MASTERS THESIS

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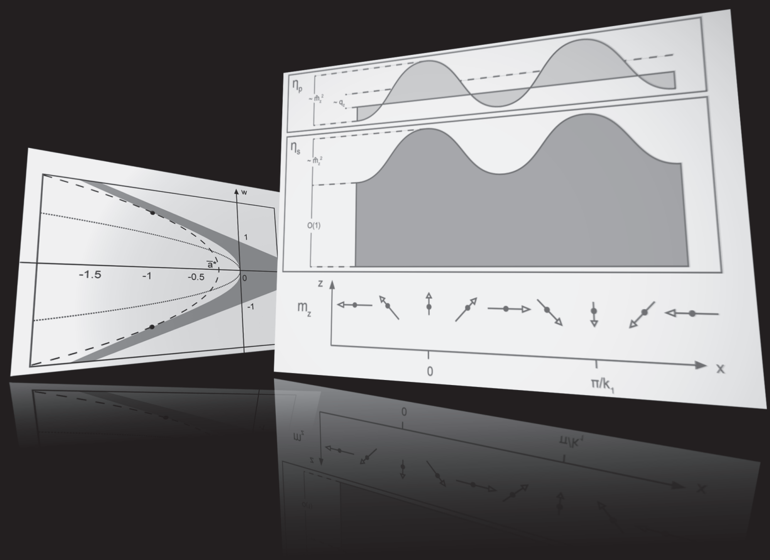

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ABSTRACT

In non-centrosymmetric superconductors the distinction of singlet and triplet pairing states of electrons becomes obsolete. This has strong ramification on the nature of superconducting phases and on the interplay of superconductivity and magnetically ordered states [23]. In this text, Ginzburg-Landau theory is used to analyse magnetic and superconducting phases for tetragonal and cubic crystal lattices whose unit cells possess no center of inversion. Beginning with a homogeneous magnetization, stable states of modulated magnetization (chiral ferromagnetism) are found in both material types. Free energy terms corresponding to the Moriya-Dzyaloshinskii spin-orbit interaction lead to a phase modulation in the superconductivity order parameter for homogeneous and chiral magnetic states. Additionally, we find that the inhomogeneous magnetic phases in tetragonal symmetry always give rise to spatial variations in the absolute value of the order parameter. As a consequence, the London penetration depth itself becomes modulated. In the case of the cubic system, the generation of inhomogeneous superconductivity in a modulated magnetic phase necessitates a sufficiently strong spin-orbit interaction. As a conclusion, this behaviour is analysed in a simplified model.

Contents

CHAPTER 1

Theoretical framework of Ginzburg-Landau analysis

1.1 Introduction

Superconductivity is most commonly characterized by the vanishing of electrical resistivity, and the inducing of shielding currents against external magnetic fields. The latter is known as the *Meissner-Ochsenfeld effect*. The corresponding microscopic picture describes these effects with Cooper pairs formed by two electrons of opposite lattice momenta $\mathbf{k}, -\mathbf{k}$. These Cooper pairs are bosonic, and the superconducting state is the corresponding Bose condensate.

Superconductors are classified via the symmetry properties of the Cooper pair wave function ψ [22]

$$\psi(\mathbf{r}-\mathbf{r}', ss') = f(\mathbf{r}-\mathbf{r}')\chi_{ss'}. \tag{1.1}$$

It can be separated into an orbital part $f(\mathbf{r}-\mathbf{r}')$ and a spin part $\chi_{ss'}$ (In presence of a spin-orbit interaction the spin is replaced by the pseudo-spin). The wave function in total must be antisymmetric under the exchange of the two electrons. Suppose the Hamiltonian of the system features inversion symmetry, parity is a good quantum number. In this case, the orbital part $f(\mathbf{r}-\mathbf{r}')$ is a function of either positive or negative parity. The demand of antisymmetricity forces the spin part to feature the opposite behaviour under particle exchange. This allows to distinguish states of *even parity pairing* (angular momentum $l = 0, 2, 4\ldots$ with spin-singlet, total spin $S = 0$) and *odd parity pairing* ($l = 1, 3, 5\ldots$ with spin-triplet, total spin $S = 1$). Condensates with $l = 0$ are called *conventional* superconductors, while all others are called *unconventional* superconductors [22].

The origin of the attractive interaction that leads to the formation of Cooper pairs differs with each superconductor class. The theory by Bardeen, Cooper and Schrieffer (BCS; [7], [8]), which applies for conventional superconductors, is based on the phonon-mediated coupling of electrons. In unconventional superconductors, where a strong Coulomb repulsion dominates over the energy gain by phonon exchange, alternative explanatory mechanisms such as spin fluctuation exchange are considered in the literature. No matter the underlying mechanism, the interaction opens a gap $\Delta_\mathbf{k}$ at the Fermi energy in the quasi-particle energy spectrum. This energetically favours the formation of Cooper pairs. The size of this gap varies with electron energy $\xi_{\mathbf{k}}$ and with the direction of the lattice momenta **k**. The latter anisotropy is most commonly parametrized via the gap function $\mathbf{g}_{\mathbf{k},ss'}$ as

$$\Delta_{\mathbf{k},ss'} = \Delta(\xi_{\mathbf{k},ss'})\mathbf{g}_{\mathbf{k},ss'}. \tag{1.2}$$

The topology of the gap function is crucial to the properties of the superconducting state and reflects symmetry properties of the wave function of the Cooper pairs.

Spontaneous symmetry breaking is a basic concept used to describe phase transitions. It is based on the principle that the transition to a phase of increased order brings about a break in the system's symmetry. Thereby, the ordered state is spontaneously chosen from a set of possible energy-degenerate realisations. A prominent example of spontaneous symmetry breaking is the ferromagnetic phase transition, where either rotational symmetry or crystallographic point group symmetry is broken by a magnetization vector. Another example is given by the description of a superconducting state via the Ginzburg-Landau theory [13]. In conventional superconductivity, the $U(1)$ gauge symmetry is broken via the emergence of a phase-fixing complex order parameter. In unconventional superconductors other symmetries are breakable in addition to that. These include time-reversal and parity.

Magnetism and superconductivity may be seen as antagonistic phenomena, since a magnetic field tends to break up Cooper pairs via two different mechanisms. Due to the antipodal lattice momenta, the Lorentz force acts in opposite directions on each electron. This is called orbital depairing. Additionally, both of the opposite spins of singlet pairs seek to line up with the magnetic field (paramagnetic depairing). Nevertheless, a number of materials which exhibit a coexistence of magnetism with superconductivity in a wealth of different phases were discovered [15]. Superconductivity was found to coexist with both ferromagnetism and antiferromagnetism. Among the first interesting examples discovered were ternary rare-earth compounds like the ferromagnetic $ErRh_4B_4$. They do, however, not show a true ferromagnetic phase. Instead, the magnetization is found to be oscillatory in space on length scales far larger than the lattice spacing and much smaller than the size of the Cooper pairs – the superconducting coherence-length. These magnetic phases are called chiral or helical ferromagnetism. (In this work, we will address a magnetic state with any spatial dependence of the magnetization vector as a *modulated* phase.) As a result from the modulation, Cooper pairs fail to feel a net magnetization [4]. Hence, the depairing mechanisms are suppressed.

