \alpha x$ and $\tilde{y} = \alpha y$, which also yields an extra $\alpha$ in front of $\sin \theta$ and $\cos \theta$. We multiply the equation by $4m/\alpha^2$ to remove the prefactor in front of the first term. We introduce $\tau = 4ma/\alpha^2$ and $\tilde{q}_y = q_y/\alpha$. The normalised GL equation for $\psi(\tilde{x})$ is then given by

$$-\frac{\partial^2 \psi}{\partial \tilde{x}^2} - 2i\alpha \sin \theta \frac{\partial \psi}{\partial \tilde{x}} + (\tau + \tilde{q}_y^2 - 2\alpha\tilde{q}_y \cos \theta) \psi(\tilde{x}) = 0.$$ (5.5)

Similar to Section 3.4.2, we want to absorb the constant terms coming from the $y$-derivatives into $T_c(h, \alpha)$. To do this, we write $a = \tau\alpha^2/4m$ and equate it to the definition of the GL coefficient $a = a_0(T_c(h, \alpha) - T_c(h, 0))/T_c(h, 0)$. Solving for $\tau$, we find that $\tau$ can be interpreted as a correction to the critical temperature recovery as

$$T_c(h, \alpha) = T_c(h, 0) \left( 1 + \frac{\alpha^2 \tau}{4ma_0} \right).$$ (5.6)
The parameter $\tau$ lies in the range $0 \leq \tau \leq 1$. When $\tau = 1$, the correction is uniform and we find our original results from the GL model, given by (5.2). Including the angle-dependency results in a smaller temperature recovery.

The normalised ferromagnet width becomes $\tilde{L}_x = \alpha L_x$. We note that $\alpha$, which takes the interaction between the SOC and the exchange field into account, vanishes outside the ferromagnet (when $|\tilde{x}| > \tilde{L}_x/2$). This gives rise to three different solutions to (5.5). Under the assumption that the order parameter decays outside the ferromagnet (i.e. $\psi(\tilde{x}) \to 0$ as $\tilde{x} \to \pm \infty$), the solution is

$$
\psi(\tilde{x}) = \begin{cases} 
C_1 e^{q_1 \tilde{x}}, & \text{for } \tilde{x} < -\tilde{L}_x/2, \\
(C_1 \cos(R\tilde{x}) + C_2 \sin(R\tilde{x})) e^{i\lambda \tilde{x}/2}, & \text{for } \tilde{x} \in [-\tilde{L}_x/2, \tilde{L}_x/2], \\
C_4 e^{-q_1 \tilde{x}}, & \text{for } \tilde{x} > \tilde{L}_x/2,
\end{cases}
$$

with $\lambda = 2\alpha \sin \theta$, $R = \frac{1}{2} \sqrt{\lambda^2 + 4q_1^2}$, $q_1 = \sqrt{\tau + \tilde{q}_y^2}$ and $q_2 = \sqrt{-2\alpha \tilde{q}_y \cos \theta - \tau - \tilde{q}_y^2}$.

The coefficients $C_1$, $C_2$, $C_3$ and $C_4$ will be determined by the boundary conditions, i.e. continuity of the wave function $\psi$ and its covariant derivative $\partial \psi$ across the interfaces $\tilde{x} = \pm \tilde{L}_x/2$. In matrix notation, these boundary conditions are

$$
\begin{bmatrix}
\cos\left(\frac{1}{2} R\tilde{L}_x\right) e^{-i\lambda \tilde{L}_x/4} & -\sin\left(\frac{1}{2} R\tilde{L}_x\right) e^{-i\lambda \tilde{L}_x/4} & -e^{-q_1 \tilde{L}_x/2} & 0 \\
R \sin\left(\frac{1}{2} R\tilde{L}_x\right) e^{-i\lambda \tilde{L}_x/4} & R \cos\left(\frac{1}{2} R\tilde{L}_x\right) e^{-i\lambda \tilde{L}_x/4} & -q_1 e^{-q_1 \tilde{L}_x/2} & 0 \\
\cos\left(\frac{1}{2} R\tilde{L}_x\right) e^{i\lambda \tilde{L}_x/4} & \sin\left(\frac{1}{2} R\tilde{L}_x\right) e^{i\lambda \tilde{L}_x/4} & 0 & -q_1 e^{-q_1 \tilde{L}_x/2} \\
-R \sin\left(\frac{1}{2} R\tilde{L}_x\right) e^{i\lambda \tilde{L}_x/4} & R \cos\left(\frac{1}{2} R\tilde{L}_x\right) e^{i\lambda \tilde{L}_x/4} & 0 & q_1 e^{-q_1 \tilde{L}_x/2}
\end{bmatrix}
\begin{bmatrix}
C_1 \\
C_2 \\
C_3 \\
C_4
\end{bmatrix}
= \begin{bmatrix}
0 \\
0 \\
0 \\
0
\end{bmatrix}.
$$

Setting the determinant of the matrix equal to zero, we find

$$
\tan(R\tilde{L}_x) = \frac{2Rq_1}{R^2 - q_1^2}.
$$

We want to solve this equation to obtain the critical temperature recovery $\tau$ as a function of magnetisation angle $\theta$. Since $\tan(R\tilde{L}_x)$ is a periodic function, there are multiple solutions. The tangent has a maximum when $R = \pi(n + \frac{1}{2})/\tilde{L}_x$, with $n \in \mathbb{Z}$. Substituting this into (5.7) and solving for $\tau$, we obtain

$$
\tau(n) = \alpha^2 \sin^2 \theta - 2\alpha \tilde{q}_y \cos \theta - \tilde{q}_y^2 - \left(\frac{\pi}{\tilde{L}_x}\right)^2 (n + \frac{1}{2})^2.
$$

We note that $\tau(n)$ is a periodic, descending function in $n$. We are interested in the maximum value of $\tau$, which corresponds to the lowest value of $n$. To find it, we solve (5.8) numerically for $\tau(0) \leq \tau \leq \tau(1)$.

### 5.4 Angular dependency of $T_c$: the comparison

The critical temperature recovery $\tau$ from the GL model is plotted in Fig. 5.2a. From the quasiclassical model in the one-dimensional limit* we obtain $\Delta T_c \equiv |T_c(h, \alpha) - T_c(0, \alpha)|/T_c(0, \alpha)$, which is plotted alongside the GL model in Fig. 5.2b. Both of them are plotted as a function of $\theta$ for several values of the relevant width $\tilde{L}_x$. The relevant width is the region where superconductivity, magnetism and SOC coexist. This is the ferromagnet strip width in the GL model and the entire superconducting strip in the quasiclassical model.

We first consider the similarities between the two models. We recall that the strip is oriented along $y$, such that $\theta = 0$ corresponds to a magnetic field perpendicular to the strip and $\theta = \pm \pi/2$ to a magnetic

*The angle-dependency of the critical field in the quasiclassical model is investigated in Section 4.5.3. Here we focus on the critical temperature instead of the critical field. To do this, we fix $|h|/T_c(0, \alpha) = 0.5$ and compute the critical temperature horizontally (see the first paragraph of Section 4.4 for details).
5.4. Angular dependency of $T_c$: the comparison

Figure 5.2: The angular dependency of the critical temperature, obtained from two different models. (a) An infinite ferromagnetic strip on a superconducting film in the Ginzburg-Landau formalism. The recovery $\tau$ of the superconducting critical temperature as a function of the in-plane magnetisation angle $\theta$, with width $L_x = \alpha L_x$ and $\alpha = 1$. (b) A one-dimensional superconducting strip with spin-orbit coupling in an in-plane applied field in the quasiclassical Usadel formalism. The normalised increase in critical temperature resulting from spin-orbit coupling $\Delta T_c = |T_c(h, \alpha) - T_c(h, 0)|/T_c(h, 0)$ as a function of the in-plane field angle $\theta$, for strip width $L_x$ (in units of $\xi$). This graph is calculated using the one-dimensional limit of the quasiclassical model in the main text, with $\alpha = 2$ and the magnetic field magnitude is fixed to $|h|/T_c(0, \alpha) = 0.5$. In both graphs, the line fitted through the points is $\tau(\theta, L_x) = A(L_x) \sin^2 \theta + B(L_x)$, which serves as a guide to the eye. We note that $\alpha$ and $L_x$ are normalised differently in the two models, and are therefore not directly comparable.

field along the strip. Using both models, the critical temperature reaches a minimum when $\theta = 0$ and a maximum when $\theta = \pm \pi/2$. The physics behind this is explained in Section 4.5.3. The critical temperature as a function of angle has approximately a $\sin^2 \theta$ dependence in both models.

Another similarity is the size-dependence. When decreasing the width, the suppression for $\theta = 0$ becomes stronger in both models. The limit where $L_x \to \infty$ corresponds to a bulk system. The bulk is isotropic and both models lose their angle-dependency. Furthermore, $\tau \to 1$. The decrease in critical temperature vs. sample size is discussed in Section 4.5.2.

Next we address the differences between the two models. The GL model shows an absolute temperature recovery $\tau$ (i.e. all graphs in Fig. 5.2a are offset compared to each other). In the quasiclassical model, all parameters are normalised by $T_c(0, \alpha)$, such that it gives the relative change in $\Delta T_c$ (i.e. all graphs in Fig. 5.2b have the same value at $\theta = \pm \pi/2$).

Another difference is the normalisation of the relevant width $\tilde{L}_x$, which is normalised with respect to $\alpha$ in the GL model, whereas it is normalised with respect to $\xi$ in the quasiclassical model. This implies that the parameters $L_x$ and $\alpha$ in the two models are different parameters.

To conclude, the two models show the same qualitative behaviour of critical temperature as a function of magnetic field angle and sample size. This means that, even though the models consider SOC in different ways and the models themselves are vastly different, they are consistent with each other.
Chapter 6

Boosting and controlling the $p$-wave $T_c$ in a S/F/P junction

“You can’t stop the waves, but you can learn to surf.”
— John Kabat Zinn about $p$-wave superconductivity

A practical obstacle in studying $p$-wave superconductors is the very low critical temperature $T_c$. We predict that the $T_c$ of an intrinsic $p$-wave superconductor can be significantly enhanced by coupling it via an atomically thin ferromagnetic layer to a conventional $s$-wave or a $d$-wave superconductor with a higher critical temperature. We show that this $T_c$-boost is tunable via the direction of the ferromagnet exchange field. Moreover, we show that the enhancement in $T_c$ can also be achieved using the Zeeman-effect of an external magnetic field. Our findings provide a way to increase $T_c$ in $p$-wave superconductors in a controllable way and make the exotic physics associated with such materials more easily accessible experimentally.

The results discussed in this chapter are published in

Controllable enhancement of $p$-wave superconductivity via magnetic coupling to a conventional superconductor.

Author contributions: I derived the equations, did the calculations and wrote the paper. Lina Johnsen had previously worked on lattice models [142] and supported me throughout this project. She shared her expertise on these models and showed me a way to implement matrices in Matlab to make the code more efficient. She also provided critical comments that significantly improved the paper. Jacob Linder and Jason Robinson co-supervised the project, with Jacob focusing on details of the model and Jason focusing on the interpretation. During my time at Trondheim where I started this project, I had daily meetings with Jacob to develop and refine the model.
6.1 Chapter in an image

(a) Figure 6.1: (a) The electrons in a s-wave superconductor (S) form $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$ singlet Cooper pairs, whereas they form $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$ triplets in a $p_x + ip_y$ superconductor (P). The S and P have different critical temperatures $T_{sc}$ and $T_{pc}$, respectively, with $T_{sc} > T_{pc}$. In a S/P junction, the Cooper pairs cannot mix and there is no proximity effect. The $T_c$ of both layers is unaffected. (b) We introduce a ferromagnetic interlayer (F) with exchange field along the $p$-wave $d$-vector (the $z$-axis). The F converts the singlets from S into $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$ triplets through the process of spin mixing. These triplets can enter the P. Extra Cooper pairs in the P result in a boost in $T_{pc}$. (c) If we rotate the exchange field along an axis perpendicular to the $p$-wave $d$-vector (the $y$-axis), the singlets are converted into $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ triplets. These are different from the P’s native triplet and therefore cannot enter. $T_{pc}$ is unaffected. This implies that $T_{pc}$ can be tuned by rotating the F exchange field.

6.2 Attempts to raise the $p$-wave $T_c$

Superconductivity is often described as conventional or unconventional, depending on the symmetry of the underlying order parameter. Conventional spin-singlet superconductors have a s-wave order parameter that is isotropic in momentum space. Unconventional superconductors can instead have a highly anisotropic order parameter, both in magnitude and in phase (see Section 2.2.4 for an introduction). The spin-triplet $p$-wave ($p_x + ip_y$) order parameter is a prototypical example [143], which is of high interest due to its edge-states. Such edge-states may arise at interfaces of unconventional superconductors where reflection causes the order parameter to change sign [144–146] with energies lying midgap at the normal-state Fermi level. Previous work has shown that edge-states arising from a $p$-wave superconductor can be topologically protected from decoherence [147–149], making them interesting as building blocks for qubits in topological quantum computation [150, 151].

Candidate materials for topological superconductivity include $^3$He B-phase [152], the surface of Sr$_2$RuO$_4$ [153], Cu-doped Bi$_2$Se$_3$ [154–156], p-type TlBiTe$_2$ [157] and BC$_3$ [158]. Sr$_2$RuO$_4$ is the most studied although the exact underlying superconducting order parameter remains hotly debated [143, 159, 160]. Sr$_2$RuO$_4$ has a critical temperature $T_c$ of 1.5 K [47] and is sensitive to disorder [161], making it challenging to utilise.
A way to locally increase the $T_c$ of Sr$_2$RuO$_4$ is via the 3 K phase, which involves embedding Ru inclusions into Sr$_2$RuO$_4$ [162]. Similar local $T_c$ enhancement has been predicted near dislocations [163]. The 3 K phase was later attributed to local stress induced by the Ru inclusions [164] and can be mimicked in pure Sr$_2$RuO$_4$ by applying uniaxial pressure [165, 166]. Piezoelectric-based techniques achieve an even higher compression and raise the $T_c$ globally to 3.4 K [167, 168]. By linking the uniaxial strain to spin and charge fluctuations, the latter could serve as a further mechanism for increasing $T_c$ [164].

Finding a general method to enhance $T_c$ of unconventional superconductors in order to more easily access their interesting physics is an important, yet challenging goal. Proximity enhancement of $T_c$ in $s$-wave systems has been predicted theoretically [169] and recently shown experimentally [170]. However, in a junction between a singlet and triplet superconductor, there is no enhancement of the critical temperature in the low-$T_c$ superconductor, since singlet Cooper pairs do not couple to triplet pairs and vice versa [171, 172].

To couple singlet and triplet superconductors, a spin-active interface is required to facilitate conversion between singlet and triplet Cooper pairs. This process is known as spin mixing. A brief introduction to spin mixing is given in Section 2.5.3. A more detailed explanation can be found in Refs. [173, 174]. Ferromagnets [9, 25, 65] and spin-orbit coupling [32, 71, 175] are commonly used for generating spin-triplet Cooper pairs from conventional superconducting pairing. In particular, both ferromagnets [48, 176, 177] and spin-orbit coupling [178, 179] have been used to study the Josephson effect in $s$-wave/$p$-wave (S/P) junctions.

In our work, we present a method to boost $T_c$ of a triplet superconductor. The key is to couple a low-$T_c$ triplet superconductor to a higher-$T_c$ spin-singlet superconductor (either $s$-wave or $d$-wave) via a ferromagnetic interface (F). The underlying physics of this process is sketched in Fig. 6.1. Moreover, we show that the $T_c$-boost is controllable by rotating the F exchange field. Finally, we show that the enhancement of $T_c$ is also obtained via a Zeeman effect from an external magnetic field.

### 6.3 Lattice model for a S/F/P junction

We model a two-dimensional S/F/P junction using the tight-binding Bogoliubov-de Gennes framework [180–184] with a square $N_x \times N_y$ lattice structure, as illustrated in Fig. 6.2. The interface normal is parallel to the $x$-axis and we assume periodic boundary conditions along $y$.

The physics at each site and interactions between adjacent sites are expressed in the second quantisation electron creation ($c_i^\dagger$) and annihilation ($c_i$) operators at lattice site $i = (i_x, i_y)$ with spin $s$. The number operator $n_{is} \equiv c_i^\dagger c_is$ counts the number of electrons occupying state $i$ with spin $s$. The Hamiltonian that describes the S/F/P junction has five contributions:

![Figure 6.2: Schematic illustration of the two-dimensional S/F/P cubic $N_x \times N_y$ lattice structure, with layer thicknesses of $N_{x,S}$, $N_{x,F}$ and $N_{x,P}$ lattice sites, respectively. The $y$-direction is translationally invariant by using periodic boundary conditions and $N_y \gg N_x$.](image-url)
1. The hopping term describes hopping between nearest-neighbours. The hopping amplitude $t_{ij}$ is the probability of an electron moving from site $j$ to $i$, i.e., an electron being created at site $i$ and annihilated at site $j$. The hopping Hamiltonian is

$$H_t = - \sum_{\langle i,j \rangle, s} t_{ij} c_{is}^\dagger c_{js}.$$ 

We assume that the hopping amplitude is the same everywhere ($t_{ij} = t$). In two dimensions, every lattice site has four nearest-neighbours and $H_t$ reduces to

$$H_t = -t \sum_{i,s} c_{is}^\dagger c_{i+\hat{x},s} + c_{is}^\dagger c_{i-\hat{x},s} + c_{is}^\dagger c_{i+\hat{y},s} + c_{is}^\dagger c_{i-\hat{y},s}. \tag{6.1}$$

2. The chemical potential $\mu_i$ is a material parameter that generally differs between the different layers. It acts as a constant offset to the electronic spectrum and is given by

$$H_\mu = - \sum_{i,s} \mu_i n_{is}. \tag{6.2}$$

3. The $s$-wave superconductor is modelled by the attractive on-site interaction $U_i$ between electrons with opposite spin (with $U_i > 0$), which is

$$H_U = - \sum_i U_i n_{i\uparrow} n_{i\downarrow}. \tag{6.3}$$

4. More complicated superconducting symmetries, such as $p$-wave and $d$-wave, are modelled using the nearest-neighbour interaction $V_{ij}$ (with $V_{ij} > 0$). Generally, the nearest-neighbour interaction can contain all possible spin and momentum dependence interactions. Here, we focus on $p_x + ip_y$ symmetry corresponding to opposite-spin pairing ($\uparrow\downarrow + \downarrow\uparrow$). Therefore, the nearest-neighbour Hamiltonian is written as

$$H_V = -\frac{1}{2} \sum_{\langle i,j \rangle, s} V_{ij} n_{is} n_{j,-s}. \tag{6.4}$$

5. The ferromagnet is introduced using the Heisenberg model (see Section 2.3.2). The ferromagnetic exchange field $h$ interacts with the spin as

$$H_h = \sum_i h_i \cdot s_i$$

where the spin density $s_i$ at lattice site $i$ is determined by the probability of an electron changing its spin from $s'$ to $s$ in accordance with the Pauli spin matrices $\sigma = (\sigma_x, \sigma_y, \sigma_z)$, that is

$$s_i = \sum_{s,s'} c_{is}^\dagger \sigma_{ss'} c_{is'}.$$ 

The ferromagnet Hamiltonian is then given by

$$H_h = \sum_{i,s,s'} c_{is}^\dagger (h_i \cdot \sigma)_{ss'} c_{is}. \tag{6.5}$$

We note that $H_U$, $H_V$ and $H_h$ are only present in their respective regions.
6.3.1 Mean-field approximation

The superconducting terms \( H_U \) and \( H_V \) contain quadratic terms which are decoupled using the Hartree-Fock mean-field approximation. This method assumes that the exact value of a product of operators can be approximated by a small fluctuation around its expectation value, i.e., \( c_i^\dagger c_i^\dagger = \langle c_i^\dagger c_i^\dagger \rangle + \delta \) and \( c_i^\dagger c_i = \langle c_i^\dagger c_i \rangle - \delta^\dagger \). Applying this directly to the on-site superconductor Hamiltonian (6.3) gives

\[
H_U = \sum_i U_i c_i^\dagger c_i^\dagger c_i^\dagger c_i \approx \sum_i U_i \left( \langle c_i^\dagger c_i \rangle \langle c_i^\dagger c_i \rangle - \delta^\dagger \langle c_i^\dagger c_i \rangle + \delta \langle c_i^\dagger c_i \rangle \right),
\]

where we neglected second order fluctuations in \( \delta \) [185]. We introduce the \( s \)-wave superconducting gap \( \Delta_i \equiv U_i \langle c_i^\dagger c_i \rangle \) such that \( H_U \) becomes

\[
H_U = \sum_i \frac{\vert \Delta_i \vert^2}{U_i} + \Delta_i c_i^\dagger c_i + \Delta_i^* c_i^\dagger c_i.
\]

The details of this step are shown in Appendix C.1. The first term gives a constant contribution \( E_U \) to the total energy, and can therefore be neglected when calculating eigenvalues and eigenvectors.