More recently, pressure-induced superconductivity was found in magnetically ordered phases of heavy-fermion systems such as UGe_2 and $CeIn_3$. While the magnetic moments in $ErRh_4B_4$ are induced by localised f-electrons, the charge-carrying electrons in materials with band-magnetism are simultaneously responsible for the magnetic ordering itself. Heavy-fermion systems belong to the latter category. However, their large quasi-particle mass distinguishes them from other itinerant magnetic materials, where the band electrons move unimpededly [11].

Non-centrosymmetric superconductors feature a unit cell that lacks inversion symmetry. $CePt_3Si$ was the first known superconductor of this nature, discovered by Bauer et al. in 2004 [9]. It exhibits antiferromagnetic order below 2.2 K and has a superconducting transition temperature of 0.75 K. Since 2004 non-centrosymmetric materials have been subject to many further theoretical and experimental studies [23].

The interest in these materials has arisen from the deep impact that the lack of parity symmetry has on the superconducting state. According to Anderson's theorems, two symmetries, time-inversion and parity, were believed to be indispensable in the formation of Cooper pairs; where parity is required only for triplet pairing [3], [20]. One way to easily break time-reversal symmetry is in the application of a magnetic field. Parity however, is breakable in the bulk under the sole condition that the material intrinsically lacks inversion symmetry. Such a system is called non-centrosymmetric.

Because parity is not a good quantum number in these materials, the orbital part $f(\mathbf{r}-\mathbf{r}')$ of the Cooper pair wave function (1.1) is neither a pure even nor a pure odd function. To maintain the overall antisymmetricity, the spin part $\chi_{ss'}$ must also reveal a mixed symmetry under particle exchange. Hence, the key feature common to non-centrosymmetric materials is that the distinction between spin singlet and spin triplet states becomes obsolete. The resulting pairing state allows the circumnavigation of the consequences of Anderson's theorems. In addition it also offers us an explanation which reconciles the contradictory experimental results – some of which are in favour of singlet and others in favour of triplet pairing. The lack of inversion symmetry points towards to the former, while the excess of paramagnetic limiting favours the latter [23].

We discussed the emergence of the parity mixing based on symmetry arguments. However, it can also be understood from the anisotropic nature of the spin-orbit interaction in non-centrosymmetric materials [23]. It allows for matrix elements that induce transitions between the two spin-states.

This work aims at an investigation of the interplay between superconductivity and ferromagnetism in non-centrosymmetric materials with cubic and tetragonal crystal structure. We proceed based on the analysis of the Ginzburg-Landau free energy functional. Our discussion is applicable to band-magnets as well as to materials with localised magnetic moments. Nonetheless, heavy-fermion systems do indeed provide us with examples of a more promising nature. The only known instance of this class of materials is the monoclinic heavy-fermion UIr [2]. Notwithstanding, should one allow a broader classification scheme, the incommensurate antiferromagnet $CeRhSi_3$ would be included as a further example [5], [16], [18].

1.2 Phase transitions in Landau theory

Landau's theory aims to model second-order phase transitions within a phenomenological description. Guided by the change of an external parameter, e.g. the temperature, the system undergoes a transition from a high-symmetry (unordered) state to an ordered state with lower symmetry. Ergo this mechanism is called spontaneous symmetry breaking. An order parameter Ψ is introduced as a measure of the strength of the ordered phase. The basic idea is the analysis of the free energy difference between the ordered state F_o and the normal state F_n in the transition vicinity. Since the theory is valid only for small Ψ, the free energy difference can be expanded like

$$F_o - F_n = \int \mathrm{d}^3 r \left(\alpha\,|\Psi|^2 + \beta\,|\Psi|^4\right) = V\left(\alpha\,|\Psi|^2 + \beta\,|\Psi|^4\right) \tag{1.3}$$

where V is the volume of the system. We assumed that neither Ψ nor the phenomenological expansion parameters α and β vary spatially. Because the free energy must be bounded from below towards arbitrarily big values of $|\Psi|$, we demand $\beta > 0$. In the system, the state that is realised is where (1.3) takes its minimal value, i.e.

$$\begin{aligned} |\Psi| &= 0 && \text{if } \alpha > 0 \\ |\Psi| &= \sqrt{-\frac{\alpha}{2\beta}} && \text{if } \alpha < 0 \end{aligned} \tag{1.4}$$

Obviously the phase-transition occurs at $\alpha = 0$. As temperature will be the driving force of the transition in our considerations, the minimal temperature expansion of the phenomenological parameters that remodels this behaviour is

$$\begin{aligned} \alpha(T) &= \alpha'(T - T_c) \quad \alpha' > 0 \\ \beta(T) &= \beta_0 > 0 \end{aligned} \tag{1.5}$$

Hence, the whole theory is only valid near the transition temperature T_c. The resulting temperature dependence of the order parameter is $|\Psi| \propto \sqrt{T_c - T}$, which is in strong agreement with observations and is a typical signature for spontaneous symmetry breaking. The values of the expansion parameters (α', β_0) cannot be connected to measurable quantities from the Landau theory alone. This theory being phenomenological offers results more qualitative rather than quantitative.

1.3 Symmetry aspects of the free energy functional

We shall use a more advanced form of the Landau theory than the one introduced above. Firstly, we allow the order parameter to vary in space, giving rise to terms in the free energy that contain spatial derivatives of the order parameter. Secondly, the symmetry of the crystal structure is taken into account in the construction of the free energy expansion. We require that all linear independent terms in the free energy transform as real scalar quantities under all *preserving* symmetry transformations of the system.

1.3.1 Spatial symmetries

The crystallographic point group of a system contains all spatial symmetries, such as inversions on certain planes and rotations of some fixed angles around certain axes. In this work, crystals with tetragonal (point group D_{4h}) and cubic (point group O_h) lattice symmetries are investigated. The point group splits into irreducible representations (denoted by $\Gamma_i^{\pm}$, where + or − denote the behaviour under parity). The elements of $\Gamma_i^{\pm}$ leave a subspace, which is spanned by their basis function(s), invariant. Thus, all functions in that subspace possess the symmetries that are contained in the irreducible representation.

Each point group comprises an irreducible representation Γ_1^+ that contains full point group symmetry. Therefore, each linear independent term in the free energy must belong to Γ_1^+. All quantities that feature in the free energy, such as the order parameter and the derivative operator $\nabla = \left(\partial_x, \partial_y, \partial_z\right)^T$, belong to an irreducible representation. This means that they share the transformational behaviour of the appropriate subspace. Coupling coefficient tables, as found in [19], allow the construction of all possible combinations of these quantities that belong to Γ_1^+. In practice, the expansion is confined to terms up to a certain power – both in the order parameter and in the derivative.

In our discussion, special attention is drawn to parity. The point groups D_{4h} and O_h feature a center of inversion symmetry. As we want to study non-centrosymmetric systems we must allow terms which have all possible symmetries but negative parity. In the isotropic case, this would mean that they belong to the irreducible representation Γ_1^-. However, should inversion symmetry be broken along one axis only, these terms might belong to a different irreducible representation. So as to ensure more control on the impact of non-centrosymmetricity, we introduce instead odd-parity real lattice order parameters ζ_z (for the tetragonal system, along the z-direction) and ζ_1 (for the cubic system). These order parameters are used to compose Γ_1^+-terms in the free energy which would be otherwise impossible. Physically, they represent the symmetry of the gap function of superconductivity $\mathbf{g_k}$.

1.3.2 Magnetism

Before we can analyse the interplay between superconductivity and magnetism, we must determine all magnetic phases possible in the material within a Landau theory. In order to do so, we express the free energy for magnetism with the magnetization $\mathbf{m}$ as a real, three-dimensional order parameter.

$$F[\mathbf{m}](T) = F_n(T) + \int \mathrm{d}^3 r\, f_{mag}$$

The aim is to determine the conditions in terms of the phenomenological expansion parameters, like α and β in section 1.2, under which possible phases arise. These phases can be either of homogeneous magnetization or possess a spatially modulated structure. A helix-like arrangement would be an example of the latter. The procedure we follow in finding these states reflects why we address ferromagnetism rather than antiferromagnetism: we seek the closest stable solutions near homogeneous magnetism by expanding the appropriate equations around $\mathbf{k} = 0$ in Fourier space. In the antiferromagnetic case however, we would have to start from a wavevector of antiferromagnetic order.

Non-centrosymmetricity in particular allows for terms that are linear in the derivative and proportional to the magnetization squared. Their counterpart in the microscopic picture are the so-called Moriya-Dzyaloshinskii (MD) spin-orbit coupling terms in the Hamiltonian $H_{MD} = \sum_{\langle i,j\rangle} \mathbf{D}_{ij}(\mathbf{S}_i \times \mathbf{S_j})$ [24]. This interaction may lead to a spiral magnetic moment with a single helicity (helical spin-density wave). The terms arise from the perturbative treatment of an orbital anisotropic exchange interaction between neighbouring magnetic moments. The first order perturbation leads to a pseudo-dipole interaction and the second order produces H_{MD}. The vector-valued tensor $\mathbf{D}_{ij}$ is antisymmetric under interchange of i and j, and does not vanish if there is *no inversion symmetry* of the crystal field with respect to center between the two spins. The isotropic case is the Heisenberg Hamiltonian $H_H = J\sum_{\langle i,j\rangle} \mathbf{S_i}\cdot\mathbf{S_j}$.

1.3.3 Superconductivity: Parity mixing

The Landau theory of superconductivity is the so called Ginzburg-Landau theory and can be derived as a limiting case of the BCS theory for conventional superconductivity. The complex-valued order parameter of superconductivity η represents the quantum mechanical wave function of of the condensate of superconducting Cooper pairs. Hence, its absolute value square is a measure of the density of the superconducting charge carriers. However, note that η does *not* correspond to the wave function of a single Cooper pair.

According to the microscopic explanation of superconductivity, there are two possible pairing states: spin-singlet and spin-triplet Cooper pairs. To allow for that, we introduce two order parameters to describe the superconducting state: one for singlet pairing η_s and one for triplet pairing η_p. The first features positive parity, the second one negative. The starting point in our expansion is the generic form of the free energy functional as given in [22]. This accounts for the coupling to a magnetic field $\mathbf{B}$ or a given magnetic state with the magnetization $\mathbf{m}$. Based on the free energy of the normal state $F_n(T)$, the phase transition brings about contributions of the following form:

$$F[\eta_s,\eta_p,\mathbf{A}](T) = F_n(T) + \int \mathrm{d}^3 r \left(f_{sc} + f_{coupling} + \frac{(\nabla\times\mathbf{A})^2}{8\pi} \right) \tag{1.6}$$

To include a magnetic field $\mathbf{B}$ (with vector potential $\mathbf{A}$), the terms are formulated using the gauge invariant derivative. We work in units with Planck's constant $h = 1$.

$$\mathbf{D} \equiv \nabla - \mathrm{i}\frac{4\pi e}{c}\mathbf{A}$$

An important consequence of non-centrosymmetricity is the mixing of the superconductivity order parameters for singlet and triplet pairing via certain terms in the free energy. This is because the lattice order parameters ζ_z and ζ_1 are able to compensate for the negative parity of the product $\eta_s\eta_p$. Moreover, coupling terms between magnetism and superconductivity which are linear in the magnetization are permitted in $f_{coupling}$. They originate from the Moriya-Dzyaloshinskii (MD) spin-orbit interaction allowed by non-centrosymmetricity.

1.3.4 Other symmetries

Barring the spatial symmetries discussed above, the linearly independent terms of the free energy functional must feature additional physically relevant symmetries. These must be taken care of separately:

- Although η_s and η_p are complex valued, the free energy must remain real.
- Under a $U(1)$ *gauge transformation* Φ, the superconducting order parameter picks up a phase factor $\eta_{s,p} \xrightarrow{\Phi} \eta_{s,p}e^{\mathrm{i}\phi}$. So that the free energy remains a scalar quantity, each term must contain the order parameter as often as it contains its complex conjugate. Thus, only even powers of the order parameters are allowed.
- Under *time inversion* K, the order parameters turn into their complex conjugate $\eta_{s,p} \xrightarrow{K} \eta^*_{s,p}$, and the magnetization $\mathbf{m}$ and the magnetic field pick up a minus sign. Since all terms in the free energy are real, we automatically take care of the change in η_s and η_p under time inversion. The minus sign in $\mathbf{m}$ is relevant in the terms of $f_{coupling}$ which are linear in $\mathbf{m}$.

In principle, the action of spin rotations as a further symmetry operation must be taken into account. However, we assume that a sufficiently strong spin-orbit coupling (stiff spin) ties orbital and spin rotations together. This symmetry is thus already accounted for in the consideration of spatial symmetries.