The nearest-neighbour superconductor Hamiltonian (6.4) is treated in a similar fashion. We introduce the pair correlation function between electrons located at sites \( i \) and \( j \) with opposite spin as \( F_{ij}^{s,-s} \equiv \langle c_i^s c_j^{-s} \rangle \). The nearest-neighbour Hamiltonian \( H_V \) is expressed in the pair correlation function as

\[
H_V = -\frac{1}{2} \sum_{(i,j),s} V_{ij} \left( \vert F_{ij}^{s,-s} \vert^2 + F_{ij}^{s,-s} F_{ij}^{s,-s} + \left( F_{ij}^{s,-s} \right)^* c_i^s c_j^{-s} \right).
\]

The first term is again a constant energy contribution, \( E_V \). We expand the summation over \( s \) and use symmetry relations to simplify the remaining terms (see Appendix C.2). We obtain

\[
H_V = E_V - \sum_{(i,j)} V_{ij} \left[ F_{ij}^{s,i \rightarrow j} c_i^\dagger c_j + \left( F_{ij}^{s,i \rightarrow j} \right)^* c_i c_j \right].
\]

Since \( V_{ij} \) only acts on the nearest-neighbours, the summation over \( j \) yields four terms, similar to the hopping Hamiltonian (6.1). For brevity, we refer to the terms originating from \( \left( F_{ij}^{s,i \rightarrow j} \right)^* \) as “h.c.” (hermitian conjugate). \( H_V \) becomes

\[
H_V = E_V - \sum_i V_{i,i+\hat{x}} F_{i,i+\hat{x}}^+ c_i^\dagger c_{i+\hat{x}} + V_{i,i-\hat{x}} F_{i,i-\hat{x}}^+ c_i^\dagger c_{i-\hat{x}} + V_{i,i+\hat{y}} F_{i,i+\hat{y}}^+ c_i^\dagger c_{i+\hat{y}} + V_{i,i-\hat{y}} F_{i,i-\hat{y}}^+ c_i^\dagger c_{i-\hat{y}} + \text{h.c.}
\]

6.3.2 The Hamiltonian in \( k \)-space

In our system, the interfaces are located along \( x \) and we assume periodic boundary conditions in the infinite \( y \)-direction. We write \( k_y = 2\pi n / N_y \), where \( n \in \mathbb{Z} \). To implement the periodic boundary condition, we use the Fourier transform

\[
c_{is} = \frac{1}{\sqrt{N_y}} \sum_k c_{ik_x,k_y,s} e^{ik_y s}.
\]

The sum over \( k_y \) spans the first Brillouin zone, such that \( k_y \in [-\pi, \pi] \). We also note that, if the function inside the summation does not depend on \( i_y \), the sum over \( i_y \) gives

\[
\frac{1}{N_y} \sum_{i_y,k_y,k'_y} f(k_y,k'_y) e^{-i(k_y-k'_y)i_y} = \sum_k f(k_y,k'_y) \delta_{k_y,k'_y}.
\]
Applying the Fourier transform (6.8) and using (6.9), the individual Hamiltonian contributions become

\[ H_t = -t \sum_{i,j,k,s} c_{ik}^\dagger c_{jk} (\delta_{i,j+1} + \delta_{i,j-1} + 2 \cos(k_y) \delta_{ij}), \]

\[ H_\mu = -\sum_{i,k,s} \mu_i c_{ik}^\dagger c_{ik}, \]

\[ H_U = E_U + \sum_{i,k} \Delta_i c_{ik}\dagger c_{ik}, \]

\[ H_V = E_V + \sum_{i,j,k} F_{ijk} c_{ik}\dagger c_{jk} \]

where \( F_{ijk} = -V_{ij} \left[ F_i^{x+} \delta_{i,j+1} + F_i^{x-} \delta_{i,j-1} + \left( F_i^{y+} e^{i\theta} + F_i^{y-} e^{-i\theta} \right) \delta_{ij} \right], \]

\[ H_h = \sum_{i,k,s} (h_i \cdot \sigma)_{ss'} c_{ik}^\dagger c_{ik'}, \]

where we have dropped the subscripts \( i = i_x, j = j_x \) and \( k = k_y \) and introduced the notation \( F_i^{x,\pm} \equiv F_i^{x,\pm \pm} \) and \( F_i^{y,\pm} \equiv F_i^{y,\pm \pm}. \) The broken translation symmetry in the \( x \)-direction leads to non-diagonal terms in \( H_t \) and \( H_U \) in the \( x \)-indices. In \( H_t \), the \( \delta_{i,j+1} \) and \( \delta_{i,j-1} \) represent hopping to nearest-neighbours in \( x \), whereas the \( 2 \cos(k_y) \) is the standard electronic spectrum (the dispersion relation). The full derivation of \( H_V \) in (6.13) is given in Appendix C.2.

### 6.3.3 Diagonalisation

To diagonalise the full Hamiltonian \( H \), we first have to express it in its current basis of single-electron creation and annihilation operators. We define the basis \( B_{ik}^\dagger = [c_{ik}^\dagger \ c_{ik} \ c_{i,-k} \ c_{i,-k}^\dagger] \), such that the Hamiltonian \( H_V \) can be written as

\[ H = E_U + E_V + \frac{1}{2} \sum_{i,j,k} B_{ik}^\dagger H_{ijk} B_{jk} \]

with

\[ H_{ijk} = \begin{bmatrix}
\varepsilon_{ijk} + h_i^x \delta_{ij} & (h_i^x - ih_i^y) \delta_{ij} & 0 & \Delta_i \delta_{ij} + F_{ijk} \\
(h_i^x - ih_i^y) \delta_{ij} & \varepsilon_{ijk} - h_i^x \delta_{ij} & 0 & -\Delta_i \delta_{ij} - F_{ijk} \\
0 & -\Delta_i \delta_{ij} - F_{ijk} & \varepsilon_{ijk} - h_i^x \delta_{ij} & 0 \\
\Delta_i^* \delta_{ij} + F_{ijk}^* & 0 & -\varepsilon_{ijk} - h_i^y \delta_{ij} & \Delta_i \delta_{ij} + F_{ijk}
\end{bmatrix}, \]

where \( \varepsilon_{ijk} = -t \delta_{i,j+1} - t \delta_{i,j-1} - (2t \cos(k) + \mu_i) \delta_{ij} \) and \( F_{ijk} \) is given in (6.14). The derivation of the \( F_{ijk} \) matrix elements is shown in Appendix C.2. We define a new basis \( W_k \), which stacks the \( N_z \) separate \( B_{ik} \) vectors into one long vector, i.e. \( W_k^\dagger = [B_{1k}^\dagger \ B_{2k}^\dagger \ \ldots \ B_{N_z,k}^\dagger] \), such that

\[ H = E_U + E_V + \frac{1}{2} \sum_k W_k^\dagger H_k W_k. \]

The matrix \( H_k \) is Hermitian and is diagonalised numerically with eigenvalues \( E_{nk} \) and eigenvectors \( \gamma_{nk} \) as

\[ H = E_U + E_V + \frac{1}{2} \sum_{n,k} E_{nk} \gamma_{nk}^\dagger \gamma_{nk}. \]

Diagonalising the Hamiltonian effectively transforms the system from the single-electron operator basis (denoted by \( c, c^\dagger \)) to the Bogoliubov quasiparticle basis (denoted by \( \gamma, \gamma^\dagger \)). Since Bogoliubov quasiparticles are part electron and part hole, the Bogoliubov operators are linear combinations of electron creation and annihilation operators. The coherence factors \( u, v, w \) and \( x \) are associated with the probability of
electron-like and hole-like states with spin-up and spin-down being occupied. The Bogoliubov creation operator is

$$\gamma_{nk} = \sum_i \left( u_{ink} c_{ik}^\dagger + v_{ink} c_{ik} + w_{ink} c_{i,-k}^\dagger + x_{ink} c_{i,-k} \right).$$  \hfill (6.20)

However, in the summation in (6.19), not all $\gamma_{nk}$ are independent for all $k$-values. Since Cooper pairs impose momentum restrictions on the pairing, there is a symmetry relation between quasiparticles with $+k$ and $-k$. The symmetries in the diagonalisation are explored in Appendix C.3. We find that $\gamma_{n,-k} = \gamma_{nk}$ and $E_{n,-k} = -E_{nk}$. To account for this, we split the sum over $k$ in (6.19) in $k > 0$ and $k < 0$ and $k = 0$ and use these symmetry relations to rewrite them. We obtain

$$H = E_U + E_V + \sum_{n,k>0} E_{nk} \left( \gamma_{nk}^\dagger \gamma_{nk} - \frac{1}{2} \right) + \sum_{E_{n0} \geq 0} E_{n0} \left( \gamma_{n0}^\dagger \gamma_{n0} - \frac{1}{2} \right),$$

where the notation $\sum_{E_{n0} \geq 0}$ is the summation over all positive eigenvalues, including one zero-energy eigenvalue.

Taking the inverse of (6.20), the single-electron operators are related to quasiparticles as

$$c_{ik}^\dagger = \sum_n u_{ink} \gamma_{nk}, \quad c_{i,-k}^\dagger = \sum_n w_{ink} \gamma_{nk},$$

$$c_{ik} = \sum_n v_{ink} \gamma_{nk}, \quad c_{i,-k} = \sum_n x_{ink} \gamma_{nk}. \hfill (6.21)$$

These expressions are the main ingredient to evaluate the pair correlations in terms of the eigenvalues and eigenvectors of the system.

### 6.3.4 Self-consistent solution

The Hamiltonian $H_k$ depends on the $s$-wave superconducting gap $\Delta_i$ and the pair correlations $F_i^{x\pm}$ and $F_i^{y\pm}$ which are initially unknown. By substituting (6.21) we express $\Delta_i$, $F_i^{x\pm}$ and $F_i^{y\pm}$ in the eigenvalues and eigenvectors of $H_k$. The self-consistent calculation consists of choosing initial values for $\Delta_i$, $F_i^{x\pm}$ and $F_i^{y\pm}$, diagonalising $H_k$ to obtain the eigenvectors and eigenvalues, using these to calculate new values for $\Delta_i$, $F_i^{x\pm}$ and $F_i^{y\pm}$, substituting these back into $H_k$ and repeating this procedure until $\Delta_i$, $F_i^{x\pm}$ and $F_i^{y\pm}$ have converged.

The $s$-wave gap $\Delta_i$ in terms of the eigenvectors and eigenvalues is

$$\Delta_i = U_i \langle c_{i\dagger} c_i \rangle = \frac{U_i}{N_y} \sum_k \langle c_{ik}^\dagger c_{i,-k} \rangle = \frac{U_i}{N_y} \left( \langle c_{0\dagger} c_{0} \rangle + \sum_{k>0} \langle c_{ik}^\dagger c_{i,-k} \rangle + \sum_{k<0} \langle c_{ik} c_{i,-k}^\dagger \rangle \right)$$

$$= \frac{U_i}{N_y} \left( \langle c_{0\dagger} c_{0} \rangle + \sum_{k>0} \langle c_{ik}^\dagger c_{i,-k} \rangle + \langle c_{i,-k}^\dagger c_{ik} \rangle \right)$$

$$= \frac{U_i}{N_y} \left( \sum_n u_{in0} x_{n0}^* \langle \gamma_{n0} \gamma_{n0}^\dagger \rangle + \sum_{k>0,n} u_{ink} x_{mk}^* \langle \gamma_{nk} \gamma_{nk}^\dagger \rangle + v_{nk} w_{nk}^* \langle \gamma_{nk}^\dagger \gamma_{nk} \rangle \right).$$

As explained in Appendix C.3, we arrange the eigenvectors in the diagonalising matrix such that the first $2N_x$ are positive and the last $2N_x$ are negative. Then, $u_{i,2N_x+n,0} = w_{i0}^* x_{i+1,2N_x+n,0} = v_{i0}^* x_{i+1,0}$ and $\gamma_{2N_x+n,0} = \gamma_{i0}$. The Fermi-Dirac function is defined as the expectation value of independent $\gamma$-operators as $f(E_{nk}) = \langle \gamma_{nk}^\dagger \gamma_{nk} \rangle$. The $s$-wave gap becomes

$$\Delta_i = \frac{U_i}{N_y} \left( K_0 + \sum_{k>0,n} u_{ink} x_{mk} [1 - f(E_{nk})] + v_{nk} w_{nk}^* f(E_{nk}) \right), \hfill (6.22)$$
with $K_0 = \sum_{E_n \geq 0} u_{in0} x_{in0}^* [1 - f(E_{n0})] + v_{in0} w_{in0} f(E_{n0})$, which is the term corresponding to $k = 0$.

The nearest-neighbour pair correlations are expressed in terms of the eigenvectors in a similar manner, as shown in Appendix C.4. They are

$$F_i^{x\pm} = \frac{1}{N_y} \left( K_{x0} + \sum_{k > 0, n} u_{ink} x_{i\pm1,nk}^* [1 - f(E_{nk})] + v_{i\pm1,nk} w_{ink}^* f(E_{nk}) \right),$$  \hspace{1cm} (6.23)

$$F_i^{y\pm} = \frac{1}{N_y} \left( K_{y0} + \sum_{k > 0, n} u_{ink} x_{i\pm1,nk}^* [1 - f(E_{nk})]\epsilon^{\pm ik} + v_{i\pm1,nk} w_{iink}^* f(E_{nk})\epsilon^{\mp ik} \right),$$  \hspace{1cm} (6.24)

with $K_{x0} = \sum_{E_n \geq 0} u_{in0} x_{i\pm1,0}^* [1 - f(E_{n0})] + v_{i\pm1,0} w_{i0} f(E_{n0})$ and $K_{y0} = \sum_{E_n \geq 0} u_{i0} x_{i0}^* [1 - f(E_{n0})] + v_{i0} w_{i0} f(E_{n0})$.

### 6.3.5 Superconducting order parameters

After convergence, the self-consistency solutions (6.22), (6.23) and (6.24) are used to calculate the superconducting order parameters. The self-consistent $s$-wave gap (6.22) is directly the on-site $s$-wave order parameter, as described in (2) in the main text. Linear combinations of the pair amplitudes $F_i^{x\pm}$ and $F_i^{y\pm}$ provide order parameters with distinct symmetry properties. These linear combinations originate from the spherical harmonic symmetry projected onto the lattice, as illustrated in Fig. 6.3.

The order parameters for $p_x$-wave, $p_y$-wave and $d$-wave ($d_{x^2-y^2}$) at lattice site $i$ are, respectively,

$$\Delta_{p_x, i} = VF_{p_x, i} = \frac{V}{2} \left( F_i^{x+(T)} - F_i^{x-(T)} \right),$$  \hspace{1cm} (6.25)

$$\Delta_{p_y, i} = VF_{p_y, i} = \frac{V}{2} \left( F_i^{y+(T)} - F_i^{y-(T)} \right),$$  \hspace{1cm} (6.26)

$$\Delta_{d, i} = VF_{d, i} = \frac{V}{4} \left( F_i^{x+(S)} + F_i^{x-(S)} - F_i^{y+(S)} - F_i^{y-(S)} \right),$$  \hspace{1cm} (6.27)

![Figure 6.3](image)

**Figure 6.3:** Symmetries of the nearest-neighbour pair correlations $F_x^+$, $F_x^-$, $F_y^+$ and $F_y^-$ based on the spherical harmonics for different superconducting pairing symmetries.
The superscripts correspond to spin-singlet (S) and spin-triplet (T) symmetries. Hence \( F^{(S)} \) has to be anti-symmetric under spin exchange, while \( F^{(T)} \) is symmetric. Therefore, they are defined as

\[
F^{(S)}_{ij} = \frac{F_{ij} + F_{ji}}{2}, \quad F^{(T)}_{ij} = \frac{F_{ij} - F_{ji}}{2}.
\] (6.28)

The pair correlations \( F_{p_x,i}, F_{p_y,i} \) and \( F_{d,i} \), have their own critical temperatures \( T_{p_x}^{c}, T_{p_y}^{c} \) and \( T_{d}^{c} \), respectively, in the sense that they become smaller than some tolerance level at a specific temperature. The highest \( T_c \) of a pair correlation determines the temperature at which the material becomes superconducting. The full expressions of the symmetry-dependent pair correlations are given in Appendix C.5.

### 6.3.6 Stabilising superconducting symmetries

To stabilise the desired superconducting symmetry in the nearest-neighbour model, we choose the initial conditions in accordance with Fig. 6.3. However, this is not enough to assure a certain symmetry. The pair correlations also depend on the model parameters: on the electronic bandwidth via the hopping amplitude \( t \), on the Fermi energy via the chemical potential \( \mu \), on the nearest-neighbour interaction \( V \) and on temperature \( T \). Fig. 6.4b shows the phases of a bulk superconductor.

Electrons forming Cooper pairs have energies close to the Fermi surface. By considering the shape of the Fermi surface for different values of \( \mu \) (shown in Fig. 6.4a), we predict the most energetically favourable symmetry. The orbital functions of the superconducting symmetries are [186]

\[
\begin{aligned}
&\text{s-wave} \quad \omega_s(k) = \cos(k_x) + \cos(k_y), \\
&\text{d-wave} \quad \omega_d(k) = \cos(k_x) - \cos(k_y), \\
&\text{p}_x\text{-wave} \quad \omega_{p_x}(k) = \sin(k_x), \\
&\text{p}_y\text{-wave} \quad \omega_{p_y}(k) = \sin(k_y).
\end{aligned}
\] (6.29)

As a result of particle-hole symmetry, the superconducting symmetries are symmetric around \( \mu = 0 \), which corresponds to half-filling. The Fermi surface near the band edge (\( \mu \approx \pm 4t \)) corresponds to \( \vec{k} = (\pm \pi, \pm \pi) \) or \( (0, 0) \), for which \( |\omega_s(k)| \) is maximised and s-wave is stable. Half filling (\( \mu \approx 0 \)) corresponds to the square \( \vec{k} = (\pm \pi, 0), (0, \pm \pi) \) for which d-wave is favoured. For intermediate filling (\( \mu \approx \pm 2t \)), the Fermi surface gets close to \( k_x = \pm \pi/2 \) and \( k_y = \pm \pi/2 \), for which \( p_x \) or \( p_y \) symmetry is preferred [186].