1.4 Variation equations

The following related conditions need to be satisfied for the systems phase to be realised:

- The absolute value and spatial distribution of the order parameter must be such that the free energy functional takes the lowest possible value.
- The state must have the highest transition temperature among all possible phases.

Hence, the variational equation of the free energy functional with respect to the order parameter is a differential equation that determines all possible states. In case of a spatially homogeneous phase, the variation reduces to the usual derivative. Temperature dependence is introduced via a linear expansion of the coefficient of the leading second order term in the free energy functional (as discussed in 1.2). All other coefficients are assumed to be temperature independent.

Since magnetism has a three-dimensional order parameter $\mathbf{m}$, the variation results in a system of three equations which have to be satisfied simultaneously:

$$\frac{\delta F}{\delta m_j(\mathbf{r})} \equiv \frac{\partial F}{\partial m_j(\mathbf{r})} - \sum_{i=x,y,z} \nabla_i \frac{\partial F}{\partial(\nabla_i m_j)} \stackrel{!}{=} 0 \qquad \text{for } j = x, y, z. \tag{1.7}$$

For superconductivity we have to satisfy a set of two variation equations, one for each order parameter:

$$\begin{aligned}\frac{\delta F}{\delta \eta_s^*(\mathbf{r})} &\equiv \frac{\partial F}{\partial \eta_s^*(\mathbf{r})} - \sum_{i=x,y,z} \nabla_i \frac{\partial F}{\partial(\nabla_i \eta_s^*)} \stackrel{!}{=} 0 \\ \frac{\delta F}{\delta \eta_p^*(\mathbf{r})} &\equiv \frac{\partial F}{\partial \eta_p^*(\mathbf{r})} - \sum_{i=x,y,z} \nabla_i \frac{\partial F}{\partial(\nabla_i \eta_p^*)} \stackrel{!}{=} 0.\end{aligned} \tag{1.8}$$

In both cases this is a system of linear homogeneous differential equations in the independent variables η_s, η_p or m_x, m_y, m_z, provided terms only up to second power in the order parameters are included. After a transformation to Fourier space, the operator is a matrix which must have a vanishing determinant in order to yield a non-trivial solution. The highest temperature at which the determinant vanishes defines the critical or transition temperature.

We can also view this as an eigenvalue problem for this linear operator with a temperature dependent eigenvalue $\epsilon_{\mathbf{k}}(T)$. The transition temperature T_c is then given by the zero of the smallest eigenvalue. We can expand the eigenvalue in a Taylor series in a chosen small quantity such as ζ_1, ζ_z, a finite $\mathbf{k}$-vector, or a given magnetization (in case of superconductivity). This enables us to directly tell whether or not the corresponding physical effect enhances or reduces the eigenvalue and thus reduces or enhances the transition temperature.

Restrictions on the phenomenological parameters in the free energy arise from our enforcing that

- the superconducting state without magnetization shall be homogeneous,
- the magnetic state in absence of non-centrosymmetricity shall be homogeneous and that
- the free energy is bounded from below so as to avoid arbitrarily strong modulations of the order parameter.

Furthermore, the coefficients must be such that the total free energy is bounded from below so as to sidestep the complication of arbitrarily large absolute values of the order parameter.

Our objective with this theory is the determination of a qualitative spatial picture of the possible phases of

- superconductivity (with f_{sc}),
- magnetism (with f_{mag}), and
- superconductivity in the previously obtained magnetic phases $\mathbf{m}(\mathbf{r})$ (with $f_{sc} + f_{coupling}$)

Furthermore, the dependence of the transition temperature as a function of the phenomenological parameters (and the magnetization in the latter case) can be determined.

1.5 Solving strategies

The determination of the solution of variation equations (1.7) and (1.8) with the help of a Fourier transformation is a straightforward algebraic problem, provided the coefficients have no spatial dependence. However, if there exists a modulated magnetic phase, the magnetization that appears in $f_{coupling}$ is not constant and thus the algebra becomes more involved. We make use of two equivalent approaches, one in Fourier space (section 1.5.1), and one in real space (section 1.5.2).

1.5.1 Bloch's theorem and weak magnetization

Differential equations with periodic coefficients are a familiar problem in solid state physics: A standard way to solve for an electron wave function in a weak potential of a periodic crystal lattice is the *nearly free electron method* (NFE). It is based on Bloch's theorem which postulates that the solution inherits the periodicity of the coefficients. The mathematical equivalent is Floquet's theorem [10]. Although the physical situation is different in our case, the mathematical question is the same and we shall also call our treatment the NFE method. Let us consider a one-dimensional problem with the coefficients' periodicity described by a wavevector k_0. Bloch's theorem states that the function for which we need to solve can be written as

$$\eta_{s,k}(x) = \sum_n s_n(k) e^{\mathrm{i}K_n x} \tag{1.9}$$

$$\eta_{p,k}(x) = \sum_n p_n(k) e^{\mathrm{i}K_n x}. \tag{1.10}$$

The wavevector $K_n = k + 2nk_0,\ n \in \mathbb{Z}$ is composed of $k \in [-k_0, k_0]$ which is confined to the first Brillouin zone and gives an overall modulation and a second contribution that creates functions with the same periodicity as the equations' coefficients themselves. The variable n labels the linearly independent *modes*.

Our further assumption is that the potential, which in our case is a modulated magnetization $\mathbf{m}(\mathbf{r})$, is weak compared to the other coefficients. Without modulation, we would only have to solve for the modes s_0 and p_0 – the coupling to higher modes is due to the potential. However, higher modes are suppressed by the weakness of the coupling potential, provided the value of k is not close to the boundary of the Brillouin zone or to other points of degeneracy in higher bands. To determine an approximate solution, it is sufficient to keep track of the modes s_n and p_n up to a particular order only (we take $n \le 1$). In this case, a homogeneous linear system of six equations is to be solved (two phases – singlet and triplet – with three mods).

1.5.2 Mathieu's equation

In case the periodic potential given by magnetization has a simple sine or cosine modulation and we are able to reduce the problem to a single dimension, we can find an exact solution if we cast it in the form of Mathieu's equation:

$$\boxed{0 = \eta''(x) + a\eta(x) + 2w\cos(2x)\eta(x)} \tag{1.11}$$

This is a second order homogeneous differential equation for $\eta(x)$. Since the coefficients are periodic in x, Floquet's theorem applies (see [1]). The theorem states that the two linear independent solutions can be written in the form

$$\eta(x) = e^{\mathrm{i}rx} P(x) \qquad\qquad \eta(x) = e^{-\mathrm{i}rx} P(-x), \tag{1.12}$$

where r is the *characteristic exponent* and depends on a and w in a nontrivial way. $P(x)$ is a periodic function with the same period as the equation coefficients (π in our case). This is equivalent to Bloch's theorem as discussed in the previous section, where r corresponds to k.

Mathieu's equation is not analytically solvable in closed form. Thus the two linear independent solutions define special functions, most commonly phrased as the *real normalised Mathieu-Sine* $\mathrm{S}(a, w, x)$ and *Mathieu-Cosine* $\mathrm{C}(a, w, x)$. Both are aperiodic functions which deviate from sine and cosine the greater w becomes (see figure 1.2). Note that the solution is bounded, for real values of r only. If r is a

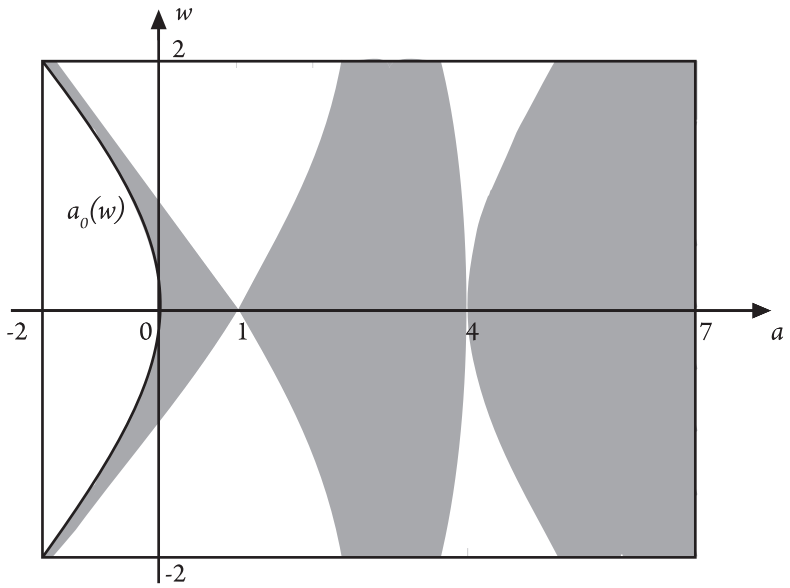

Figure 1.1: Stability diagram for Mathieu's equation (4.4). The parameter regions for which stable (bounded) solutions exist are indicated with grey. Solutions at the edges of stability regions are periodic. The parameters defining the edges are called characteristic values, such as the curve $a_0(w)$ for stability region of zeroth order.

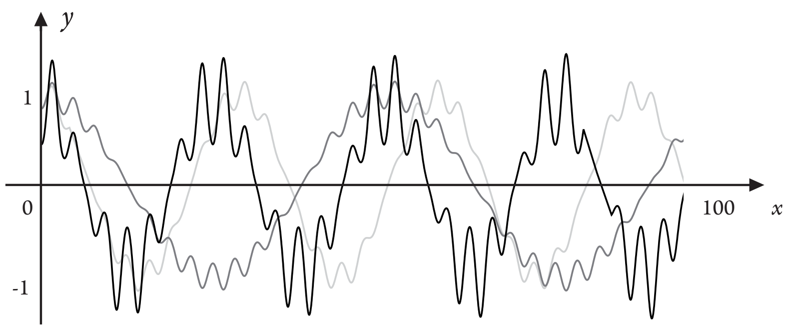

Figure 1.2: Three different examples of Mathieu-Cosine $\mathrm{C}(a,w,x)$: light grey $\mathrm{C}(0,0.3,x)$; grey $\mathrm{C}(-0.03,0.3,x)$; black $\mathrm{C}(-0.6,1.2,x)$. Although the action of both parameters a and w are related, a tends to change the period, whereas the graph becomes more pitted in its deviation from a cosine with increasing w.

complex number the solution either decays or grows exponentially and is called *unstable*, otherwise it is a *stable* solution. The parameter ranges for a and w which give stable solutions define the stability region of equation (1.11). Furthermore, the edges of the stability regions define the *characteristic values* for the parameters $a_n(w)$, where n is the order of the stability region. The solution of the Mathieu equation with characteristic values has π or 2π periodicity. The expansion of $a_0(w)$, indicated by the bold line in figure 1.1, is given by [1]:

$$a_0(w) = -\frac{w^2}{2} + \frac{7}{128}w^4 + \dots \tag{1.13}$$

The expansion of the periodic solution on the edge of the zeroth order stability region reads:

$$\mathrm{ce}_0(x, w) = \frac{1}{\sqrt{2}}\left[1 - \frac{w}{2}\cos 2x + w^2\left(\frac{\cos 4z}{32} - \frac{1}{16}\right) + \dots\right] \tag{1.14}$$

In our context, a will be a temperature dependent parameter, which becomes renormalised by the modulated magnetization, while w is proportional to the magnetization squared and can thus be seen as a (small) perturbation. Additional difficulty comes into play because we have two unknowns η_s and η_p and thus a coupled system of two Mathieu equations.

CHAPTER 2

Tetragonal crystal symmetry

The aim of this chapter is to study how the presence of a magnetic phase alters superconductivity in a crystal with a tetragonal unit cell. In order to do so, we first analyse homogeneous superconductivity and magnetism independently (sections 2.1 and 2.2). Afterwards, we study the impact of each of the calculated magnetic phases on the superconductivity order parameter (sections 2.3 and 2.4).

The most symmetric tetragonal point group D_{4h} will be used. We assume that parity is violated in the z-direction only (the crystallographic c-axis), since this axis already stands out from the others by crystal symmetry. Accordingly we introduce a (small) lattice order parameter ζ_z as measure of the strength of the parity violation. This order parameter can be taken to represent a polar vector in the crystallographic c-direction, describing the dipole moment of the non-centrosymmetric crystal field. In terms of the gap function (see (1.2)), this corresponds to an anisotropy taken to be

$$\mathbf{g}_{\mathbf{k}} = \mathbf{e}_z \times \mathbf{k}. \tag{2.1}$$

2.1 Homogeneous superconductivity

We determine the Ginzburg-Landau free energy density of superconductivity f_{sc} in the absence of magnetic fields or magnetic order. We force the superconducting state to be homogeneous. Its parity properties and transition temperature will be analysed, and we focus in particular on the implications of non-centrosymmetricity.

2.1.1 Expansion of the free energy f_{sc}

In principle, the dimensions of the singlet and triplet order parameters are not predetermined. They can, however, be chosen according to the dimensions of the irreducible point group representations that reveal the symmetries of the order parameters. For simplicity, we choose η_s and η_p to be one-dimensional (see Table 2.1). Higher dimensions allow the description of superconducting phases in greater detail. For example the distinction between spin-up and spin-down state of triplet Cooper pairs can be included.