![Figure 6.4](image_url)

**Figure 6.4:** (a) The Fermi surface in the tight-binding model as a function of chemical potential \( \mu \) in units of the hopping amplitude \( t \). (b) Stable superconducting phases as a function of \( T_c \) and \( \mu \) in units of \( t \). The nearest-neighbour interaction is \( V = 1.5 \). Adapted from Kuboki et al [186].
In a bulk superconductor, \( p_x \) and \( p_y \) are degenerate. Ginzburg-Landau analysis [186] shows that the complex combination \( p_x \pm ip_y \) removes nodes in the Fermi surface such that the system gains condensation energy, which is why \( p_x \pm ip_y \) pairing is favoured over \( p_x \pm p_y \). The same reasoning explains the coexisting states \( d \pm p_x \) and \( s \pm p_x \) (equivalent to \( d \pm p_y \) and \( s \pm p_y \) in bulk superconductors). The mixed \( (d + p_x) \)-region is much wider than the \( (s + p_x) \)-region, since \( d \)-wave has nodes while \( s \)-wave does not and therefore, a larger energy gain is obtained for \( d + p_x \) pairing [186]. Coexisting \( d \) and \( p \) order parameters have been predicted in superconductor/(anti)ferromagnet bilayers, where the proximity effect induces imbalance of spin-up and spin-down electron densities [187].

To stabilise the \( p_x + ip_y \) pairing, the parameters in \( P \) are chosen in accordance with free energy minimisation [186] and previously used values for \( \text{Sr}_2\text{RuO}_4 \) [182] as \( V/t = 1.5 \) and \( \mu_P/t = 1.8 \). The \( P \) thickness \( N_{x,P} = 10 \) is the smallest for which we can comfortably stabilise \( p \)-wave pairing. The parameters in \( S \) are calibrated to give \( T_c^s \approx 10T_c^p \) (in bulk systems), which is realistic for common \( s \)-wave superconductors like Nb. We find \( U/t = 5.3 \) and \( \mu_S/t = 1.2 \). Since superconductivity in \( S \) is stronger than in \( P \), it can be stabilised in a thinner layer and we use \( N_{x,S} = 5 \). We note that the used value for \( U \) is too large to be realistic for an actual BCS superconductor and is a result of downscaling the lattice to a computationally manageable system size. Nevertheless, it is the relative ratio of the critical temperatures that is important to enhance \( T_c \) of the \( p \)-wave superconductor and for this reason we expect that our predictions hold for larger system sizes as well. The parameters in \( F \) are optimised to give the largest effect, i.e., \( h_z/t = 0.9 \) and \( \mu_F/t = 1.4 \). We use \( N_{x,F} = 1 \) to model an atomically thin ferromagnet.

### 6.4 Numerical method

The numerical method to iteratively calculate the pair correlations and order parameters vs. temperature has been touched upon throughout the previous section. This section gives a step-by-step overview and introduces some Matlab syntax.

1. **Parameters.** Define the parameters for the \( S \), \( F \) and \( P \) regions. For the \( P \) region, it is crucial to choose \( \mu \) and \( V \) such that \( p \)-wave symmetry is stabilised. The parameters for the \( S \) region are chosen such that \( T_c^s \approx 10T_c^p \). A discussion on the parameters is given in Section 6.3.6.

2. **Initiate the numerics.** Define the list of temperatures that will go on the horizontal axis. Define empty lists of the same length in which to store the order parameters. This makes the calculation more robust. Define the list of \( k \) values used for the summation over the momentum. The \( k = 0 \) term will be calculated separately. The other \( k \) terms are defined in a list as \( \text{linspace}(\pi/\text{Ny}, \pi, \text{Ny}) \).

3. **Conditions for the while-loop.** The iterative calculation is done using a while-loop, which stops when one of three criteria is met. Define two convergence tolerances: the absolute tolerance as \( 10^{-8} \), the relative tolerance as \( 10^{-6} \) (two orders larger for testing).* To prevent the loop from getting stuck, also introduce a maximum number of iterations, equal to 10000.

4. **Loop over temperature.** For every temperature, the following has to be reset: Set the number of iterations to 0. Define the difference between the current and previous pair correlation as a large number (100 is sufficient). This difference will be recorded after every iteration and compared to the tolerance. Reset the while-loop conditions by setting the three boolean operators to 1. Reset the absolute tolerance as 100 is sufficient. However, when the pair correlations get very small, we divide by a number that is very close to zero. To prevent numerical converging issues due to this, we use the absolute tolerance.

* In many cases, using only the relative tolerance is sufficient. However, when the pair correlations get very small, we divide by a number that is very close to zero. To prevent numerical converging issues due to this, we use the absolute tolerance.
as \texttt{while c1 \&\& c2 \&\& c3}, where the boolean operators \texttt{c1}, \texttt{c2} and \texttt{c3} correspond to the absolute tolerance, relative tolerance and maximum number of iterations, respectively. The boolean operators are 1 at the start of the loop and turn to 0 when their respective conditions are met. The \texttt{\&\&} signifies that only one of the conditions has to be met to stop the while-loop.

6. **Constructing the Hamiltonian.** Define the Hamiltonian matrix as an empty $4N_x \times 4N_x$ matrix using \texttt{zeros}(4*Nx,4*Nx). Fill the matrix according to (6.18). The Matlab command \texttt{repmat} does this efficiently by making vectors with repeated entries (e.g. for every lattice site). For example, the hopping term on the upper diagonal is implemented as

$$H_{1}(16*Nx+1:4*Nx+1:end) = \texttt{repmat([-t, -t, t, t],1,Nx-1)};$$

7. **Eigenvalues and eigenvectors.** Calculate the eigenvalues and eigenvectors of the Hamiltonian for a single $k$. The eigenvalues are used in the Fermi-Dirac distribution (note that only positive eigenvalues are taken for $k = 0$). The weights $u$, $v$, $w$ and $x$ introduced in (6.20) are obtained from the eigenvectors as

$$[\text{eigvec, eigval}] = \texttt{eig(H)};$$

$$u = \texttt{eigvec(1:4:4*Nx,:);}$$

$$v = \texttt{eigvec(2:4:4*Nx,:);}$$

$$w = \texttt{eigvec(3:4:4*Nx,:);}$$

$$x = \texttt{eigvec(4:4:4*Nx,:);}$$

where $u$, $v$, $w$ and $x$ are $N_x \times 4N_x$ matrices.

8. **Pair correlations.** Using the $u$, $v$, $w$, $x$ and the Fermi-Dirac distribution, calculate $\Delta_i$ using (6.22), $F_i^{\pm}$ using (6.23) and $F_i^{xy}$ using (6.24). Note that the pair correlations take the sum over both $k$ and $n$. The sum over $n$ is taken by simply summing over the matrix entries, which yields $1 \times N_x$ vectors for $\Delta_i$ and $F_i^{\pm}$, and a $1 \times (N_x - 1)$ vector for $F_i^{xy}$ (due to the broken translational symmetry in $x$). The diagonalisation (step 7) and calculation of the pair correlations are done separately for every $k$ and the results are summed using a for-loop.

9. **Singlet and triplet components.** The pair correlations in the previous step are symmetrised according to (6.28) (full expressions are given in Appendix C.5). Again, the summation over $n$ is done by summing over the matrix entries and the summation over $k$ is done in a for-loop (the same for-loop as used in the previous step to make it more efficient).

10. **Convergence criteria.** The pair correlations obtained in step 8 are used to check whether the convergence criteria are met. The pair correlations are compared with those of the previous iteration to see whether the relative and absolute tolerance have been met, that is,

$$\left\| \frac{F_{n+1} - F_n}{F_n} \right\| < 10^{-6}, \quad \|F_{n+1} - F_n\| < 10^{-8},$$

where $F_n$, $F_{n+1}$ are general pair correlations after $n$ and $n+1$ iterations, respectively, and the $\|$ brackets represent the Euclidean norm. If the convergence criteria are not met, the current pair correlations are fed into the calculation at step 6 and the process is repeated.

11. **Order parameters.** After convergence is reached, the order parameters are calculated. The order parameters for $p_x$ and $p_y$ are given by (6.25) and (6.26), respectively, and are calculated using the singlet and triplet components obtained in step 9. Note that due to the broken translational symmetry in $x$, the components $F_i^{\pm(T)}$ have dimension $1 \times (N_x - 1)$ as opposed to the required $1 \times N_x$. To calculate the $p_x$ order parameter correctly, a zero is added at the beginning of $F_i^{\pm(T)}$ and at the end of $F_i^{\mp(-T)}$. 
12. **Spatial profile.** The entire calculation so far has been for one temperature. If one is interested in the spatial profile of the order parameters, the calculation ends here and the order parameters can be plotted as a function of $x$.

13. **Temperature dependence.** If one is interested in the order parameter as a function of temperature, save the value of the order parameter in step 11 in the middle of the relevant layer (meaning, the $s$-wave order parameter in the middle of S and the $p_x$- and $p_y$-wave order parameters in the middle of P). Repeat the calculation from step 4 for the full temperature range.

### 6.5 Boosting and controlling the $p$-wave $T_c$

This section contains the results obtained using the lattice model. We first introduce the concept of midgap surface states, which will be used in the discussion of the results. We then calculate the $p$-wave $T_c$ in multiple junctions, show that it can be boosted and controlled in the S/F/P junction and compare it to a S/P junction in an external field.

#### 6.5.1 Midgap surface states

The behaviour of the $p$-wave pair correlations is closely linked to the presence of midgap surface states in P. Midgap surface states are surface states with zero energy relative to the Fermi level [144].

Midgap surface states were first proposed as a bound state in a normal metal/superconductor junction [144]. We consider a one-dimensional junction along $x$ consisting of vacuum for $x < 0$; a normal metal located between $x \in [0, d_N]$, where the normal metal thickness $d_N$ is much smaller than the mean free path; and a superconductor for $x > d_N$. We look at a particle in the normal metal with momentum $k_\perp$ perpendicular to the interfaces. This particle alternately experiences Andreev reflection at the superconductor interface and normal reflection at the free surface (interface with vacuum). This bound state is sketched in Fig. 6.5a. Andreev reflection changes an electron with momentum $k_\perp$ into a hole with momentum $-k_\perp$. Normal reflection only changes the sign of $k_\perp$. Having an alternating sequence of two types of reflections implies that the pair correlations either alternate sign or keep the same sign, depending on the superconducting symmetry. Treating the free surface by an image method as illustrated in Fig. 6.5b, we extend the pair correlation $F$ by $F(k_\perp, -x) = F(-k_\perp, x)$. This is equal to $-F(k_\perp, x)$ in the case of the alternating sign, giving a pair correlation that is odd in $x$ and $k_\perp$. This is precisely the symmetry condition that gives rise to midgap states: $F(k_\perp) = -F(-k_\perp)$ [144, 146].

![Figure 6.5: (a) Bound state in a normal metal/superconductor junction. Particles experience normal reflection at the free surface (vacuum interface) and Andreev reflection at the interface with the normal metal. Upon Andreev reflection, the nature of the particle changes from electron (filled dot, solid line) to hole (open dot, dashed line) and vice versa. (b) The image method: an incoming electron from the left ($x < 0$) with momentum $k_\perp > 0$ is equivalent to an incoming electron from the right ($x > 0$) with momentum $k_\perp < 0$.](image)

Hence, it is the symmetry condition and not the precise form of the pair correlations that determines whether midgap states are present. For the same reason, since the midgap states are independent of $d_N$, the argument still holds in the absence of the normal metal, i.e., for a single superconductor.
The symmetry condition \( F(k) = -F(-k) \) leads to the midgap states as well as to the suppression of the pair correlations at the surface [146]. The two electrons in a Cooper pair have opposite momentum and therefore experience an opposite sign after reflection. This causes pair breaking near the surface and the pair correlations are locally suppressed [145, 188].

The midgap states have many experimental consequences [144]. Most notably, quasiparticle tunneling gives a direct way to observe midgap states which show up as a zero bias conductance peak in the density of states [144, 146, 189]. When the midgap surface states are topologically protected, they are associated with Majorana bound states [150, 190], but this topic is beyond the scope of this project.

### 6.5.2 \( p \)-wave pair correlations

We will now calculate the spatial and temperature dependence of the \( p \)-wave pair correlations in a single P and in N/P, S/P and S/F/P junctions.

**Single P**

We first consider the pair correlations close to the surface of a finite two-dimensional \( p_x + ip_y \) superconductor shown in Fig. 6.7a. In a single P (interfaced with vacuum), electrons are reflected with opposite momentum in the \( x \)-direction (\( k_x \rightarrow -k_x \)), while the momentum in the \( y \)-direction is conserved. The \( p_x \) orbital symmetry \( \sin(k_x) \) is odd under inversion of \( k_x \) and obeys the symmetry condition for having a midgap surface state [144, 146]. Consequently, this causes pair breaking and results in the cancellation of \( F_{p_x} \) near the surface [145, 188]. As a result, there are more electrons present to form Cooper pairs in the \( y \)-direction and \( F_{p_y} \) increases close to the surface.

To study the temperature-dependence of \( F_{p_x} \) and \( F_{p_y} \), we consider a system where P is thin (\( N_x, P \) small) enough that the midgap surface states of the two surfaces partially overlap. If P is interfaced by vacuum on either side, \( F_{p_x} \) vanishes at both interfaces and is severely or even fully suppressed over the whole width of the superconductor. Hence, its \( T_c \) (taken in the middle of P) is suppressed as well, as shown in Fig. 6.7e.

![Energy spectrum of a single \( p \)-wave superconductor](image)

**Figure 6.6:** Energy spectrum of a single \( p \)-wave superconductor, adapted from [145]. By comparing the energy in the normal state (dashed) to superconducting state (solid, coloured), we determine where energy is gained and lost. For example, the negative midgap states have a higher energy than the normal state, such that it costs energy to occupy them. The non-trivial energy-dependence of the midgap states eventually result in the re-entrant behaviour of \( F_{p_x}(T) \).
An interesting feature is the non-monotonic re-entrance behaviour of $F_{px}(T)$ which has been linked to the presence of midgap surface states in a thin P in the literature [145, 146, 190]. Hara and Nagai [145] use the simplified energy spectrum shown in Fig. 6.6 to compare the normal state energy (dashed black lines) to the superconducting state energy (solid coloured lines). They discuss two different re-entrance effects here: as a function of system size $L$ and temperature $T$.

At zero temperature, the system is filled up to the Fermi level ($E = 0$). The negative band has a lower energy than the normal state. Therefore, occupying the negative band minimises the energy. The negative midgap states ($E < 0$) have a higher energy than the normal state, such that occupying the midgap states increases the energy. The momentum $K$ associated with the midgap states is proportional to the system size $L$. When the system size becomes smaller, the midgap region becomes wider. When the energy increase from occupying the midgap states overtakes the energy decrease from occupying the negative band, the critical size $L_c$ is reached and the normal state is energetically favourable, resulting in a suppression of $T_c$ [145]. Hence, the re-entrance effect is the result of a small system. We have confirmed this with our code: when we increase the system size numerically, the suppression disappears.

In Fig. 6.7e, we observe the re-entrance effect as a function of temperature for a fixed system size. At finite temperature, the positive midgap states ($E > 0$) become occupied. They have a lower energy than the normal state, such that occupying them results in a decrease in energy. This explains the re-entrance effect as a function of temperature [145, 190].

We note that the explanation of the re-entrance effect by Hara and Nagai [145] is based on a simplified band structure. To get a more in-depth understanding of the effect, it would be necessary to consider the actual band structure of materials and interfaces with different dimensions, for example, by implementing density functional theory [191].

**N/P and S/P junctions**

By bringing the P into contact with a normal metal (N) in Fig. 6.7b, $F_{px}$ is no longer fully cancelled at the interface since Cooper pairs can enter the N via the proximity effect, resulting in a suppression of the midgap states. In fact, replacing the vacuum with any conducting material suppresses the midgap states since the reflection probability goes from 1 to $< 1$. On the other hand, $F_{py}$ simply decreases at the interface since Cooper pairs can now tunnel into N. Both $F_{px}$ and $F_{py}$ decay exponentially in N.

In Fig. 6.7c, we replace N with a conventional superconductor S, forming a S/P junction. The proximity effect is strongly suppressed [171, 172] and spans only a few lattice sites on either side of the interface. Consequently, $F_{px}$ and $F_{py}$ reach their bulk values close to the interface. Like the N/P case, midgap surface state reflections are also suppressed in S/P and $F_{px}$ overtakes $F_{py}$.

The temperature-dependence of the pair correlations in both N/P and S/P is similar. Placing the P in contact with either (instead of a vacuum), $F_{px}$ can be recovered by reducing midgap surface state reflections, as seen in Fig. 6.7f-g. The $T_c$ in this case matches the $T_c$ of a bulk P.

**The S/F/P junction**

Finally, by sandwiching a F in between the S and P, as shown in Fig. 6.7d, conversion of $s$-wave singlets into $p_x$-wave triplets takes place and $F_{px}$ is boosted at the interface. The effect of increasing the exchange field is two-fold: it enhances singlet-to-triplet pair conversion and weakens the effect of the midgap surface state [189], resulting in an increase in $F_{px}$.

The temperature-dependence of the pair correlations in the S/F/P junction shows an additional effect on top of the $T_c$ recovery seen in the N/P and S/P junctions. The S has a higher $T_c$ than P; for our parameters, $T_c^S \approx 10T_c^P$. Once the intrinsic $T_c$ of P is exceeded, there is still a small amount of triplets coming from the S/F interface, stabilising $F_{px}$ above its intrinsic $T_c$. This results in a tail in $T_c^{px}$, as seen in Fig. 6.7h. For the optimal parameters, it is possible to nearly double $T_c^{px}$. Only $T_c^{px}$ is boosted while $T_c^{py}$ remains the same as a result of the structural symmetry. In this setup, translational symmetry is broken along $x$. The S/F bilayer converts even-frequency $s$-wave singlets into even-frequency $p_x$-wave triplets and odd-frequency $s$-wave triplets [142]. The latter do not contribute to the $T_c$-enhancement discussed here. Since there is no symmetry breaking in the $y$-direction, there is no conversion to $p_y$-wave
6.5. Boosting and controlling the $p$-wave $T_c$

Figure 6.7: Spatial pair correlation profiles $\text{Re}(F_{px})$ (solid) and $\text{Im}(F_{py})$ (dashed) at the interface of (a) vacuum/P, (b) N/P, (c) S/P and (d) S/F/P at zero temperature. The pair correlations versus normalised temperature for (e) thin single P, (f) thin-layer N/P, (g) S/P and (h) S/F/P junctions ($N_{x,N} = N_{x,S} = 5$, $N_{x,F} = 1$, $N_{x,P} = 10$). The thin single P is severely suppressed. The suppression is recovered in N/P and S/P. Singlet-triplet conversion in S/F/P results in a tail in $T_c$. The parameters for all graphs are $N_y = 200$, $\mu_S/t = \mu_S/t = 1.2$, $U/t = 5.3$, $\mu_V/t = 1.4$, $h_z/t = 0.9$, $\mu_V/t = 1.8$ and $V/t = 1.5$. 

(a) Vac. P
(b) N P
(c) S P
(d) S F P
(e) Re($F_{px}$) — solid; Im($F_{py}$) — dashed
(f) N P
(g) S P
(h) S F P

$x$

$T/t$
alongz Figure 6.8: can be tuned externally, while conductivity. The exchange field direction is tunable via an applied magnetic field, meaning that observation which could lead to interesting device concepts and a means to further probe exchange field direction.

triplets originating from P into singlets. Since the S is isotropic, this contribution is independent of the parameters, as sketched in Fig. 6.5.3 Controlling $T_c$ via magnetisation direction

Triplet superconductivity is generally described by the $\hat{d}$-vector $d \equiv [(\Delta_{\downarrow\downarrow} - \Delta_{\uparrow\uparrow})/2, -i(\Delta_{\uparrow\downarrow} + \Delta_{\downarrow\uparrow})/2, \Delta_{\downarrow\uparrow}]$ [9]. We consider $p_x + ip_y$ pairing, which happens between opposite spin electrons such that $d$ is along $\hat{z}$. We study the effect of changing the F exchange field direction $h$ with respect to $\hat{d}$. The S is isotropic and the $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$ spin-singlet Cooper pair is rotationally invariant. The three spin-triplet states $|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle$, $|\uparrow\downarrow\rangle$ and $|\downarrow\downarrow\rangle$ transform into each other when the quantisation axis changes [9, 26] (see Section 2.5.3). We choose the quantisation axis to be along $h$. This means that the exchange field $h_z$ converts singlets to $|\uparrow\downarrow\rangle + |\downarrow\downarrow\rangle$ triplets polarised along the $z$-axis. This is the native triplet Cooper pairs of the P and hence boosts $T_p^v$.

By changing the exchange field direction from $h_z$ to $h_x$ or $h_y$, singlets are converted to $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$ triplets with a quantisation axis along the $x$ and $y$ axis, respectively. In the reference frame of the $p_x + ip_y$-wave superconductor, this corresponds to $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ triplets. The cases with $h_z$ and $h_y$ are sketched in Fig. 6.1. The $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ triplets suppress $T_p^v$, as seen in Fig. 6.8. For the optimal parameters, $T_p^v$ corresponding to $h_z$ is double the $T_p^v$ for $h_x$ or $h_y$. Vice versa, the F also converts triplets originating from P into singlets. Since the S is isotropic, this contribution is independent of the exchange field direction.

The fact that the $T_c$-enhancement is controlled by the exchange field direction is an important observation which could lead to interesting device concepts and a means to further probe $p$-wave superconductivity. The exchange field direction is tunable via an applied magnetic field, meaning that $T_p^v$ can be tuned externally, while $T_c^v$ remains largely unchanged. This can serve as a switch in a device.

Figure 6.8: The pair correlations versus normalised temperature for S/F/P with the exchange field in F (a) along $\hat{z}$ and (b) along $\hat{y}$. Rotating the exchange field changes $T_c$ dramatically. The parameters are $N_{F,S} = 5$, $N_{S,F} = 1$, $N_{S,P} = 10$, $N_F = 200$, $\mu_S/t = 1.2$, $U/t = 5.3$, $\mu_F/t = 1.4$, $h_z/t = h_y/t = 0.9$, $\mu_F/t = 1.8$ and $V/t = 1.5$. 
Similarly, to observe a Josephson current in a S/F/P junction, an exchange field component parallel to the $\vec{d}$-vector of the triplet order parameter (here pointing along $z$) is required [177]. By extension, one could control the Josephson current by rotating an applied magnetic field.

### 6.5.4 $T_c$-boost via external magnetic field

Finally, we compare the S/F/P junction to a S/P junction with an external field $B_z$ along $\hat{z}$. When the superconductors are much smaller than the magnetic penetration depth $\lambda$, the orbital effect of $B_z$ is quenched and superconductivity coexists with a Zeeman-splitting throughout both superconductors up to the Clogston-Chandrasekhar limit [90, 91]. This results in a spin polarisation across the whole junction. Since $F_{pz}$ and $F_{py}$ have different magnitudes and different $T_c$, they also have different critical fields $B^{pz}_c$ and $B^{py}_c$, respectively; with $B^{pz}_c > B^{py}_c$.

By applying the field, first $F_{pz}$ decreases. Since less Cooper pairs are converted from $F_{pz}$ to $F_{py}$, this goes accompanied with a net increase in $F_{pz}$. Naturally, the $F_{pz}$-to-$F_{py}$ conversion stops at $B^{pz}_c$, at which $F_{pz}$ reaches its maximum. This case is shown in Fig. 6.9. Similar to $h_z$, $B_z$ facilitates singlet-to-triplet conversion and $T^{pz}_c$ shows a tail. Interestingly, the magnitude of $F_{pz}$ in S/P with $B_z$ is significantly larger than in S/F/P, due to the lack of $F_{pz}$-to-$F_{py}$ conversion.

However, $B_z$ also introduces a gradient of $F_z$ over the full width of the P (positive at the S/P interface, zero in the middle, negative at the P/vacuum interface). The magnitude of $F_z$ at the interfaces is approximately half the magnitude of $F_{pz}$, which is significant, especially since the interesting physics unique to P superconductivity are generally situated at the edges. In this respect, the S/F/P structure is favorable since it maintains the pure $p$-wave correlations in the P throughout the regime of increased critical temperature. Increasing $B_z$ further, our model shows LOFF oscillations in the P (see Section 2.5.2 for details).

![Figure 6.9: Comparison between the pair correlations in a S/F/P (a) with exchange field $h_z$ and (b) S/P in an external field $B_z$, versus normalised temperature. The external field is chosen as $B_z/t = B^{pz}_c = 0.3$, for which $F_{pz}$ is maximised. The parameters are $N_{x,S} = 5$, $N_{x,F} = 1$, $N_{x,P} = 10$, $N_y = 200$, $\mu_S/t = 1.2$, $U/t = 5.3$, $\mu_F/t = 1.4$, $h_z/t = 0.9$, $\mu_F/t = 1.8$ and $V/t = 1.5$.](image-url)
6.6 Conclusions & Outlook

We have shown that the $T_c$ of a spin-triplet $p$-wave superconductor is controllable in a S/F/P junction, where S has a higher $T_c$ than P. A ferromagnetic interlayer facilitates singlet-to-triplet conversion, providing the P with triplets even above its intrinsic $T_c$. This shows up as a tail in the order parameter-temperature phase diagram. Rotating the F exchange field direction with respect to the $p$-wave $d$-vector controls the triplets, and therefore, $T_c$. An exchange field parallel to $d$ is able to nearly double $T_c$, whereas an exchange field perpendicular to $d$ converts singlets to the wrong type of triplets and suppresses $T_c$. Hence, the exchange field direction serves as a $T_c$ switch and can by extension control a Josephson current. In our model, we considered an atomically thin F. Qualitatively similar results are expected for thicker F.

Enhancing the $T_c$ of a $p$-wave superconductor above liquid helium temperatures would have massive practical advantages from a device operation point of view. In the case of Sr$_2$RuO$_4$ with its $T_c$ of 1.5 K, the doubling of $T_c$ is still not enough, although it might be sufficient for different $p$-wave materials. Therefore, it would be interesting to explore enhancing $T_c$ further using a high-$T_c$ cuprate $d_{x^2-y^2}$-wave superconductor (D). The theoretical framework used in this paper does not allow us to address the D case. The reason is that when solved self-consistently, as is required to compute $T_c$, our model tends to stabilise $d+pz$ symmetry in D rather than pure $d$-wave [186]. However, our findings for the S/F/P case are indicative that a much larger $T_c^p$ could be possible if one is able to experimentally realize a high-$T_c$ superconductor/F/P junction.

6.6.1 Possible experiments

The easiest way to measure $T_c$ is the van der Pauw method [138], which involves growing the stack on a square insulting substrate and wire bonding a contact to each corner, as illustrated in Fig. 6.10a. The contacts will go through all three layers and measure the resistance of the entire film. Alternatively, one could pattern a Hall bar on top of the stack. The latter method is more controlled since it measures only the resistance of a small strip, but does involve more processing steps. The superconducting transition will resemble the graph shown in Fig. 6.10b, which consists of two transitions since the S or D becomes superconducting before the P.

We note that this project relies on the existence of $p$-wave superconductor thin films, which, at the time of writing, is a subject under investigation [192–194]. Possible materials combinations with Sr$_2$RuO$_4$ include the transition metal ferromagnet SrRuO$_3$ [195], the highly spin-polarized manganites such as La$_{0.7}$Ca$_{0.3}$MnO$_3$ [196, 197] and the oxide superconductors YBa$_2$Cu$_3$O$_{7-x}$ [198] and Pr$_{1.85}$Ce$_{0.15}$CuO$_4$ [199]. Other materials to consider are two-dimensional ferromagnets including Cr$_2$Ge$_2$Te$_6$ [200], CrI$_3$ [201] and VSe$_2$ [202].
References

References


[186] K. Kuboki, J. Phys. Soc. Jpn 70, 2698 (2001), note: This reference has an $i$ in their definition of $p$ compared to Equations (6.25) and (6.26), meaning that $ip_x$ and $ip_y$ in their notation are $p_x$ and $p_y$ in our notation.


Appendices
Appendix A

Generating superconducting vortices via spin-orbit coupling

A.1 Rewriting the free energy

Using that the GL order parameter can be expressed as $\psi = |\psi|e^{i\phi}$, the kinetic term $|\nabla x|^2$ is expanded as

$$\frac{1}{4m}|\nabla x|^2 = \frac{e^2}{m} \left| -\frac{i}{2e} \tilde{\mathbf{D}} + \tilde{A} \right| \psi |^2 = \frac{e^2|\psi|^2}{m} \left( \frac{1}{4e^2} (\nabla \varphi)^2 + \frac{1}{e} \tilde{\mathbf{A}} \nabla \varphi + \tilde{A}^2 \right) = \frac{1}{8\pi \lambda^2} \left( \tilde{\Phi} - \tilde{A} \right)^2,$$

where the London penetration depth $\lambda$ is defined as $\lambda^2 = m/8\pi e^2 |\psi|^2$. Similarly, the SOC term in (3.2) becomes

$$\frac{1}{4m} \cdot \left( \psi^* \nabla \psi + \psi (\nabla \psi)^* \right) = \frac{1}{8\pi \lambda^2} \frac{\alpha}{e} \cdot \left( \tilde{\Phi} - \tilde{A} \right).$$

Assuming $ds \ll \lambda$, superconductivity along $z$ is taken to be constant, such that its integral yields a factor $d_s$. We define the effective penetration depth as $\lambda_{\text{eff}} = \lambda^2/d_s$ [83]. The free energy $F = \int f(\mathbf{r})d^3\mathbf{r}$ is

$$F = F_0 + \frac{1}{8\pi \lambda_{\text{eff}}} \int \left[ \left( \tilde{\Phi} - \tilde{A} \right)^2 + \frac{\alpha}{e} \cdot \left( \tilde{\Phi} - \tilde{A} \right) \right] d^3\mathbf{r},$$

where $F_0$ is the free energy in the normal state (above $T_c$), containing the standard GL $a$ and $b$ coefficient terms, as well as the magnetic field term. This expression for the free energy clearly shows the individual contributions. For further calculations, we factorise the second term and introduce $1/2e = \phi_0/2\pi$ to obtain the more compact form

$$F = F_0 + \frac{1}{8\pi \lambda_{\text{eff}}} \int \left( \tilde{\Phi} - \tilde{A} + \frac{\alpha \phi_0}{2\pi} \right)^2 d^3\mathbf{r}. \quad (3.5)$$

A.2 Fourier transforms

The differential equation for $\tilde{A}$ is

$$-\Delta \tilde{A} = \frac{1}{\lambda_{\text{eff}}} \left( \tilde{\Phi} - \tilde{A} + \frac{\alpha \phi_0}{2\pi} \right) \delta(z). \quad (3.6)$$
We transform (3.6) to Fourier space by setting $\vec{q} = q_x \hat{x} + q_y \hat{y}$ and $\vec{k} = k \hat{z}$ and introducing the following three and two-dimensional Fourier transforms:

\[
\begin{align*}
\vec{A}_{q,k} &\equiv \int \vec{A} e^{i \vec{q} \cdot \vec{r}} e^{ikz} d^3 r \, dz, \\
\vec{A}_q &\equiv \frac{1}{2\pi} \int \vec{A}_{q,k} \, dk = \int \vec{A} e^{i \vec{q} \cdot \vec{r}} d^2 r, \\
\vec{\alpha}_q &\equiv \int \vec{\alpha} e^{i \vec{q} \cdot \vec{r}} d^2 r = \frac{4\pi \alpha}{q_x} \sin \left( \frac{q_x L}{2} \right) \delta(q_y) \hat{y}, \\
\vec{\Phi}_q &\equiv \int \vec{\Phi} e^{i \vec{q} \cdot \vec{r}} d^2 r = i\phi_0 \frac{q_x \hat{y} - q_y \hat{x}}{|q|^2} e^{i q_x L/2}. 
\end{align*}
\] (A.1)

such that the Fourier transform of (3.6) becomes

\[
\vec{A}_{q,k} = \frac{1}{|q|^2 + k^2} \lambda_{\text{eff}} \left( \vec{\Phi}_q - \vec{A}_q + \frac{\vec{\alpha}_q \phi_0}{2\pi} \right). 
\] (A.3)

By integrating over $k$, we go from the three-dimensional $\vec{A}_{q,k}$ to the two-dimensional $\vec{A}_q$, which corresponds to the Fourier transform of $\vec{A}(z = 0)$:

\[
\vec{A}_q = \vec{\Phi}_q + \vec{\alpha}_q \phi_0 / 2\pi \left( 1 + 2|q| \lambda_{\text{eff}} \right). 
\] (3.7)

$\vec{A}_q$ can be written as the sum of a vortex term and a SOC term, that is

\[
\vec{A}_q = \vec{A}_q^{\text{vor}} + \vec{A}_q^{\text{soc}} = \frac{\vec{\Phi}_q}{2\pi} \left( \frac{|q|^2}{2\pi} \lambda_{\text{eff}} \right),
\]

\[
\vec{A}_q = \frac{\vec{\alpha}_q \phi_0}{2\pi} \left( 1 + 2|q| \lambda_{\text{eff}} \right).
\]

A.3 The current density

The Maxwell equation $\vec{j} = -\nabla \times \vec{A}/4\pi$ in Fourier space becomes

\[
\vec{j}_q = \frac{|q|^2}{2\pi} \vec{A}_q = \frac{|q|^2}{2\pi} \left( \vec{A}_q^{\text{vor}} + \vec{A}_q^{\text{soc}} \right) = \vec{j}_q^{\text{vor}} + \vec{j}_q^{\text{soc}}.
\]

The quantity of interest is the current generated due to SOC. Transforming $\vec{j}_q^{\text{soc}}$ to real space gives

\[
\vec{j}_{\text{soc}}(x) = \frac{\alpha \phi_0 \hat{y}}{4\pi^3} \int \frac{\sin \left( \frac{q_x L}{2} \right) |q|^2}{1 + 2|q| \lambda_{\text{eff}}} \frac{q_x \delta(q_y) e^{-i \vec{q} \cdot \vec{r}} d^2 q}{|q|^2}.
\]

The integral over $q_y$ vanishes. To take the absolute value of $|q|$ into account, we split the integral into $(-\infty, 0)$ and $(0, \infty)$. Rewriting the result, we find

\[
\vec{j}_{\text{soc}}(x) = \frac{\alpha \phi_0 \hat{y}}{4\pi^3 \lambda_{\text{eff}}} \int_0^\infty \frac{\sin \left( \frac{p x}{\lambda_{\text{eff}}} \right) + \sin \left( \frac{p (x + 1)}{\lambda_{\text{eff}}} \right)}{1 + 2p} \, dp
\]

with $\vec{j}_{0,\text{soc}} = \alpha \phi_0 / 4\pi^3 \lambda_{\text{eff}}$ and $p = q_x \lambda_{\text{eff}}$. 

\[\text{(3.8)}\]
A.4 The local magnetic field

The Maxwell equation $\vec{h} = \vec{\nabla} \times \vec{A}$ in Fourier space is given by

$$\vec{h}_{q,k} = i(\vec{q} + \vec{k}) \times \vec{A}_{q,k}. \quad (A.4)$$

We substitute $\vec{A}_q$ [given by (3.7)] into $\vec{A}_{q,k}$ [given by (A.3)]. To get the SOC contribution to the local magnetic field, we ignore the vorticity ($\overline{\Phi}_q = 0$). We obtain

$$\vec{h}_{q,k}^{\text{soc}} = \frac{2i|\vec{q}|}{(|\vec{q}|^2 + k^2)(1 + 2|\vec{q}| \lambda_{\text{eff}})}(\vec{q} + \vec{k}) \times \overline{\alpha}_q. \quad (A.5)$$

It follows from the cross product that the magnetic field has a $\hat{x}$- and $\hat{z}$-component, i.e. $\vec{h} = h_x \hat{x} + h_z \hat{z}$, where $h_x$ and $h_z$ are found by taking the inverse Fourier transforms of (A.5). We are interested in the magnetic field at the surface of the superconductor and take $z = 0$.

The $\hat{x}$-component gives an improper integral over $k$, of which the Cauchy principal value is equal to zero. Therefore, $h_x^{\text{soc}} = 0$. The $\hat{z}$-component is given by

$$h_z^{\text{soc}} = \frac{i \alpha \phi_0}{2 \pi^2} \int \frac{\delta(q_y)}{|\vec{q}|^2 + k^2} \frac{|\vec{q}| \sin \left( \frac{1}{2} q_x L \right)}{1 + 2|\vec{q}| \lambda_{\text{eff}}} e^{-i\vec{q} \cdot \vec{r}} d^2 \vec{q} dk$$

where we have used that the integral over $q_y$ vanishes and the integral over $k$ yields $\pi/|q_x|$. We split the remaining integral in $(-\infty, 0)$ and $(0, \infty)$ to take the absolute value into account. Rewriting the result gives

$$h_z^{\text{soc}}(x) = h_0^{\text{soc}} \frac{\pi}{2 \lambda_{\text{eff}}} \int_0^{\infty} \frac{\cos \left( \frac{1}{2} p \frac{|x|}{\lambda_{\text{eff}}} \right)}{1 + 2p} dp \quad (3.9)$$

with $h_0^{\text{soc}} = \frac{\alpha \phi_0}{2 \pi^2 \lambda_{\text{eff}}}$.

A.5 The interaction energy

The interaction energy has two contributions. The first one is the combined superconductivity and SOC term originating from the first integral in (3.5), which we name $E^{\text{int.s}}$. The contribution from the magnetic field, given by the second integral in (3.5), will be referred to as $E^{\text{int.h}}$. Since the magnetic field gives a volume integral, while the other term is described by a surface integral, we evaluate them separately and take the sum in the end.