Parameter	Representation	Dimension	Basis function
η_s	Γ_1^+	1	$x^2+y^2+z^2$
η_p	Γ_2^-	1	z
ζ_z	Γ_2^-	1	z
D_z	Γ_2^-	1	z
D_x, D_y	Γ_5^-	2	x, y

Table 2.1: Representations of parameters in tetragonal symmetry

According to the symmetry considerations explained in section 1.3, the free energy of superconductivity has the following expansion in η_s and η_p. As in [21] we included all possible terms of the form "η^2", "η^4", "$D\eta^2$" and "$D^2\eta^2$". In this section and in the ones which follow vectors with index $\perp$ (e.g. $\mathbf{D}_\perp, \nabla_\perp, \mathbf{m}_\perp$) denote two-vectors with x- and y-components only.

$$\begin{aligned} f_{sc} \;=\;& a_s|\eta_s|^2 + a_p|\eta_p|^2 + b_s|\eta_s|^4 + b_p|\eta_p|^4 + c_1|\eta_s|^2|\eta_p|^2 \\ & c_2\left(\eta_s^{*2}\eta_p^2 + \eta_s^2\eta_p^{*2}\right) + d\zeta_z\left(\eta_s^*\eta_p + \eta_s\eta_p^*\right) + \\ & \delta_0\left(\eta_s D_z^*\eta_p^* + \eta_s^* D_z\eta_p\right) + \delta_s\zeta_z\left(\eta_s D_z^*\eta_s^* + \eta_s^* D_z\eta_s\right) + \delta_p\zeta_z\left(\eta_p D_z^*\eta_p^* + \eta_p^* D_z\eta_p\right) + \\ & \gamma_{s,\perp}|\mathbf{D}_\perp\eta_s|^2 + \gamma_{s,z}|D_z\eta_s|^2 + \gamma_{p,\perp}|\mathbf{D}_\perp\eta_p|^2 + \gamma_{p,z}|D_z\eta_p|^2 + \\ & \gamma_{0,z}\zeta_z\left((D_z\eta_s)^* D_z\eta_p + D_z\eta_s (D_z\eta_p)^*\right) + \gamma_{0,\perp}\zeta_z\left((\mathbf{D}_\perp\eta_s)^*\cdot\mathbf{D}_\perp\eta_p + \mathbf{D}_\perp\eta_s\cdot(\mathbf{D}_\perp\eta_p)^*\right) \end{aligned} \tag{2.2}$$

Here we have introduced 16 phenomenological parameters, one for each linearly independent term which shows Γ_1^+-symmetry. For the remainder of this work, the indices s and p denote that the parameter belongs to a term constructed either from η_s or η_p. The index 0 indicates terms in which singlet and triplet order parameters are mixed. The term proportional to d is the term responsible for parity mixing and therefore represents the spin-orbit interaction.

Aside from a_s and a_p, all parameters are assumed to be temperature independent. The former are expanded to first order in temperature:

$$\begin{aligned} a_s &= a_s'(T - T_{cs}) \\ a_p &= a_p'(T - T_{cp}) \end{aligned} \tag{2.3}$$

In doing so, we assume that singlet and triplet pairing can arise at different temperatures T_{cs} and T_{cp} in general. To mimic the phase transition behaviour as discussed in section 1.2, both a_s' and a_p' are positive. Since the expansion of the free energy is symmetric in the indices s and p, without loss of generality we can from here onwards assume that the singlet pairing transition temperature is greater than the triplet pairing transition temperature

$$T_{cs} > T_{cp}. \tag{2.4}$$

Terms with phenomenological parameters $\gamma_{n,\bullet}$ ($n = s,\ p;\ \bullet = z,\ \perp$) are important if superconductivity varies in space. So as to avoid an instability (arbitrary strong modulations of η_s or η_p), these stiffness parameters are taken to be positive.

2.1.2 Analysis of second order terms in the free energy

Restrictions on the expansion parameters in (2.2) arise from the conditions under which a homogeneous superconducting phase can be realised. So as to avoid exotic solutions in the form of heavy modulations of the order parameter, the homogeneous solution of the variation equations must have the highest critical temperature T_c and thus will come about. Neglecting terms of third order in $\eta_{s,p}$, the variation equations in the absence of a magnetic field read ($\mathbf{D} = \nabla$)

$$\begin{aligned} 0 &= a_s\eta_s + d\zeta_z\eta_p + \delta_0\nabla_z\eta_p - \gamma_{s,z}\nabla_z^2\eta_s - \gamma_{0,z}\zeta_z\nabla_z^2\eta_p - \\ &\quad \gamma_{s,\perp}\nabla_x^2\eta_s - \gamma_{0,\perp}\zeta_z\nabla_x^2\eta_p - \gamma_{s,\perp}\nabla_y^2\eta_s - \gamma_{0,\perp}\zeta_z\nabla_y^2\eta_p \\ 0 &= a_p\eta_p + d\zeta_z\eta_s - \delta_0\nabla_z\eta_s - \gamma_{p,z}\nabla_z^2\eta_p - \gamma_{0,z}\zeta_z\nabla_z^2\eta_s - \\ &\quad \gamma_{p,\perp}\nabla_x^2\eta_p - \gamma_{0,\perp}\zeta_z\nabla_x^2\eta_s - \gamma_{p,\perp}\nabla_y^2\eta_p - \gamma_{0,\perp}\zeta_z\nabla_y^2\eta_s. \end{aligned} \tag{2.5}$$

They can be written in $\mathbf{k}$-space ($\eta_{s,p} = \int \mathrm{d}^3 r e^{\mathrm{i}\mathbf{kr}}\hat{\eta}_{s,p}(\mathbf{k})$)

$$\begin{aligned} \hat{A}_s\hat{\eta}_s + \hat{B}\hat{\eta}_p &= 0 \\ \hat{A}_p\hat{\eta}_p + \hat{B}^\dagger\hat{\eta}_s &= 0, \end{aligned} \tag{2.6}$$

where we have defined the following operators

$$\begin{aligned} \hat{A}_s &:= a_s + \gamma_{s,z}k_z^2 + \gamma_{s,\perp}\left(k_x^2 + k_y^2\right) \\ \hat{A}_p &:= a_p + \gamma_{p,z}k_z^2 + \gamma_{p,\perp}\left(k_x^2 + k_y^2\right) \\ \hat{B} &:= \zeta_z d + \mathrm{i}\delta_0 k_z + \zeta_z\gamma_{0,z}k_z^2 + \zeta_z\gamma_{0,\perp}\left(k_x^2 + k_y^2\right). \end{aligned} \tag{2.7}$$

To calculate the shape of the state and the transition temperature from this homogeneous linear system of two equations, we perform a calculation that will be repeatedly done in this work – for superconductivity as well as for magnetism.

We use the temperature expansion of a_s and a_p as given by (2.3), and examine the expression near the transition temperature of the singlet state T_{cs}. Under the assumption (2.4), a_p is positive.

For the system (2.6) to have a non-trivial solution, the determinant must vanish ($\hat{A}_s\hat{A}_p - \hat{B}\hat{B}^\dagger = 0$). Since $\hat{A}_s$ and $\hat{A}_p$ are linear in temperature, there will be two temperatures at which the determinant vanishes. The greater of them is defined as the *transition temperature*.

Let us first consider the system with inversion symmetry by setting $\zeta_z = 0$. In this case, the critical temperature of homogeneous (singlet) superconductivity is expected to be T_{cs}. At this temperature, the determinant of the system (2.6) reads

$$\begin{aligned} &\left(k_x^2 + k_y^2\right)a_p\gamma_{s,\perp} + k_z^2\left(a_p\gamma_{s,z} - \delta_0^2\right) + \left(k_x^2 + k_y^2\right)k_z^2\left(\gamma_{s,\perp}\gamma_{p,z} + \gamma_{p,\perp}\gamma_{s,z}\right) + \\ &\left(k_x^2 + k_y^2\right)^2\gamma_{s,\perp}\gamma_{p,\perp} + k_z^4\gamma_{s,z}\gamma_{p,z} = 0. \end{aligned} \tag{2.8}$$

So as avoid real solutions of (2.8) at finite $\mathbf{k}$, all terms in (2.8) must be positive definite. Hence, the following condition clearly follows:

$$\boxed{a_p'(T_{cs} - T_{cp})\gamma_{s,z} > \delta_0^2}\,. \tag{2.9}$$

Let us now turn to the case of non-centrosymmetricity with $\zeta_z \neq 0$. Using the linear temperature expansion of a_s and a_p, the greater solution of $\hat{A}_s\hat{A}_p - \hat{B}\hat{B}^\dagger = 0$ is given by:

$$\begin{aligned} T_c \;=\;& \frac{T_{cs}+T_{cp}}{2} - (k_x^2+k_y^2)\gamma_{\perp,+} - k_z^2\gamma_{z,+} + \\ & \left\{ \left(\frac{T_{cs}-T_{cp}}{2}\right)^2 + \frac{d^2\zeta_z^2}{a_s'a_p'} + (k_x^2+k_y^2)\left(\frac{2d\gamma_{0,\perp}\zeta_z^2}{a_s'a_p'} + \gamma_{\perp-}(T_{cs}-T_{cp})\right) \right. \\ & + k_z^2\left(\frac{2d\gamma_{0,z}\zeta_z^2}{a_s'a_p'} - \gamma_{z-}(T_{cs}-T_{cp}) + \frac{\delta_0^2}{a_s'a_p'}\right) + (k_x^2+k_y^2)k_z^2\left(2\gamma_{\perp-}\gamma_{z-} + \frac{2\gamma_{0,\perp}\gamma_{0,z}\zeta_z^2}{a_s'a_p'}\right) \\ & \left. + (k_x^2+k_y^2)^2\left(\gamma_{\perp-}^2 + \frac{\gamma_{0,\perp}^2\zeta_z^2}{a_s'a_p'}\right) + k_z^4\left(\gamma_{z-}^2 + \frac{\gamma_{0,z}^2\zeta_z^2}{a_s'a_p'}\right)\right\}^{1/2} \end{aligned} \tag{2.10}$$

Where we have used the abbreviations

$$\gamma_{\bullet\pm} = \frac{\gamma_{s,\bullet}}{2a_s'} \pm \frac{\gamma_{p,\bullet}}{2a_p'} \qquad \bullet = z, \perp\,. \tag{2.11}$$

To ensure that the homogeneous solution ($\mathbf{k} = 0$) has the highest transition temperature we impose the following conditions:

$$\left(\frac{\partial T_c}{\partial k_i^2}\right)_{\mathbf{k}=0} < 0 \qquad\qquad \lim_{k_i\to\infty}\frac{T_c}{k_i^2} < 0 \qquad \forall i = x, y, z \tag{2.12}$$

Using (2.9), this determines the following four additional constraints on the parameters (the first two only apply if the quantity on the left is positive):

$$\boxed{2\gamma_{s,\perp}\frac{a_p'(T_{cs}-T_{cp})}{d\gamma_{0,\perp} - \frac{4\gamma_{\perp+}d^2}{T_{cs}-T_{cp}}} > \zeta_z^2} \qquad \boxed{2\gamma_{s,z}\frac{a_p'(T_{cs}-T_{cp})}{d\gamma_{0,z} - \frac{4\gamma_{z+}d^2}{T_{cs}-T_{cp}}} > \zeta_z^2}$$

$$\boxed{\gamma_{s,\perp}\gamma_{p,\perp} > \gamma_{0,\perp}^2\zeta_z^2} \qquad \boxed{\gamma_{s,z}\gamma_{p,z} > \gamma_{0,z}^2\zeta_z^2} \tag{2.13}$$

All these conditions give restrictions on the absolute value of ζ_z. The strength of non-centrosymmetricity thus seems to be limited in order to allow for stable superconductivity.

If we assume ζ_z to be sufficiently small, the transition temperature can be expanded and reads

$$\boxed{T_c = \frac{T_{cs}+T_{cp}}{2} + \sqrt{\left(\frac{T_{cs}-T_{cp}}{2}\right)^2 + \frac{d^2\zeta_z^2}{a_s'a_p'}} \approx T_{cs} + \zeta_z^2\frac{d^2}{a_s'a_p'(T_{cs}-T_{cp})}} \tag{2.14}$$

This shows clearly that non-centrosymmetricity always acts in favour of a higher transition temperature and thus mixes the singlet and the triplet phases. From (2.6) we can read off the mixing ratio for homogeneous superconductivity in the vicinity of the transition (to lowest order in ζ_z):

$$\boxed{\frac{\eta_p}{\eta_s} = -\left.\frac{\hat{B}^\dagger}{\hat{A}_p}\right|_{\mathbf{k}=0} = -\frac{\zeta_z d}{a_p'(T_{cs}-T_{cp})}} \tag{2.15}$$

Hence, triplet pairing exists for temperatures above T_{cp}, where the ratio is controlled by the non-centrosymmetricity parameter ζ_z and – as mentioned before – by the mixing coefficient d. As a consequence, states with defined parity (either triplet pairing or singlet pairing) are not solutions in systems without inversion symmetry.