We first consider the magnetic field term. We use (A.4) to find the Fourier transform of $h^2$, which is

$$h_{q,k}^2 = h_{q,k} \cdot h_{-q,-k} \sim \left[ (\vec{q} + \vec{k}) \times (\overline{\Phi}_q + \overline{\alpha}_q) \right] \cdot \left[ (\vec{q} + \vec{k}) \times (\overline{\Phi}_q^* + \overline{\alpha}_q^*) \right]$$

where we used that $\overline{\Phi}_q = \overline{\Phi}_q^*$ and $\overline{\alpha}_q = \overline{\alpha}_q^*$. We apply the vector identity $(a \times b) \cdot (c \times d) = (a \cdot c)(b \cdot d) - (a \cdot d)(b \cdot c)$. Since the vortices and SOC are both located in-plane, we have $\vec{k} \cdot \Phi_q = \vec{k} \cdot \Phi_q^* = \vec{k} \cdot \overline{\alpha}_q = \vec{k} \cdot \overline{\alpha}_q^* = 0$. The $\vec{q} \cdot \Phi_q$ term turns out to be zero as well. Since $\vec{q} \perp \vec{k}$, we reduce $(\vec{q} + \vec{k})^2 = \vec{q}^2 + \vec{k}^2$. The remaining terms in $h_{q,k}^2$ are

$$h_{q,k}^2 \sim |\Phi_q|^2 + \overline{\alpha}_q \cdot \Phi_q^* + \overline{\alpha}_q^* \cdot \Phi_q + |\overline{\alpha}_q|^2 - (\vec{q} \cdot \overline{\alpha}_q)(\vec{q} \cdot \overline{\alpha}_q^*).$$

The interaction between the vortices and SOC is given by the two mixed terms $\overline{\alpha}_q \cdot \Phi_q^* + \overline{\alpha}_q^* \cdot \Phi_q$. The contribution of the interaction to the energy, originating from the magnetic field (including pre-factors)
is given by
\[
E_{q,k}^{\text{int.}} = \frac{1}{8\pi} \left( \frac{2|q|}{1 + 2|q|\lambda_{\text{eff}}} \right)^2 \frac{1}{|q|^2 + k^2} \left( \frac{\alpha_q}{2e} \cdot \Phi_q^* + \frac{\alpha_q^*}{2e} \cdot \Phi_q \right).
\]

We substitute \(\alpha_q\) and \(\Phi_q\) from Eqs. (A.1) and (A.2). We take the inverse Fourier transform and set \(e^{iq_xx} = e^{iq_yy} = e^{ik_z} = 1\). We obtain
\[
E_{q,k}^{\text{int.}} = \frac{\alpha_0^2}{4\pi^4} \int \frac{\delta(q_y)}{|q_x|^2 + k^2} \frac{\sin^2 \left( \frac{1}{2} q_x L \right)}{(1 + 2|q_x|\lambda_{\text{eff}})^2} d^2q d\mathbf{k}
= \frac{\alpha_0^2}{4\pi^4} \int_{-\infty}^{\infty} \frac{\sin^2 \left( \frac{1}{2} q_x L \right)}{|q_x|(1 + 2|q_x|\lambda_{\text{eff}})^2} dq_x,
\]
(A.6)
where we have used that the integral over \(q_y\) vanishes and the integral over \(k\) gives \(\pi/|q_x|\). To write \(E_{q,k}^{\text{int.}}\) in the same form, we substitute (3.7) in the integrand, such that
\[
\left( \Phi - \Phi_\mathbf{A} + \frac{\alpha_0 \phi_0}{2\pi} \right)^2 = \left[ \frac{2|q|\lambda_{\text{eff}}}{1 + 2|q|\lambda_{\text{eff}}} \left( \Phi_q^* + \frac{\alpha_q \phi_0}{2\pi} \right) \right]^2.
\]
We work out the brackets and only keep the mixed terms \(\alpha_q \cdot \Phi_q^* + \alpha_q^* \cdot \Phi_q\). The corresponding interaction energy is given by
\[
E_{q,k}^{\text{int.}} = \frac{\alpha_0^2 \lambda_{\text{eff}}}{2\pi^3} \int_{-\infty}^{\infty} \frac{\sin^2 \left( \frac{1}{2} q_x L \right)}{|q_x|(1 + 2|q_x|\lambda_{\text{eff}})^2} dq_x.
\]
We are interested in the total interaction energy \(E^\text{int}\), which is given by the sum of Eqs. (A.6) and (A.7). Again splitting the integral into \((-\infty, 0)\) and \((0, \infty)\), we finally obtain the total interaction energy
\[
E^\text{int} = \frac{\alpha_0^2 \lambda_{\text{eff}}}{2\pi^3} \int_{0}^{\infty} \frac{\sin^2 \left( \frac{1}{2} q_x L \right)}{q_x(1 + 2q_x\lambda_{\text{eff}})} dq_x.
\]
(A.8)
This interaction energy only describes the interaction with a vortex at \(x = L/2\). To describe the interaction with a vortex at a general position \(x = x_0\), we translate the Fourier transform of the vortex as follows:
\[
\Phi_q(x_0) = e^{iq_xx_0} \Phi_q(0) = e^{iq_x(x_0 - L/2)} \Phi_q(\frac{1}{2}L).
\]
We repeat the calculation for this general \(x_0\). Since this holds for all \(x_0 \in \mathbb{R}\), we may replace \(x_0\) by \(x\). We can now express the interaction energy as a function of \(x\) as
\[
E^\text{int}(x) = -E_0^\text{int} \int_0^\infty \frac{\sin \left( \frac{pL}{\lambda_{\text{eff}}} \right) \sin \left( \frac{px}{\lambda_{\text{eff}}} \right)}{p(1 + 2p)} dp
\]
with \(E_0^\text{int} = \alpha_0^2/2\pi^3\).

**Estimate for a thick ferromagnet**

The objective of calculating the interaction energy is to derive a criterion for vortex generation. To do this, we estimate (3.10) in the case of a thick ferromagnet, i.e. \(L \gg \lambda_{\text{eff}}\). We introduce the substitutions \(y = 2q\lambda_{\text{eff}}, p = L/4\lambda_{\text{eff}}\) and \(C = -\alpha_0^2/2\pi^3\). Since \(L \gg \lambda_{\text{eff}}, p \gg 1\). We split the integral range in
\[ E^{\text{int}} = C \int_0^{1/p} \frac{\sin^2(py)}{y(1 + y)} \, dy + C \int_{1/p}^{\infty} \frac{\sin^2(py)}{y(1 + y)} \, dy. \] (A.9)

Since \( p \gg 1 \), the range \([0, 1/p]\) is very small. On this small interval, \( \sin^2(py) \) is bounded by \( p^2 y^2 \). Since \( y \ll 1 \), we estimate the denominator by \( 1 + y \approx 1 \). We obtain

\[
C \int_0^{1/p} \frac{\sin^2(py)}{y(1 + y)} \, dy < C p^2 \int_0^{1/p} \frac{y}{1 + y} \, dy \approx C p^2 \int_0^{1/p} \frac{y}{2} \, dy = \frac{C}{2p}.
\]

For the second integral in (A.9), we use \( \sin^2(py) = \frac{1}{2}(1 - \cos(2py)) \), which yields again two integrals. The first one can be estimated as

\[
\int_{1/p}^{\infty} \frac{1}{y(1 + y)} \, dy = \ln(y) - \ln(1 + y) \bigg|_{1/p}^{\infty} \approx \ln(p).
\]

To evaluate the integral with \( \cos(2py) \), we introduce another substitution \( u = 2py \). Carefully taking the integration limits into account, we get

\[
\int_{1/p}^{\infty} \frac{\cos(2py)}{y(1 + y)} \, dy = \int_{2}^{\infty} \frac{\cos u}{u} \, du + \int_{2}^{\infty} \frac{\cos u}{u + 2p} \, du.
\]

For \( p \gg 1 \), the first term is just a constant smaller than 1, while the second term vanishes. To summarise, the first integral in (A.9) follows \( \sim 1/p \), whereas the second integral \( \sim \ln(p) \). Hence, for \( p \gg 1 \), the interaction energy for thick ferromagnets can be estimated by

\[
E^{\text{int}} \approx \frac{\alpha \phi_0^2}{4\pi^3} \ln \left( \frac{L}{4\lambda_{\text{eff}}} \right).
\] (A.10)

A.6 The lower critical field

To derive a criterion for spontaneous generation of vortices, we first derive an expression for the lower critical field \( h_{c1} \) in presence of SOC. Following page 65 of Ref. [83], the Gibbs function writes

\[
G = n_L (E^{\text{vor}} + E^{\text{int}}) - B h \frac{4\pi}{4\pi},
\]

where \( n_L \) is the number of lines, which is related to the induction \( B \) as \( B = n_L \phi_0 \). \( E^{\text{vor}} \) is the energy of vortices [83] and \( E^{\text{int}} \) is the interaction energy between the vortices and SOC. At the transition from the Meissner state to the vortex state, \( h = h_{c1} \) and \( G = 0 \). We find

\[
h_{c1} = \frac{4\pi}{\phi_0} (E^{\text{vor}} + E^{\text{int}}).
\]

A.7 Ginzburg-Landau equation

We consider the free energy \( F = \int f \, d^2r \) where \( f \) is given by (3.2). For simplicity, we neglect the magnetic terms \( A \) and \( \tilde{h} \). Since the SOC is directed along the interface, i.e. \( \tilde{A} \parallel \tilde{y} \), (3.2) simplifies to

\[
f = a|\psi|^2 + \frac{b}{2}|\psi|^4 + \frac{1}{4m} \left( \left| \frac{\partial \psi}{\partial x} \right|^2 + \left| \frac{\partial \psi}{\partial y} \right|^2 \right) + \frac{i\alpha}{4m} \left( \psi \frac{\partial \psi^*}{\partial y} - \psi^* \frac{\partial \psi}{\partial y} \right).\]
The Ginzburg-Landau (GL) equation is obtained by minimising the free energy $F$ using the Euler-Lagrange method. We use that $|\psi|^2 = \psi\psi^* = \psi^*\psi$. Minimising with respect to $\psi^*$, all terms containing $\psi^*$ disappear. The GL equation in the absence of a magnetic field is

$$a\psi + b|\psi|^2\psi - \frac{1}{4m} \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) - \frac{i\alpha}{2m} \frac{\partial \psi}{\partial y} = 0. \quad (3.15)$$

Minimising $F$ with respect to $\psi$ results in the complex conjugate of (3.15).

At $T_c$, the order parameter becomes small, such that the quadratic and higher order terms are negligible and the GL equation is linearised, i.e., the $b|\psi|^2\psi$ term is neglected. We use $\psi(x, y) = \psi(x)e^{iq_yy}$ and introduce the substitutions $T = 4ma/\alpha^2$, $\kappa = q_y/\alpha$, $x \mapsto ax$, $L \mapsto \alpha L$. The linearised GL equation becomes

$$\begin{cases} 
(\tau + (\kappa + 1)^2 - 1) \psi(x) - \frac{d^2 \psi}{dx^2} = 0 & \text{for } |x| < \frac{1}{2}L, \\
(\tau + \kappa^2) \psi(x) - \frac{d^2 \psi}{dx^2} = 0 & \text{for } |x| > \frac{1}{2}L.
\end{cases}$$

The wave function satisfying the boundary conditions $\psi(x) = \psi(-x)$ and $\lim_{x \to \pm \infty} \psi(x) = 0$ is

$$\psi(x) = \begin{cases} 
\psi_1 \cos \left( \sqrt{\tau - (\kappa + 1)^2x} \right) & \text{for } |x| < \frac{1}{2}L, \\
\psi_2 \exp \left( -\sqrt{\tau + \kappa^2x} \right) & \text{for } |x| > \frac{1}{2}L.
\end{cases} \quad (A.11)$$

We define $\kappa = -1 + \varepsilon$, where $\varepsilon > 0$ is a small difference between the modulation vector and $\alpha$. We impose continuity of $\psi(x)$ and $\psi'(x)$ at $x = \pm L/2$, which results in a relation between $\tau$ and $\varepsilon$. Maximising $\varepsilon$ with respect to $\tau$ (i.e. $d\tau/d\varepsilon = 0$), we find $\tau \approx 1 - (\pi/L)^2$ and $\varepsilon \approx \pi^2/(\sqrt{2}\alpha^4 + \pi^2)$. We express $\psi_2$ in terms of $\psi_1$ and set $\psi_1 = 1$.

The current density is obtained from $\vec{j} = -\partial f/\partial \vec{A}$. After minimising $f$, we set $\vec{A} = 0$ and obtain

$$\vec{j} = \frac{ie}{2m} \left[ \psi^* \nabla \psi - \psi \nabla \psi^* \right] + \frac{2\alpha^2}{\alpha^2} |\psi|^2. \quad (3.16)$$

We substitute $\psi(x, y) = \psi(x)e^{iq_yy}$, with $\psi(x)$ given by (A.11) and $q_y = \kappa\alpha = \alpha(-1 + \varepsilon)$, where $\varepsilon$ allows for a small variation from the optimal $q_y = -\alpha$ (which is only an estimate). Since $\psi(x) \in \mathbb{R}$, the component $j_x = 0$.

In the regions $|x| > L/2$, there is no SOC, which implies the last term in (3.16) vanishes and $\varepsilon = 0$. For $|x| < L/2$, we have $q_y = \alpha(-1 + \varepsilon)$, which yields a current density proportional to $\varepsilon$. The resulting current density is

$$\vec{j}(x) = \begin{cases} 
\frac{e\alpha}{m} |\psi(x)|^2 \hat{y} & \text{for } |x| > L/2, \\
-\frac{e\alpha\varepsilon}{m} |\psi(x)|^2 \hat{y} & \text{for } |x| < L/2,
\end{cases} \quad (3.17)$$

where $\varepsilon$ is found self-consistently.

### A.8 Modulated critical temperature

After obtaining the GL equation, we can use it to investigate the transition temperature $T_c$. We write the wave function as $\psi(x, y) = \psi(x)\psi(y)$ and solve it in two steps. We first assume $\psi(x)$ to be constant and optimise for $\psi(y)$. We then use the optimised value of $\psi(y)$ to find $\psi(x)$.

For the first step, we assume superconductivity is uniform in the $x$-direction, and a plane wave in the $y$-direction, i.e. $\psi(x, y) = \psi_0 e^{iq_yy}$. We linearise the GL equation (3.15) since we consider the regime close to the critical temperature. Since the wave function no longer depends on $x$, the $x$-derivative is zero. Substituting the wave function into our linearised GL equation, we obtain a quadratic equation in...
A.9. The coherence length

\[ q_y, \quad a_0 \frac{T - T_c}{T_c} + \frac{1}{4m} q_y^2 + \frac{\alpha}{2m} q_y = 0. \]

Taking the derivative with respect to \( q_y \) and setting it equal to zero, we find that \( T - T_c \) has a maximum for \( q_y = -\alpha \).

We use this value for \( q_y \) to consider the general case in which we no longer assume uniformity in \( x \). We use a wave function of the form \( \psi(x, y) = \psi(x)e^{-iyy} \). We substitute this into the GL equation (3.15) and apply separation of variables. Since we are now solving for \( \psi(x) \), the derivatives with respect to \( y \) will become a constant set to \( T_c \). We distinguish between the regions with and without SOC. In the presence of SOC (\( \alpha > 0 \)), the \( y \)-dependent terms in the GL equation (3.15) become

\[-\frac{1}{4m} \frac{\partial^2 \psi}{\partial y^2} - i\alpha \frac{\partial \psi}{2m \partial y} = \frac{\alpha^2}{4m} \psi.\]

In the absence of SOC (\( \alpha = 0 \)) only the \( \frac{\partial^2 \psi}{\partial y^2} \) term remains, which gives a contribution of \( \frac{\alpha^2}{4m} \).

For a fixed value of \( \alpha \), these terms can be considered as a constant offset to \( T_c \). We obtain

\[ T_{c+} = T_c \left( 1 + \frac{\alpha^2}{4ma_0} \right). \quad (3.18) \]

### A.9 The coherence length

The \( y \)-dependent terms contain the SOC. Instead of taking the SOC into account explicitly through the \( y \)-terms, we include SOC implicitly by substituting the modulated critical temperature \( T_{c+} \) into the GL equation (3.15) as follows:

\[ a_0 \frac{T - T_{c+}}{T_c} \psi + b|\psi|^2 \psi - \frac{1}{4m} \frac{d^2 \psi}{dx^2} = 0. \quad (A.12) \]

Far inside the superconductor (for \( x \gg 0 \)), we expect superconductivity to be homogeneous, meaning \( \psi \) is constant and we can neglect the second derivative with respect to \( x \). We obtain

\[ |\psi|^2 = -\frac{a_0}{b} \frac{T - T_{c+}}{T_c}. \]

We note that \( T \ll T_c < T_{c+} \) such that \( |\psi|^2 > 0 \). For convenience of writing, we define \( \psi_\infty \equiv \sqrt{|\psi|^2} \), i.e.,

\[ \psi_\infty \equiv \sqrt{\frac{a_0}{b} \frac{T - T_{c+}}{T_c}}. \]

Using this, we write the wave function as \( \psi(x) = \psi_\infty f(x) \), where \( 0 \leq f(x) \leq 1 \) takes the spatial variation into account. We substitute this into (A.12) and divide by \( |a|\psi_\infty \). We obtain

\[ \frac{a}{|a|} f + \frac{|b|\psi_\infty^2}{|a|} f^3 - \frac{1}{4m|a|} \frac{\partial^2 \psi}{\partial x^2} = 0. \]

The first term is equal to \( a/|a| = \text{sign}(a) = -1 \). The second term simply yields \( 1 \). We define the prefactor of the third term as the temperature dependent coherence length \( \xi(T) \), which is equal to

\[ \xi^2(T) = \frac{1}{4m a_0} \frac{T_c}{T - T_{c+}}. \quad (3.19) \]
An important property of the coherence length is that it diverges as $T \to T_c^+$, which is indeed the case for this expression for $\xi(T)$.

### A.10 The half-plane wave function

Using the wave function $\psi(x) = \psi_\infty f(x)$ and the coherence length in (3.19), we can rewrite the GL equation in terms of $f$. For $x > 0$, we get

$$-\xi^2(T) \frac{d^2 f}{dx^2} - f + f^3 = 0. \tag{A.13}$$

where $\xi$ is defined in (3.19). We multiply (A.13) by $df/dx$ and rewrite it as

$$-\xi^2(T) \frac{d}{dx} \left( \frac{df}{dx} \right)^2 - \frac{d}{dx} \left( \frac{f^2}{2} \right) + \frac{d}{dx} \left( \frac{f^4}{4} \right) = 0.$$

We integrate this equation. Since $\lim_{x \to \infty} f(x) = 1$, the integration constant is equal to $-\frac{1}{2}$ and (A.13) becomes

$$\xi^2(T) \left( \frac{df}{dx} \right)^2 = \frac{1}{2} (1 - f^2)^2.$$

Taking the square root of both sides of the equation and rewriting the constants on one side, we find

$$\frac{df}{dx} = \pm \frac{1 - f^2}{\sqrt{2\xi(T)}}. \tag{A.14}$$

We have defined $f$ to lay between $0 \leq f \leq 1$, such that $1 - f^2 \geq 0$. The function $f$ should be an increasing function of $x$ and have its maximum for large values of $x$, which implies we expect the derivative to be positive and therefore, we choose the $+$ sign. The solution of (A.14) is

$$f(x) = \tanh \left( \frac{x}{\sqrt{2\xi}} + c_1 \right) = \frac{e^{\sqrt{2x/\xi}e^{2c_1}} - 1}{e^{\sqrt{2x/\xi}e^{2c_1}} + 1}, \tag{A.15}$$

where $c_1$ is a constant determined by the boundary condition $f(0) = f_0$ as follows,

$$e^{2c_1} = \frac{1 + f_0}{1 - f_0}, \quad \Rightarrow \quad c_1 = \frac{1}{2} \ln \left( \frac{1 + f_0}{1 - f_0} \right). \tag{A.16}$$

The value of $f_0$ will be determined later from continuity of $df/dx$ at $x = 0$. We first consider the region $x < 0$, for which there is no $T_c$ enhancement. The GL equation is

$$a_0 \frac{T - T_c}{T_c} \psi + b|\psi|^2 \psi - \frac{1}{4m} \frac{\partial^2 \psi}{\partial x^2} = 0. \tag{A.17}$$

We substitute $\psi(x) = \psi_\infty f(x)$, use $\xi(T)$ from (3.19), and follow the same steps as before. The boundary condition $\lim_{x \to -\infty} f(x) = 0$ results in the integration constant being equal to 0. Dividing by $\psi_\infty^2$ and multiplying by $\xi^2$, we get

$$\xi^2(T) \left( \frac{df}{dx} \right)^2 = \tau f^2 + \frac{1}{2} f^4, \quad \tau \equiv \frac{T - T_c}{|T - T_c|}.$$
We solve these differential equations for \( f(x) \) and use that the wave function is continuous at \( x = 0 \) and equal to \( f(0) \equiv f_0 \), for some \( 0 < f_0 < 1 \). Substituting \( f(x) \) back into \( \psi(x) = \psi_\infty f(x) \), we find

\[
\psi(x) = \begin{cases} 
- \frac{4\tau c_2 e^{\sqrt{\tau x}/\xi}}{2\tau c_2^2 e^{2\sqrt{\tau x}/\xi} - 1} & \text{for } x < 0, \\
\tanh \left( \frac{x}{\sqrt{2\xi}} + c_1 \right) & \text{for } x > 0,
\end{cases}
\]

with \( c_1 \) given by (A.16) and \( c_2 \) is determined by the boundary condition \( f(0) = f_0 \) as

\[
c_2 = -\frac{2\tau + \sqrt{4\tau^2 + 2\tau f_0^2}}{2\tau f_0}.
\]

Finally, \( f_0 \) is obtained from continuity of the \( df/dx \) at \( x = 0 \) and is equal to \( f_0 = 1/\sqrt{2(\tau + 1)} \).

### A.11 The half-plane current

We substitute the total current (3.21) into Biot-Savart’s law \( \vec{A} = \int \vec{j}/\sqrt{x^2 + y^2} \, d\vec{l} \) and introduce the dimensionless lengths \( x \mapsto x/\lambda_{\text{eff}}, y \mapsto y/\lambda_{\text{eff}} \) to obtain a dimensionless form. The implicit equation for \( A_y(x, z) \) in the \( z = 0 \) plane is given by

\[
A_y(x, z = 0) = \int_{-\infty}^{\infty} \frac{j_0}{\sqrt{x^2 + y^2}} \, dy - \frac{1}{4\pi} \int_{-\infty}^{\infty} \int_{0}^{\infty} \frac{A_y(x')}{\sqrt{(x - x')^2 + y^2}} \, dx' \, dy.
\]

This expression is for a ferromagnet covering the half-plane, i.e. \( x \in [0, \infty) \). To avoid divergence issues, we consider a ferromagnetic strip instead, i.e. \( x \in [0, L] \). This means that at the other end of the strip we have to add a current \(-j_0 \delta(x - L) \vec{y}\). The integration range for \( x' \) is now \([0, L]\). Since these integrals are even in \( y \), we use that the integral over \((-\infty, \infty)\) is equal to twice the integral over \([0, \infty)\). The expression for \( A_y(x) \) becomes

\[
A_y(x) = 2j_0 \int_{0}^{\infty} \frac{1}{\sqrt{x^2 + y^2}} - \frac{1}{\sqrt{(x - L)^2 + y^2}} \, dy - \frac{1}{2\pi} \int_{0}^{L} \int_{0}^{\infty} \frac{A_y(x')}{\sqrt{(x - x')^2 + y^2}} \, dx' \, dy.
\]

To remove the prefactor, we substitute \( A_y \mapsto A_y/2j_0 \). Performing integration over \( y \), we obtain

\[
A_y(x) = \ln |x - L| - \ln |x| + \frac{1}{2\pi} \int_{0}^{L} A_y(x') \ln |x - x'| \, dx'.
\]

(A.22)
Appendix B

The phase diagram of superconductors with spin-orbit coupling

B.1 Residual theorem

To evaluate the integral over the kinetic energy, we factorise the denominator of \( F_{1+} \) as

\[
F_{1+}(\omega_n, \varepsilon_k) = \frac{\Delta}{(\omega_n + i\hbar)^2 + \varepsilon_k^2 + \Delta^2}
\]

\[
= \frac{\Delta}{(\varepsilon_k + \sqrt{(\omega_n + i\hbar)^2 + \Delta^2})(\varepsilon_k - \sqrt{(\omega_n + i\hbar)^2 + \Delta^2})}.
\]

From which we identify the two poles \( \varepsilon_k = \pm i \sqrt{(\omega_n + i\hbar)^2 + |\Delta|^2} \). Applying the Residual Theorem to the pole \( \varepsilon_k = i \sqrt{(\omega_n + i\hbar)^2 + |\Delta|^2} \), we obtain

\[
\int_0^\infty F_{1+}(\omega_n, \varepsilon_k) \, d\varepsilon_k = 2\pi i \cdot \frac{\Delta}{2i \sqrt{(\omega_n + i\hbar)^2 + \Delta^2}} = \frac{\pi \Delta}{\sqrt{(\omega_n + i\hbar)^2 + \Delta^2}}.
\]

The self-consistency equation has now reduced to

\[
\Delta = \pi VT \sum_n \frac{\Delta}{\sqrt{(\omega_n + i\hbar)^2 + \Delta^2}}.
\]

(4.1)

B.2 From kernel to self-consistency equation

The kernel is

\[
K(T, \Delta, h) = \pi VT \sum_n \frac{1}{\sqrt{(\omega_n + i\hbar)^2 + \Delta^2}} = 1.
\]

(4.2)

In the presence of a magnetic field, the critical temperature becomes dependent on the magnetic field as well, i.e. \( T_c = T_c(h) \). Hence, we define two critical temperatures: \( T_{c0} = T_c(0) \) and \( T_c = T_c(h) \). The kernel is equal to 1 at the every phase transition, meaning that both \( K(T_c, 0, h) = 1 \) and \( K(T_{c0}, 0, 0) = 1 \). Therefore, \( K(T_c, 0, h) = K(T_{c0}, 0, 0) \). To allow for certain mathematical manipulations, we subtract
We consider the Debye frequency to be much larger than the temperatures of interest, i.e. \( \omega_D \gg T_{c0}, T_c \). Hence, we may use that \( \omega_D \approx k_B T_c \) such that the cut-off reduces to \( N = \omega_D / T_c \). We find
\[
K(T_{c0},0,0) - K(T_c,0,0) = \pi V \left[ T_{c0} \sum_{n=0}^{\omega_D / T_{c0}} \frac{1}{(2n+1)\pi} - \frac{1}{(2n+1)\pi T_c} \right] = V \left[ \sum_{n=0}^{\omega_D / T_{c0}} \frac{1}{2n+1} - \sum_{n=0}^{\omega_D / T_c} \frac{1}{2n+1} \right].
\]

The sum can be evaluated in terms of the digamma function \( \psi_0 \) as
\[
\sum_{n=0}^{N} \frac{1}{2n+1} = \frac{\psi_0(N + \frac{3}{2})}{2} + \gamma \ln 2
\]
where \( \gamma \) is the Euler-Mascheroni constant. Plugging this back into \( K(T_{c0},0,0) - K(T_c,0,0) \), we find that the terms with \( \gamma \) and \( \ln 2 \) cancel.

\[
K(T_{c0},0,0) - K(T_c,0,0) = \frac{V}{2} \left[ \psi_0 \left( \frac{\omega_D}{T_{c0}} + \frac{3}{2} \right) - \psi_0 \left( \frac{\omega_D}{T_c} + \frac{3}{2} \right) \right].
\]

We consider the Debye frequency to be much larger than the temperatures of interest, i.e. \( \omega_D \gg T_{c0}, T_c \). Hence, we may use that \( \omega_D \rightarrow \infty \). In this approximation, the digamma function is given by
\[
\lim_{N \rightarrow \infty} \psi_0 \left( N + \frac{3}{2} \right) = \ln(N) + \frac{1}{N} - \ldots
\]

Using this, \( K(T_{c0},0,0) - K(T_c,0,0) \) reduces to
\[
K(T_{c0},0,0) - K(T_c,0,0) = \frac{V}{2} \left[ \ln \left( \frac{\omega_D}{T_{c0}} + \frac{3}{2} \right) - \ln \left( \frac{\omega_D}{T_c} + \frac{3}{2} \right) \right] = \frac{V}{2} \ln \left( \frac{T_c}{T_{c0}} \right).
\]

The right hand side of (B.1) is
\[
K(T_c,0,h) - K(T_c,0,0) = \pi V T_c \sum_m \left( \frac{1}{|\omega_n + i\hbar|} - \frac{1}{|\omega_n|} \right)
\]
Substituting everything back into (B.1), we obtain the self-consistency equation
\[
\ln \left( \frac{T_c}{T_{c0}} \right) = 2\pi T_c \sum_m \left( \frac{1}{|\omega_n + i\hbar|} - \frac{1}{|\omega_n|} \right).
\]

**B.3 The Usadel equations near \( T_c \)**

We start from the transport equation for \( f \) and \( g \),
\[
\frac{D}{\pi} \nabla (g \nabla f + f \nabla g) + 2i\omega_n f = \hat{\Delta} \hat{g} - g \hat{\Delta} + \hat{\sigma} f - f \hat{\sigma}^*.
\]
Close to $T_c$, we approximate $g$ by $g = -i\pi \sigma_0 \text{sgn}(\omega_n)$, such that $\hat{g} = i\pi \sigma_0 \text{sgn}(\omega_n)$ and $\nabla \hat{g} = 0$. We divide by $-i \text{sgn}(\omega_n)$. The transport equation reduces to
\[ D\nabla^2 f - 2|\omega_n| f = -2\pi \Delta - i \text{sgn}(\omega_n) \left( \tilde{h} \cdot \hat{\sigma} f - f \tilde{h} \cdot \hat{\sigma}^* \right). \]

We substitute $f = (f_s + \tilde{f}_t \hat{\sigma}) e^{i\sigma_y}$ and $\Delta = \Delta_s e^{i\sigma_y}$ and divide by $i\sigma_y$. We split the resulting equation in two equations: a scalar equation for $f_s$ and a vector equation for $\tilde{f}_t$, i.e.
\[
\begin{cases}
D\nabla^2 f_s - 2|\omega_n| f_s = -2\pi \Delta_s - i \text{sgn}(\omega_n) \left( \tilde{h} \hat{\sigma} f_t \hat{\sigma} - f_t \tilde{h} \hat{\sigma} \hat{\sigma}^* \right) \\
D\nabla^2 \tilde{f}_t \hat{\sigma} - 2|\omega_n| \tilde{f}_t \hat{\sigma} = 2i \text{sgn}(\omega_n) \tilde{h} f_s \hat{\sigma}
\end{cases}
\]

(B.2)

The equation for $f_s$ can be simplified by applying (B.5) to the magnetic field term, which becomes
\[
\tilde{h} \hat{\sigma} f_t \hat{\sigma} - f_t \tilde{h} \hat{\sigma} \hat{\sigma}^* = \tilde{h} f_t \hat{\sigma} + i(\tilde{h} \times \tilde{f}_t) \hat{\sigma} + f_t \tilde{h} + i(f_t \times \tilde{h}) \hat{\sigma} = 2\tilde{h} \cdot \tilde{f}_t.
\]

We divide the equation for $\tilde{f}_t$ by $\hat{\sigma}$ and group the terms. The simplified Usadel equations near $T_c$ are
\[
\begin{cases}
(D\nabla^2 - 2|\omega_n|) f_s - 2\pi \Delta_s + 2i \text{sgn}(\omega_n) \tilde{h} \cdot \tilde{f}_t, \\
(D\nabla^2 - 2|\omega_n|) \tilde{f}_t = 2i \text{sgn}(\omega_n) \tilde{h} f_s.
\end{cases}
\]

(B.11)

### B.4 Covariant derivatives

The spin-orbit coupling (SOC) is included by replacing the standard derivative by the covariant derivative $\nabla \rightarrow \nabla - i\hat{A}$, where $\nabla$ is the standard derivative and $\hat{A}$ the spin-orbit field vector. This replacement is made in both the Usadel equations and the boundary conditions.

The spin-orbit field goes accompanied with a very convoluted notation. We define $\hat{A}$ as a $4 \times 4$ matrix in particle-hole $\otimes$ spin space, which contains the spin-orbit field $\hat{A}$, consisting of $2 \times 2$ matrices $A_x$, $A_y$ and $A_z$. These matrices can be expressed in spin space as $A_k = \hat{A}_k \hat{\sigma}$. The element $\hat{A}_k^p$ of the spin-orbit field has real space coordinate $r$ and spin space coordinate $s$. In matrix-form,
\[ \hat{A} = \begin{bmatrix} A_x & 0 \\ 0 & -A^*_x \end{bmatrix}, \quad \hat{A} = \begin{bmatrix} A_x \\ A_y \\ A_z \end{bmatrix}, \quad \begin{bmatrix} A_x \hat{\sigma} \\ A_y \hat{\sigma} \\ A_z \hat{\sigma} \end{bmatrix} = \begin{bmatrix} A_x^\sigma + A_y^\sigma y + A_z^\sigma z \\ A_y^\sigma x + A_y^\sigma y + A_z^\sigma z \\ A_z^\sigma x + A_y^\sigma y + A_z^\sigma z \end{bmatrix}. \]

In our system, we consider Rashba spin-orbit coupling $\hat{H}_{\text{SOC}} = \alpha(\hat{s} \cdot \hat{\sigma}) \cdot \hat{n}$, with $\hat{s} = (s_x, s_y, 0)^T$, $\hat{n} = (p_x, p_y, p_z)^T$ and $\alpha = \tilde{\alpha} \zeta$, such that $\hat{H}_{\text{SOC}} = \alpha (s_z p_y - s_y p_z)$. In spin-orbit field notation, this gives
\[
\begin{bmatrix} \hat{A}_x \\ \hat{A}_y \\ \hat{A}_z \end{bmatrix} = \begin{bmatrix} \alpha \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} A_x = -\alpha \sigma_y \\ A_y = \alpha \sigma_z \\ A_z = -\alpha \sigma_x \end{bmatrix} \quad \begin{bmatrix} A_x^\sigma = -\alpha \\ A_y^\sigma = \alpha \\ A_z^\sigma = -\alpha \end{bmatrix}.
\]

The Green’s function $\hat{g}$ is a matrix in the $4 \times 4$ spin $\otimes$ particle-hole space with the structure [129]
\[ \hat{g} = \begin{bmatrix} g & f \\ f & \tilde{g} \end{bmatrix}, \]

where $\hat{g}$ and $\tilde{f}$ are the particle-hole conjugates of the Green’s function $g$ and $f$. Applying the covariant derivative to $\hat{g}$ gives
\[
\nabla \hat{g} \rightarrow \nabla \hat{g} + i \left[ \hat{A}, \hat{g} \right] = \nabla \begin{bmatrix} g & f \\ f & \tilde{g} \end{bmatrix} - i \left[ \begin{bmatrix} \hat{A} & \hat{A} \\ -\hat{A} & \hat{A} \end{bmatrix} \begin{bmatrix} g & f \\ f & \tilde{g} \end{bmatrix} \right].
\]

(B.3)
We are particularly interested in applying the covariant derivative to the anomalous Green’s function $f = (f_\tau + \bar{f}_\tau) i \sigma^y$, i.e. the top-right term in (B.3),

$$\nabla f \mapsto \nabla (f_\tau + \bar{f}_\tau) i \sigma^y - i \left( A(f_\tau + \bar{f}_\tau) i \sigma^y + (f_\tau + \bar{f}_\tau) i \sigma^y A^* \right).$$

We right-multiply the last term by $\sigma^y \sigma^y = 1$ to take $i \sigma_y$ outside of the brackets. We use that $A_k = \tilde{A}_k \bar{\sigma}$ and $A_k^* = \tilde{A}_k^* \bar{\sigma}^*$, with $k \in \{x, y, z\}$. We assume the SOC is Hermitian, such that $\tilde{A}_k$ is real and $\tilde{A}_k = \tilde{A}_k^*$. Combining this, we obtain

$$\partial_k f \mapsto \left( \partial_k (f_\tau + \bar{f}_\tau) - i \tilde{A}_k \bar{\sigma}(f_\tau + \bar{f}_\tau) - i (f_\tau + \bar{f}_\tau) \sigma^y \tilde{A}_k \bar{\sigma}^* \sigma^y \right) i \sigma^y.$$

Since $\bar{\sigma}^* = (\sigma^z, -\sigma^y, \sigma^x)^T$, we can evaluate the product of matrices as $\sigma^y \tilde{A}_k \bar{\sigma}^* \sigma^y = -\tilde{A}_k \bar{\sigma}$. We then remove the brackets around $(f_\tau + \bar{f}_\tau)$. Since $f_\tau$ is a scalar we can move it in front of $\tilde{A}_k \bar{\sigma}$, which cancels some of the terms. What remains is

$$\partial_k f \mapsto \left[ \partial_k (f_\tau + \bar{f}_\tau) - i \left( \tilde{A}_k \bar{\sigma} \tilde{f}_\tau - \tilde{f}_\tau \tilde{A}_k \bar{\sigma} \right) \right] i \sigma^y. \tag{B.4}$$

Since the vectors $\tilde{A}_k$ and $\tilde{f}_\tau$ and $\bar{\sigma}$ live in different spaces, the products between them are not all equal. More generally, using the cyclic permutation rules of the Pauli matrices, we write the product of the four matrices as

$$\tilde{a} \bar{\sigma} \cdot \tilde{b} \bar{\sigma} = (a_x \sigma_x + a_y \sigma_y + a_z \sigma_z) \cdot (b_x \sigma_x + b_y \sigma_y + b_z \sigma_z)$$

$$= a_x b_x a_y b_y a_z b_z + i (a_y b_z - a_z b_y) \sigma_x + i (a_z b_x - a_x b_z) \sigma_y + i (a_x b_y - a_y b_x) \sigma_z$$

$$= \tilde{a} \bar{\sigma} + i (\tilde{a} \times \tilde{b}) \bar{\sigma}. \tag{B.5}$$

Using the above, along with commutativity of $\tilde{A}_k$ and $\tilde{f}_\tau$ and anti-commutativity of the cross-product, we find

$$\tilde{A}_k \bar{\sigma} \tilde{f}_\tau - \tilde{f}_\tau \bar{\sigma} \tilde{A}_k \bar{\sigma} = \tilde{A}_k \bar{\sigma} \tilde{f}_\tau + i \left( \tilde{A}_k \bar{\sigma} \times \tilde{f}_\tau \right) \bar{\sigma} - \tilde{f}_\tau \tilde{A}_k \bar{\sigma} - i \left( \tilde{f}_\tau \times \tilde{A}_k \right) \bar{\sigma}$$

$$= i \left( \tilde{A}_k \bar{\sigma} \times \tilde{f}_\tau - \tilde{f}_\tau \tilde{A}_k \right) \bar{\sigma} = 2i \left( \tilde{A}_k \bar{\sigma} \times \tilde{f}_\tau \right) \bar{\sigma},$$

such that (B.4) becomes

$$\partial_k f \mapsto \left[ \partial_k (f_\tau + \bar{f}_\tau) + 2 \left( \tilde{A}_k \bar{\sigma} \times \tilde{f}_\tau \right) \bar{\sigma} \right] i \sigma^y = \left[ \partial_k f_\tau + \left( \partial_k \bar{f}_\tau + 2 \tilde{A}_k \times \tilde{f}_\tau \right) \bar{\sigma} \right] i \sigma^y.$$

We note here that only the cross-product between the SOC and the triplet component $\tilde{f}_\tau$ remains. This is because the singlet $f_\tau$ does not carry any spin and is therefore not affected by SOC. Introducing the notation $\partial_k \circ \tilde{a} = \partial_k \tilde{a} + 2 \tilde{A}_k \times \tilde{a}$, we write the covariant derivative of $f$ as

$$\partial_k f \mapsto \left[ \partial_k f_\tau + \left( \partial_k \circ \tilde{f}_\tau \right) \bar{\sigma} \right] i \sigma^y. \tag{4.12}$$

To calculate the second covariant derivative, we start from $\partial_k f = \partial_k f - i \left( \tilde{A}_k \bar{\sigma} f + f \tilde{A}_k^* \bar{\sigma} \right)$, such that the second derivative becomes

$$\partial_k^2 f \mapsto \partial_k \left[ \partial_k f - i \left( \tilde{A}_k \bar{\sigma} f + f \tilde{A}_k^* \bar{\sigma} \right) \right]$$

$$- i \tilde{A}_k \bar{\sigma} \left[ \partial_k f - i \left( \tilde{A}_k \bar{\sigma} f + f \tilde{A}_k^* \bar{\sigma} \right) \right] - i \left[ \partial_k f - i \left( \tilde{A}_k \bar{\sigma} f + f \tilde{A}_k^* \bar{\sigma} \right) \right] \tilde{A}_k \bar{\sigma}^*.$$

We use that $\tilde{A}_k^* = \tilde{A}_k$. The derivative $\partial_k$ only acts on $f$, which allows us to take some of the terms
we find the expression for the second derivative
\[
\partial^2_\k f \rightarrow \partial^2_\k f - 2i \bar{A}_k \sigma (\partial_k f) - 2i(\partial_k f) \bar{A}_k \sigma^* - 2 \bar{A}_k \sigma f \bar{A}_k \sigma^* - \bar{A}_k \sigma \bar{A}_k \sigma f - f \bar{A}_k \sigma^* \bar{A}_k \sigma^*.
\]
We expand \(f\) in its singlet and triplet components, i.e. \(f = (f_s + f_t \sigma)i\sigma^y\). Since the SOC does not interact with the singlet component, all cross terms between them vanish. We take \(i\sigma^y\) out of the brackets by multiplying some of the terms with \(\sigma^y\). Finally, we use that \(\sigma^y \bar{A}_k \sigma^* \sigma^y = -\bar{A}_k \sigma\) and obtain
\[
\partial^2_\k f \rightarrow \left[ \partial^2_\k f_s + (\partial^2_\k f_t) \sigma - 2i \bar{A}_k \sigma (\partial_k f_t) \sigma + 2i(\partial_k f_t) \sigma \bar{A}_k \sigma \right]
\]
\[
+ 2 \bar{A}_k \sigma f_t \bar{A}_k \sigma - \bar{A}_k \sigma \bar{A}_k \sigma f_t \sigma + f_t \sigma \bar{A}_k \sigma^* \bar{A}_k \sigma \right] i\sigma_y.
\]
We apply (B.5) to the second and third term, which gives
\[
2i \left[ (\partial_k f_t) \sigma \bar{A}_k \sigma - \bar{A}_k \sigma (\partial_k f_t) \sigma \right] = 4 \left( \bar{A}_k \times (\partial_k f_t) \right) \sigma.
\]
We now dissect the second line of (B.6) and notice that it contains a mix of dot products and normal products. Applying (B.5) twice to \(2 \bar{A}_k \sigma f_t \bar{A}_k \sigma\) yields
\[
2(\bar{A}_k \sigma)(f_t \sigma)(\bar{A}_k \sigma) = 2(\bar{A}_k \sigma) \left( f_t \bar{A}_k + 2i (f_t \times \bar{A}_k) \sigma \right)
\]
\[
= 2 \bar{A}_k \sigma f_t \bar{A}_k + 2i \bar{A}_k (f_t \times \bar{A}_k) - 2 \left( \bar{A}_k \times (f_t \times \bar{A}_k) \right) \sigma
\]
\[
= 2 \bar{A}_k \sigma f_t \bar{A}_k + 2 \left( \bar{A}_k \times (\bar{A}_k \times f_t) \right) \sigma
\]
(B.7)
Similarly, we write the last two terms of (B.6) as
\[
-(\bar{A}_k \sigma)(\bar{A}_k \sigma)(f_t \sigma) = -(\bar{A}_k \sigma \bar{A}_k \sigma + \left( \bar{A}_k \sigma \right)(\bar{A}_k \sigma)(f_t \sigma)
\]
\[
\left( f_t \sigma \right)(\bar{A}_k \sigma^*) = -f_t \sigma \bar{A}_k \sigma
\]
(B.8)
Taking (B.7), (B.8) and (B.9) together and using that \(\bar{a} \times (\bar{b} \times \bar{c}) = (\bar{a} \cdot \bar{c})\bar{b} - (\bar{a} \cdot \bar{b})\bar{c}\) gives
\[
2 \bar{A}_k \sigma f_t \bar{A}_k \sigma - \bar{A}_k \sigma \bar{A}_k \sigma f_t \sigma + f_t \sigma \bar{A}_k \sigma^* \bar{A}_k \sigma
\]
\[
= 3 \left( \bar{A}_k \sigma \times (\bar{A}_k \sigma \times f_t) \right) \sigma + (\bar{A}_k \sigma)(f_t \bar{A}_k) - (f_t \sigma)(\bar{A}_k \bar{A}_k)
\]
\[
= 4 \left( \bar{A}_k \times (\bar{A}_k \times f_t) \right) \sigma.
\]
Putting everything back into the second derivative (B.6) gives
\[
\partial^2_\k f \rightarrow \left[ \partial^2_\k f_s + \left( \partial^2_\k f_t + 4 \bar{A}_k \sigma \times (\partial_k f_t) + 4 \bar{A}_k \times (\bar{A}_k \times f_t) \right) \sigma \right] i\sigma_y,
\]
Extending the new notation with \(\delta_k\) as
\[
\delta_k \circ (\delta_k \circ \bar{a}) = \delta_k \circ (\delta_k \bar{a} + 2 \bar{A}_k \times \bar{a}) = \delta_k \bar{a} + 4 \bar{A}_k \times (\delta_k \bar{a}) + 4 \bar{A}_k \times \left( \bar{A}_k \times \bar{a} \right),
\]
we find the expression for the second derivative
\[
\partial^2_\k f \rightarrow \left[ \partial^2_\k f_s + \left( \delta_k \circ (\delta_k \circ f_t) \right) \sigma \right] i\sigma_y.
\]
(4.13)
B.5 The Usadel equations including SOC

To include SOC in the Usadel equations (4.11), we replace the derivative $\nabla$ by the covariant derivative $\nabla_c$,

$$\begin{align*}
(D\nabla^2 - 2|\omega_n|) f_\alpha &= -2\pi\Delta_\alpha + 2i \text{sgn}(\omega_n) \tilde{h} \cdot \tilde{f}_\alpha, \\
(D\nabla^2 - 2|\omega_n|) \tilde{f}_\alpha &= 2i \text{sgn}(\omega_n) \tilde{h} f_\alpha.
\end{align*}$$

(B.10)

where $\nabla = (\partial_x, \partial_y, \partial_z)$ and $\partial_k$ is defined in (4.12).

The scalar equation for $f_s$ is not affected by SOC. The second equation describes the triplets $\tilde{f}_\alpha = (f^x_\alpha, f^y_\alpha, f^z_\alpha)$. We divide by $\tilde{\sigma}$. Rashba SOC is described by $\tilde{A}_x = (0, \alpha, 0)$, $\tilde{A}_y = (-\alpha, 0, 0)$ and $\tilde{A}_z = (0, 0, 0)$, such that the $x$-component of the covariant derivative becomes

$$\partial^2_x f^x_\alpha + 4\tilde{A}_x \times (\partial_x \tilde{f}_\alpha) + 4\tilde{A}_x \times (\tilde{A}_x \times \tilde{f}_\alpha) = \partial^2_x f^x_\alpha \dot{x} + \partial^2_y f^y_\alpha \dot{y} + \partial^2_z f^z_\alpha \dot{z} + 4\alpha (\partial_x f^x_\alpha \dot{x} - \partial_y f^y_\alpha \dot{y} - \partial_z f^z_\alpha \dot{z}) - 4\alpha^2 (f^\alpha \dot{x} + f^\alpha \dot{y} + f^\alpha \dot{z}).$$

The $y$-component becomes the same with $x \leftrightarrow y$. We consider the superconductor in the $z$-direction to be so thin that superconductivity is constant along that direction and we do not take the derivative $\partial_z$ into account, i.e. the $z$-component is zero. We substitute the expression for the in-plane field $\tilde{h} = (h_x, h_y, 0)$. The Usadel equations (B.10) have now become

$$\begin{align*}
(D \partial^2_x f^x_\alpha + \partial^2_y f^y_\alpha) - 2|\omega_n| f^x_\alpha - 2i \text{sgn}(\omega_n) (h_x f^x_\alpha + h_y f^y_\alpha) &= -2\pi\Delta_s, \\
(D \partial^2_x f^x_\alpha + \partial^2_y f^y_\alpha + 4\alpha \partial_x f^x_\alpha - 4\alpha^2 f^x_\alpha) - 2|\omega_n| f^x_\alpha - 2i \text{sgn}(\omega_n) h_x f^x_\alpha &= 0, \\
(D \partial^2_x f^x_\alpha + \partial^2_y f^y_\alpha + 4\alpha \partial_y f^y_\alpha - 4\alpha^2 f^y_\alpha) - 2|\omega_n| f^y_\alpha - 2i \text{sgn}(\omega_n) h_y f^y_\alpha &= 0, \\
(D \partial^2_x f^x_\alpha + \partial^2_y f^y_\alpha + 8\alpha \partial_x f^x_\alpha + 8\alpha \partial_y f^y_\alpha) - 8\alpha^2 f^x_\alpha - 2|\omega_n| f^x_\alpha &= 0.
\end{align*}$$

We introduce the coherence length $\xi = \sqrt{D/2\pi T_c}$, and use it to normalise the physical quantities as $\dot{x} = x/\xi$, $\dot{y} = y/\xi$, $\alpha = k^2$ $\omega_n = (2n+1)\xi/2T_c$, $\tilde{h}_{x,y} = h_{x,y}/2\pi T_c$ and $\tilde{\Delta} = \Delta_s/T_c$. We multiply the Usadel equations by $\xi^2/D$ and substitute the normalised parameters. The normalised Usadel equations in terms of the coherence length scale are

$$\begin{align*}
\partial^2_x f^x_\alpha + \partial^2_y f^y_\alpha - 2|\omega_n| f^x_\alpha - 2i \text{sgn}(\omega_n) (\tilde{h}_x f^x_\alpha + \tilde{h}_y f^y_\alpha) &= -\tilde{\Delta}, \\
\partial^2_x f^x_\alpha + \partial^2_y f^y_\alpha + 4\tilde{\alpha} \partial_x f^x_\alpha - 4\tilde{\alpha}^2 f^x_\alpha - 2|\omega_n| f^x_\alpha - 2i \text{sgn}(\omega_n) \tilde{h}_x f^x_\alpha &= 0, \\
\partial^2_x f^x_\alpha + \partial^2_y f^y_\alpha + 4\tilde{\alpha} \partial_y f^y_\alpha - 4\tilde{\alpha}^2 f^y_\alpha - 2|\omega_n| f^y_\alpha - 2i \text{sgn}(\omega_n) \tilde{h}_y f^y_\alpha &= 0, \\
\partial^2_x f^x_\alpha + \partial^2_y f^y_\alpha - 4\tilde{\alpha} \partial_x f^x_\alpha + 8\tilde{\alpha} f^x_\alpha - 2|\omega_n| f^x_\alpha &= 0.
\end{align*}$$

(B.14)

B.6 Self-consistency equation including SOC

We start from the Usadel equations for an infinite film, given by (4.16). To find an expression for $f_s$, we rewrite the bottom two equations to express $f^x_\alpha$ and $f^y_\alpha$ in terms of $f_s$,

$$\begin{align*}
f^x_\alpha &= -\frac{i}{2\tilde{\alpha}^2} \text{sgn}(\omega_n) \tilde{h}_x f_s, & f^y_\alpha &= -\frac{i}{2\tilde{\alpha}^2} \text{sgn}(\omega_n) \tilde{h}_y f_s.
\end{align*}$$

We substitute this in the top Usadel equation and use $\text{sgn}(\omega_n)^2 = 1$. Factorising by $2\tilde{\alpha}^2 + |\omega_n|$, we find

$$\begin{align*}
f_s &= \frac{1}{2} \frac{\tilde{\Delta}}{|\omega_n| + \frac{|\tilde{h}_x|^2}{2\tilde{\alpha}^2}}.
\end{align*}$$

(B.17)
B.7. Boundary conditions

The standard self-consistency equation is [41]

\[ \Delta_x \ln \frac{T_{c0}}{T} = \pi T \sum_{n=-\infty}^{\infty} \left( \frac{\Delta_x}{\omega_n} - f_s(\omega_n) \right). \]

Dividing by \( T_{c0} \) and defining \( \tilde{\Delta} = \Delta_x/T_{c0} \), \( \tau = T/T_{c0} \) and \( \tilde{\omega}_n = (2n+1)\tau/2 \), we obtain the normalised self-consistency equation

\[ \tilde{\Delta} \ln \frac{1}{\tau} = \tau \sum_{n=-\infty}^{\infty} \left( \frac{\tilde{\Delta}}{2\tilde{\omega}_n} - f_s(\tilde{\omega}_n) \right) = 2\tau \sum_{n=0}^{\infty} \left( \frac{\tilde{\Delta}}{2\tilde{\omega}_n} - f_s(\tilde{\omega}_n) \right). \]

Substituting \( f_s \) into (4.18), we rewrite the result in terms of the digamma function \( \psi_0 \) as

\[ 2 \ln \left( \frac{1}{\tau} \right) = \left( 1 + \frac{\tilde{\alpha}^2}{\sqrt{X}} \right) \psi_0 \left( \frac{2\tilde{\alpha} + \tau + 2\sqrt{X}}{2\tau} \right) + \left( 1 - \frac{\tilde{\alpha}^2}{\sqrt{X}} \right) \psi_0 \left( \frac{2\tilde{\alpha} + \tau + 2\sqrt{X}}{2\tau} \right) - 2\psi_0 \left( \frac{1}{2} \right), \]

where we defined \( X = \tilde{\alpha}^2 - \tilde{h}^2 \) for a more compact notation. Because the properties of \( \psi_0 \) are known, we are able to find the optimum value analytically. We fix the temperature \( \tau \) and look for the corresponding magnetic field \( \tilde{h} \) that optimises the equation, i.e. that minimises its norm. This is the critical field \( \tilde{h}_c \), defined as

\[ \tilde{h}_c = \min_{\tilde{h}} \left\| \left( 1 + \frac{\tilde{\alpha}^2}{\sqrt{X}} \right) \psi_0 \left( \frac{2\tilde{\alpha} + \tau + 2\sqrt{X}}{2\tau} \right) + \left( 1 - \frac{\tilde{\alpha}^2}{\sqrt{X}} \right) \psi_0 \left( \frac{2\tilde{\alpha} + \tau + 2\sqrt{X}}{2\tau} \right) - 2\psi_0 \left( \frac{1}{2} \right) - 2 \ln \left( \frac{1}{\tau} \right) \right\|. \]

B.7 Boundary conditions

We consider a system located at \([0, L_x] \times [0, L_y]\) and assume there is no current flowing across the boundaries, i.e. \( j_x = 0 \) at \( x = 0, L_x \) and \( j_y = 0 \) at \( y = 0, L_y \). Since the current is proportional to the covariant derivative \((j_{x,y} \sim \partial_{x,y})\),

\[ \partial_k \equiv \partial_k f_x + \left( \partial_k \tilde{f}_t + 2\tilde{A}_k \times \tilde{f}_t \right) \hat{\sigma} = 0. \]

Since the singlet and triplet component are independent, we split this condition into two, i.e.

\[ \partial_k f_s = 0, \quad \left( \partial_k \tilde{f}_t + 2\tilde{A}_k \times \tilde{f}_t \right) \hat{\sigma} = 0. \]

For the triplet component we use that \( \tilde{f}_t = (f_t^x, f_t^y, f_t^z) \), \( \tilde{A}_x = (0, \tilde{\alpha}, 0) \), \( \tilde{A}_y = (-\tilde{\alpha}, 0, 0) \) and \( \tilde{A}_z = (0, 0, 0) \), such that the \( x \)-component becomes

\[ \partial_x \tilde{f}_t^x + 2\tilde{A}_x \times \tilde{f}_t^x = \partial_x f_t^x \sigma^x + \partial_x f_t^y \sigma^y + \partial_x f_t^z \sigma^z + 2\tilde{\alpha}(f_t^x \sigma^x - f_t^z \sigma^z), \]

where we used that the triplet components are expressed in the spin basis (by the Pauli matrices). The \( y \)-component is the same with \( x \leftrightarrow y \) and the \( z \)-component is zero. Therefore, the \( x \) and \( y \) terms do not mix and all individual components have to be zero. Hence, we find

\[ \begin{align*}
\text{at } x = 0, L_x : & \\
\begin{cases}
\partial_x f_s = 0, \\
\partial_x f_t^x + 2\tilde{\alpha} f_t^x = 0, \\
\partial_x f_t^y = 0, \\
\partial_x f_t^z - 2\tilde{\alpha} f_t^z = 0,
\end{cases} & \begin{cases}
\partial_y f_s = 0, \\
\partial_y f_t^y + 2\tilde{\alpha} f_t^y = 0, \\
\partial_y f_t^z - 2\tilde{\alpha} f_t^z = 0.
\end{cases}
\end{align*} \]

(4.19)
Appendix C

Boosting and controlling the $p$-wave $T_c$ in a S/F/P junction

C.1 Mean-field approximation of the on-site Hamiltonian

The on-site superconductor Hamiltonian (6.3) is given by

$$H_U = - \sum_i U_i n_{i\uparrow} n_{i\downarrow} = - \sum_i U_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} = \sum_i U_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{i\uparrow} c_{i\downarrow}.$$  

In the mean-field approximation, we approximate the operators by a small fluctuation $\delta$ around their expectation value, i.e., $c_{i\uparrow} c_{i\downarrow} = \langle c_{i\uparrow} c_{i\downarrow} \rangle + \delta$ and $c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger = \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle - \delta^\dagger$. Applying this to $H_U$ gives

$$H_U = \sum_i U_i \left( \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle \langle c_{i\uparrow} c_{i\downarrow} \rangle - \delta^\dagger \langle c_{i\uparrow} c_{i\downarrow} \rangle + \delta \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle + \delta^\dagger \delta \right).$$

We neglect the $\delta^\dagger \delta$ term corresponding to second order fluctuations [185]. Next, we rewrite the mean-field approximation as $\delta = c_{i\uparrow} c_{i\downarrow} - \langle c_{i\uparrow} c_{i\downarrow} \rangle$ and $\delta^\dagger = -c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle$. We substitute this back into $H_U$ and obtain

$$H_U = \sum_i U_i \left( \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle \langle c_{i\uparrow} c_{i\downarrow} \rangle + c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger (c_{i\uparrow} c_{i\downarrow}) + c_{i\uparrow} c_{i\downarrow} (c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger) - \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle \langle c_{i\uparrow} c_{i\downarrow} \rangle \right)$$

$$= \sum_i U_i \left( \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle \langle c_{i\uparrow} c_{i\downarrow} \rangle + c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger (c_{i\uparrow} c_{i\downarrow}) + c_{i\uparrow} c_{i\downarrow} (c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger) - \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle \langle c_{i\uparrow} c_{i\downarrow} \rangle \right).$$

We introduce the $s$-wave superconducting gap $\Delta_s \equiv U_i (c_{i\uparrow} c_{i\downarrow})$ such that $H_U$ becomes

$$H_U = \sum_i \frac{|\Delta_s|^2}{U_i} + \Delta_s c_{i\uparrow}^\dagger c_{i\downarrow} + \Delta_s^* c_{i\uparrow} c_{i\downarrow}.$$  

C.2 Nearest-neighbour Hamiltonian

The nearest-neighbour Hamiltonian $H_V$ expressed in the pair correlation functions $F_{ij}^{s,s'}$ is

$$H_V = -\frac{1}{2} \sum_{(i,j),s} V_{ij} \left( |F_{ij}^{s,-s}|^2 + F_{ij}^{s,-s} c_{is}^\dagger c_{is,-s} + \left(F_{ij}^{s,-s}\right)^* c_{is} c_{is,-s} \right).$$  

(6.6)
The first term gives a constant contribution $E_V$ to the total energy of the electron system, and can therefore be neglected when calculating eigenvalues and eigenvectors. We expand the summation over $s$ and obtain

$$H_V = E_V - \frac{1}{2} \sum_{(i,j)} V_{ij} \left( F_{ij}^{\uparrow \downarrow} c_i^\dagger c_j^\dagger + F_{ij}^{\downarrow \uparrow} c_i^\dagger c_j^\dagger + (F_{ij}^{\uparrow \downarrow})^* c_i c_j + (F_{ij}^{\downarrow \uparrow})^* c_i c_j \right)$$

Using that the nearest-neighbour interaction is symmetric ($V_{ij} = V_{ji}$) and $F_{ij}^{\uparrow \downarrow} = -F_{ij}^{\downarrow \uparrow}$, we write

$$\sum_{(i,j)} V_{ij} F_{ij}^{\uparrow \downarrow} c_i^\dagger c_j^\dagger = \sum_{(i,j)} V_{ji} F_{ji}^{\downarrow \uparrow} c_i^\dagger c_j^\dagger = \sum_{(i,j)} V_{ij} F_{ij}^{\uparrow \downarrow} c_i^\dagger c_j^\dagger.$$  \hfill (C.1)

Substituting (C.1) into $H_V$ removes the factor $\frac{1}{2}$ in front of the summation. $H_V$ simplifies to

$$H_V = E_V - \sum_{(i,j)} V_{ij} \left[ F_{ij}^{\uparrow \downarrow} c_i^\dagger c_j^\dagger + (F_{ij}^{\uparrow \downarrow})^* c_i c_j \right]$$

Since $V_{ij}$ only acts on the nearest neighbours, the summation over $j$ yields four terms, similar to the hopping Hamiltonian (6.1). For brevity, we refer to the terms originating from $(F_{ij}^{\uparrow \downarrow})^*$ as “h.c.” (hermitian conjugate). $H_V$ becomes

$$H_V = E_V - \sum_i V_{i,i+\hat{x}} F_{i,i+\hat{x}} c_i^\dagger c_{i+\hat{x}}^\dagger + V_{i,i-\hat{x}} F_{i,i-\hat{x}} c_i^\dagger c_{i-\hat{x}}^\dagger + V_{i,i+\hat{y}} F_{i,i+\hat{y}} c_i^\dagger c_{i+\hat{y}}^\dagger + V_{i,i-\hat{y}} F_{i,i-\hat{y}} c_i^\dagger c_{i-\hat{y}}^\dagger + h.c.$$  \hfill (6.7)

Applying the Fourier transform (6.8) to $H_V$ in (6.7) gives

$$H_V = E_V - \frac{1}{N} \sum_{i,x,y,k} V_{i,x,y+1} F_{x+1}^{\uparrow \downarrow} c_{x+y}^\dagger c_{x+y+1,k}^\dagger e^{-i(k_x+k_y)i_y}$$

$$+ V_{i,x,y-1} F_{x-1}^{\uparrow \downarrow} c_{x+y}^\dagger c_{x+y-1,k}^\dagger e^{i(k_x+k_y)i_y}$$

$$+ V_{i,x,y} F_{x}^{\uparrow \downarrow} c_{x+y}^\dagger c_{x+y,k}^\dagger e^{-i(k_x+k_y)i_y}$$

$$+ V_{i,x,y} F_{x}^{\uparrow \downarrow} c_{x+y}^\dagger c_{x+y,k}^\dagger e^{i(k_x+k_y)i_y} + h.c.$$
where we defined the pair correlation $F_{ijk}$ as

$$F_{ijk} = -V_{ij} \left[ F_i^{x_+} \delta_{i,j-1} + F_i^{z} \delta_{i,j+1} + (F_i^{y_+} e^{i k} + F_i^{y} e^{-i k}) \delta_{ij} \right].$$

To transform $H_V$ to electron-hole basis, we expand (6.13) as

$$H_V = E_V + \frac{1}{2} \sum_{i,j,k} F_{ijk} c_i^\dagger c_j^\dagger c_k + F_{i,j,-k} c_i^\dagger c_j c_k^\dagger + F_{i,j,k} c_i^\dagger c_j c_k + F_{i,j,-k} c_i c_j c_k^\dagger + F_{i,j,k} c_i c_j c_k$$

This notation is used to express $H_V$ in the electron creation and annihilation operator basis $B_{ik}^\dagger = [c_i^\dagger c_k^\dagger c_i c_k]$ as

$$H_V = E_V + \frac{1}{2} \sum_{i,j,k} B_{ik}^\dagger \begin{bmatrix} E_{i,j,k} & F_{i,j,k} \\ -F_{i,j,k} & -E_{i,j,k} \end{bmatrix} B_{jk},$$

**C.3 Diagonalising the Hamiltonian**

The matrix $H_k$ in (6.18) is a $4N_x \times 4N_x$ matrix with the structure

$$H_k = \begin{bmatrix} H_{1,1,k} & \cdots & H_{1,N_x,k} \\ H_{2,1,k} & \cdots & H_{2,N_x,k} \\ \vdots & \ddots & \vdots \\ H_{N_x,1,k} & \cdots & H_{N_x,N_x,k} \end{bmatrix}$$

where the individual $H_{ijk}$ entries are 4 x 4 matrices given in (6.17). From the diagonalisation in (6.19), we assume $H_k$ has eigenvalues $E_{nk}$ with eigenvectors $[u_{1nk}, v_{1nk}, w_{1nk}, x_{1nk}, u_{2nk}, \ldots, x_{N_x nk}]^T$. Then it follows from (C.2) that

$$\sum_{j=1}^{N_x} H_{ijk} \begin{bmatrix} u_{jnk} \\ v_{jnk} \\ w_{jnk} \\ x_{jnk} \end{bmatrix} = E_{nk} \begin{bmatrix} u_{ink} \\ v_{ink} \\ w_{ink} \\ x_{ink} \end{bmatrix}$$

Using the matrix (6.17), the first row and the third row of this equation read, respectively,

$$\sum_{j=1}^{N_x} (\epsilon_{ijk} + h_i^x \delta_{ij}) u_{jnk} + (h_i^x - ih_i^y) \delta_{ij} v_{jnk} + (\Delta_i \delta_{ij} + F_{ijk}) x_{jnk} = E_{nk} u_{ink},$$

$$\sum_{j=1}^{N_x} (\Delta_i^* \delta_{ij} + F_{i,j,-k}^*) v_{jnk} - (\epsilon_{ijk} + h_i^x \delta_{ij}) w_{jnk} - (h_i^x + ih_i^y) \delta_{ij} x_{jnk} = E_{nk} w_{ink}$$

**C.3.1 Diagonalising the Hamiltonian**

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We take (C.5) and substitute \( k \mapsto -k \), we complex conjugate the whole equation and multiply by \(-1\). We find

\[
\sum_{j=1}^{N_k} (\Delta \delta_{ij} + F_{ijk}) v_{jn,-k} + (\epsilon_{ij,-k} + h^2 \delta_{ij}) w_{jn,-k} + (h^2 i - i h^0) \delta_{ij} x_{jn,-k}^- = -E_{n,-k} w_{jn,-k}^\dagger
\]

which is the same as (C.4) when using the eigenvalues \(-E_{n,-k}\) and eigenvectors \([w_{1n,-k}^\dagger, x_{1n,-k}^\dagger, u_{1n,-k}^\dagger, v_{1n,-k}^\dagger, \ldots, v_{N,n,-k}^\dagger]^T\). Hence, this shows that if \( E_{nk} \) is an eigenvalue of \( H_k \) with eigenvector \([w_{nk}^\dagger, v_{nk}^\dagger, w_{1nk}, x_{1nk}, \ldots, x_{N,nk}]^T\), then \(-E_{n,-k}\) is also an eigenvalue of \( H_k \) with eigenvector \([w_{1n,-k}^\dagger, x_{1n,-k}^\dagger, u_{1n,-k}^\dagger, v_{1n,-k}^\dagger, \ldots, v_{N,n,-k}^\dagger]^T\).

We will now use this in diagonalising the Hamiltonian. We define a new basis \( \Gamma_k \) and the diagonalisation matrix \( P_k \) which contains the eigenvectors of \( H_k \) as column vectors:

\[
\Gamma_k = \begin{bmatrix} \gamma_{1k} \\ \gamma_{2k} \\ \vdots \\ \gamma_{4,N,nk} \end{bmatrix}, \quad P_k = \begin{bmatrix} u_{11k} & u_{12k} & \cdots & u_{1,N,n,k} \\ v_{11k} & v_{12k} & \cdots & v_{2,N,n,k} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N,n,1k} & \cdots & x_{N,n,N,n,k} \end{bmatrix}.
\]  

(C.6)

We transform the \( W_k \) basis used in (6.18) into this new basis by \( W_k = P_k \Gamma_k \), which is equivalent to \( \Gamma_k^\dagger = W_k^\dagger P_k \). The diagonalised Hamiltonian is

\[
H = E_U + E_V + \frac{1}{2} \sum_{n,k} E_{nk} \gamma_{nk}^\dagger \gamma_{nk}.
\]  

(6.19)

From the relation \( \Gamma_k^\dagger = W_k^\dagger P_k \), we get directly

\[
\gamma_{nk}^\dagger = \sum_i \left( u_{i,nk} c_{ik}^\dagger + v_{i,nk} c_{ik}^\dagger + w_{i,nk} c_{i,-k}^\dagger + x_{i,nk} c_{i,-k}^\dagger \right).
\]  

(C.7)

As we showed above, the Hamiltonian \( H_{-k} \) has eigenvalues \(-E_{nk}\) and eigenvectors \([w_{nk}^\dagger, x_{nk}^\dagger, u_{nk}^\dagger, v_{nk}^\dagger, \ldots, v_{N,nk}^\dagger]^T\). Using the relation \( W_{-k} = P_{-k} \Gamma_{-k} \), we find

\[
\gamma_{n,-k}^\dagger = \sum_i \left( u_{i,nk}^* c_{i,-k}^\dagger + x_{i,nk}^* c_{i,-k}^\dagger + u_{i,nk}^* c_{ik}^\dagger + v_{i,nk}^* c_{ik}^\dagger \right).
\]  

(C.8)

Comparing (C.7) and (C.8), it follows immediately that \( \gamma_{n,-k}^\dagger = \gamma_{nk} \). This shows that the \( \gamma_{nk} \) operators are not independent for all \( k \)-values. However, we can use this symmetry to express (6.19) in independent operators. We split the sum into \( k > 0 \) and \( k < 0 \).

\[
H = E_U + E_V + \frac{1}{2} \sum_{n,k>0} E_{nk} \gamma_{nk}^\dagger \gamma_{nk} + \frac{1}{2} \sum_{n,k<0} E_{nk} \gamma_{nk}^\dagger \gamma_{nk} + K_0,
\]

where the term \( K_0 \) refers to the value \( k = 0 \), which will be treated separately. In the sum over negative
k-values, we let $k \mapsto -k$. We subsequently use $\gamma_{n-k} = \gamma_{n-k}$ and $E_{n-k} = -E_{nk}$. We obtain

$$H = E_U + E_V + \frac{1}{2} \sum_{n,k \geq 0} \left( E_{nk} \gamma_{nk} \gamma_{nk} + E_{n-k} \gamma_{n-k} \gamma_{n-k} \right) + K_0$$

$$= E_U + E_V + \frac{1}{2} \sum_{n,k \geq 0} \left( E_{nk} \gamma_{nk} \gamma_{nk} - E_{nk} \gamma_{nk} \gamma_{nk} \right) + K_0$$

$$= E_U + E_V + \sum_{n,k \geq 0} E_{nk} \left( \gamma_{nk} \gamma_{nk} - \frac{1}{2} \right) + K_0. \quad (C.9)$$

For the $k = 0$ term, we assume that $H_k = H_{-k} = H_0$. If $E_{n0}$ is an eigenvalue of $H_0$, then so is $-E_{n0}$. To avoid double counting, we arrange the eigenvalues for $k = 0$ such that the first $2N_x$ are positive and the last $2N_x$ are negative. If $E = 0$ is an eigenvalue of $H_0$, it must be degenerate and we include one zero-energy eigenvalue with the first $2N_x$ and the other with the last $2N_x$. We can then write $\gamma_{2N_x+n,0} = \gamma_{n0}$. Using this, the $K_0$ term becomes

$$K_0 = \frac{1}{2} \sum_n E_{n0} \gamma_{n0} \gamma_{n0} = \frac{1}{2} \sum_{E_{n0} \geq 0} E_{n0} \left( \gamma_{n0} \gamma_{n0} - \gamma_{00} \gamma_{00} \right)$$

$$= \sum_{E_{n0} \geq 0} E_{n0} \left( \gamma_{n0} \gamma_{n0} - \frac{1}{2} \right), \quad (C.10)$$

where the notation $\sum_{E_{n0} \geq 0}$ is the summation over all positive eigenvalues of $H_0$, including one zero-energy eigenvalue.

### C.4 Expressing pair correlations in eigenvectors

The nearest neighbour pair correlation $F_{i}^{\pm} = F_{i, \pm \pm}$ is

$$F_{i}^{\pm} = \langle c_{i} \gamma_{i} c_{i} \rangle = \frac{1}{N_y} \sum_{k} \langle c_{ik} \gamma_{i} c_{i+k} \rangle$$

$$= \frac{1}{N_y} \left( \langle c_{00} c_{10} \rangle + \sum_{k > 0} \langle c_{ik} c_{i+1,k} \rangle \right)$$

$$= \frac{1}{N_y} \left( K_{x0} + \sum_{k > 0, n} u_{nk} x_{n+k}^* [1 - f(E_{nk})] + v_{n+k} w_{nk}^* f(E_{nk}) \right), \quad (6.23)$$

where $K_{x0}$ corresponds to $k = 0$ and is given by $K_{x0} = \sum_{E_{n} \geq 0} u_{n0} x_{n+1,0}^* [1 - f(E_{n0})] + v_{n+1,0} w_{n0}^* f(E_{n0})$. Similarly, $F_{i}^{\gamma \gamma} = F_{i, \gamma \gamma}$ becomes

$$F_{i}^{\gamma \gamma} = \langle c_{i} \gamma_{i} \gamma_{i} \rangle = \frac{1}{N_y} \sum_{k} \langle c_{ik} \gamma_{i} \gamma_{i+k} \rangle$$

$$= \frac{1}{N_y} \left( \langle c_{00} c_{00} \rangle + \sum_{k > 0} \langle c_{ik} \gamma_{i+k} \rangle e^{ik} + \langle c_{i-k} c_{ik} \rangle e^{ik} \right)$$

$$= \frac{1}{N_y} \left( K_{00} + \sum_{k > 0, n} u_{nk} x_{n+k}^* [1 - f(E_{nk})] e^{ik} + v_{n+k} w_{nk}^* f(E_{nk}) e^{ik} \right), \quad (6.24)$$

with $K_{00} = \sum_{E_{n} \geq 0} u_{n0} x_{n+1,0}^* [1 - f(E_{n0})] + v_{n0} w_{n0}^* f(E_{n0})$.\[\]
C.5 Symmetrised pair correlations

The symmetrised pair correlation functions for singlet symmetry, \( F^{(S)} \), and triplet symmetry, \( F^{(T)} \) are given in (6.28). We substitute the self-consistent pair correlations \( F^{x\pm}_T \) and \( F^{y\pm}_T \) from (6.23) and (6.24). The singlet pair correlations \( F^{(S)} \) become

\[
F_i^{x\pm}(S) = F_{i,i\pm\hat{x}}^{(S)} = \frac{F_{i,i\pm\hat{x}} + F_{i\pm\hat{x},i}}{2} = \frac{1}{2N_y} \sum_{k>0,n} \left( u_{ink} x_{i\pm1,nk}^* + u_{i\pm1,nk} x_{ink}^* \right) \left[ 1 - f(E_{nk}) \right] + \left( v_{i\pm1,nk} w_{ink}^* + v_{ink} w_{i\pm1,nk}^* \right) f(E_{nk}) + K_{x0}^{(S)}(S),
\]

with

\[
K_{x0}^{(S)} = \sum_{E_n \geq 0} \left( u_{i00} x_{i\pm1,00}^* + u_{i\pm1,00} x_{i00}^* \right) \left[ 1 - f(E_{n0}) \right] + \left( v_{i\pm1,00} w_{i00}^* + v_{i00} w_{i\pm1,00}^* \right) f(E_{n0}).
\]

The \( y \)-term of the singlet pair correlations is

\[
F_i^{y\pm}(S) = F_{i,i\pm\hat{y}}^{(S)} = \frac{F_{i,i\pm\hat{y}} + F_{i\pm\hat{y},i}}{2} = \frac{1}{2N_y} \sum_{k,k'} (c_{ik} c_{ik'}^*) e^{-i(k+k')y} \left( e^{\mp ik'} + e^{\mp ik} \right) = \frac{1}{N_y} \sum_k (c_{ik} c_{-k}) \cos(k) = \frac{1}{N_y} \left( \sum_{k>0,n} \left( u_{ink} x_{ink}^* [1 - f(E_{nk})] + v_{ink} w_{ink}^* f(E_{nk}) \right) \cos(k) + K_{y0} \right).
\]

The \( K_{y0} \) term is the same as in (6.24). Similarly, the triplet pair correlations \( F^{(T)} \) are expanded as

\[
F_i^{x\pm}(T) = F_{i,i\pm\hat{x}}^{(T)} = \frac{F_{i,i\pm\hat{x}} - F_{i\pm\hat{x},i}}{2} = \frac{1}{2N_y} \sum_{k>0,n} \left( u_{ink} x_{i\pm1,nk}^* - u_{i\pm1,nk} x_{ink}^* \right) \left[ 1 - f(E_{nk}) \right] + \left( v_{i\pm1,nk} w_{ink}^* - v_{ink} w_{i\pm1,nk}^* \right) f(E_{nk}) + K_{x0}^{(T)}(T),
\]

with

\[
K_{x0}^{(T)} = \sum_{E_n \geq 0} \left( u_{i00} x_{i\pm1,00}^* - u_{i\pm1,00} x_{i00}^* \right) \left[ 1 - f(E_{n0}) \right] + \left( v_{i\pm1,00} w_{i00}^* - v_{i00} w_{i\pm1,00}^* \right) f(E_{n0}).
\]

The triplet \( y \)-term is

\[
F_i^{y\pm}(T) = F_{i,i\pm\hat{y}}^{(T)} = \frac{F_{i,i\pm\hat{y}} - F_{i\pm\hat{y},i}}{2} = \frac{1}{2N_y} \sum_k \left( c_{ik} c_{-k} \right) \left( e^{\pm ik} - e^{\mp ik} \right) \pm \frac{i}{N_y} \sum_k \left( c_{ik} c_{-k} \right) \sin(k) = \pm \frac{i}{N_y} \sum_{k>0,n} \left( u_{ink} x_{ink}^* [1 - f(E_{nk})] - v_{ink} w_{ink}^* f(E_{nk}) \right) \sin(k).
\]
The $K_{00}$ terms cancel.