2.1.3 Analysis of fourth order terms in the free energy

While second order terms in the free energy govern the point of transition, terms that are proportional to "η^4" bound the absolute value of the order parameter. Since the solutions are cumbersome in complexity, we shall not delve into them here.

Furthermore, fourth order terms make an impact on the phase coherence of η_s and η_p. To study this we consider the variation equations for homogeneous superconductivity:

$$\begin{aligned} 0 &= a_s\eta_s + 2b_s\left|\eta_s\right|^2\eta_s + c_1\left|\eta_p\right|^2\eta_s + 2c_2\eta_p^2\eta_s^* + d\zeta_z\eta_p \\ 0 &= a_p\eta_p + 2b_p\left|\eta_p\right|^2\eta_p + c_1\left|\eta_s\right|^2\eta_p + 2c_2\eta_s^2\eta_p^* + d\zeta_z\eta_s. \end{aligned} \tag{2.16}$$

Using a parametrisation of the order parameters with absolute value and complex phase $\eta_s = \eta_{s,0}e^{\mathrm{i}\varphi_s}$, $\eta_p = \eta_{p,0}e^{\mathrm{i}\varphi_p}$ and $\Delta\varphi = \varphi_s - \varphi_p$, these equations read:

$$\begin{aligned} 0 &= \left(a_s + b_s\eta_{s,0}^2 + c_1\eta_{p,0}^2\right)\eta_{s,0} + \left(2c_2\eta_{s,0}\eta_{p,0}e^{-\mathrm{i}\Delta\varphi} + d\zeta_z\right)\eta_{p,0}e^{-\mathrm{i}\Delta\varphi} \\ 0 &= \left(a_p + b_p\eta_{p,0}^2 + c_1\eta_{s,0}^2\right)\eta_{p,0} + \left(2c_2\eta_{p,0}\eta_{s,0}e^{\mathrm{i}\Delta\varphi} + d\zeta_z\right)\eta_{s,0}e^{\mathrm{i}\Delta\varphi}. \end{aligned} \tag{2.17}$$

Since the first terms in both equations are real, the second terms must also be real. Its imaginary part must therefore vanish:

$$0 = 2c_2\eta_{s,0}\eta_{p,0}\sin(\pm 2\Delta\varphi) + \zeta_z d\sin(\pm\Delta\varphi) \quad \Rightarrow \Delta\varphi = 0, \pi$$

Both possibilities for $\Delta\varphi$ correspond to the change $\zeta_z d \longrightarrow -\zeta_z d$ and the solutions are therefore equivalent. In agreement with (2.15) we have

$$\begin{aligned} \Delta\varphi &= 0 \quad \text{if } d\zeta_z < 0 \\ \Delta\varphi &= \pi \quad \text{if } d\zeta_z > 0 \end{aligned} \tag{2.18}$$

stating that the mixing ratio of singlet and triplet superconductivity will always be real. The sign will depend on the sign of the spin-orbit coupling parameter d. Our result resembles the one given in [21].

2.2 Magnetic phases

In this section, we shall use a Landau theory to explore – similar to the treatment of superconductivity – possible magnetic phases in a tetragonal crystal lattice (point group D_{4h}) without inversion center. The order parameter is the real position-dependent magnetization $\mathbf{m}$. Table 2.2 lists the symmetries of all quantities that occur in the expansion of the free energy f_{mag}.

In the following expansion, we keep terms up to fourth power in $\mathbf{m}$, and derivative-terms up to "$\nabla^2 m^2$".

$$\begin{aligned} f_{mag} = \; & \alpha_\perp\mathbf{m}_\perp^2 + \alpha_z m_z^2 + \beta_1\left(\mathbf{m}_\perp^2\right)^2 + \beta_2\mathbf{m}_\perp^2 m_z^2 + \beta_3 m_z^4 + \beta_4 m_x^2 m_y^2 + \\ & \vartheta_1\zeta_z\left(m_x\nabla_z m_x + m_y\nabla_z m_y\right) + \vartheta_2\zeta_z m_z\nabla_z m_z + 2\vartheta_3\zeta_z m_z\left(\nabla_\perp\cdot\mathbf{m}_\perp\right) + \\ & \tau_1\left(\nabla_\perp\cdot\mathbf{m}_\perp\right)^2 + \tau_2\left(\nabla_x m_x - \nabla_y m_y\right)^2 + \tau_3\left(\nabla_x m_y + \nabla_y m_x\right)^2 + \\ & 2\tau_4\left(\nabla_\perp\cdot\mathbf{m}_\perp\right)\left(\nabla_z m_z\right) + \tau_5\left(\nabla_z\mathbf{m}_\perp\right)^2 + \tau_6\left(\nabla_\perp m_z\right)^2 + \tau_7\left(\nabla_z m_z\right)^2 \end{aligned} \tag{2.19}$$

Again, all expansion coefficients in (2.19) are assumed to be temperature independent, save for

$$\begin{aligned} \alpha_\perp &= \alpha'_\perp(T - T_{c\perp}) \\ \alpha_z &= \alpha'_z(T - T_{cz}). \end{aligned} \tag{2.20}$$

The temperatures $T_{c\perp}$ and T_{cz} are the critical temperatures of homogeneously magnetized states in the z-direction and in the x-y-plane in the absence of non-centrosymmetricity.

The terms with coefficients τ_i $(i = 1\ldots7)$ ensure the stiffness of the system so as to avoid arbitrary modulations in $\mathbf{m}$, similar to the superconductivity γ-terms. We can however not simply assume that they are all positive, because a weaker constraint may also guarantee stiffness. Non-centrosymmetricity also allows for ϑ-terms of the form "$m\nabla m$". These reflect the presence of MD interaction in the system, as mentioned in 1.3.2.

The variation of (2.19) with respect to m_x, m_y and m_z yields a homogeneous linear system of three equations for the Fourier components ($m_j = \int \mathrm{d}^3 r\, \hat{m}_j e^{i\mathbf{k}\cdot\mathbf{r}}$; $j = x, y, z$) with the following system matrix:

$$M = \begin{pmatrix} \alpha_\perp + k_x^2(\tau_1+\tau_2) + k_y^2\tau_3 + k_z^2\tau_5 & k_xk_y(\tau_1-\tau_2+\tau_3) & k_xk_z\tau_4 - \mathrm{i}\zeta_z k_x\vartheta_3 \\ k_xk_y(\tau_1-\tau_2+\tau_3) & \alpha_\perp + k_y^2(\tau_1+\tau_2) + k_x^2\tau_3 + k_z^2\tau_5 & k_yk_z\tau_4 - \mathrm{i}\zeta_z k_y\vartheta_3 \\ k_xk_z\tau_4 + \mathrm{i}\zeta_z k_x\vartheta_3 & k_yk_z\tau_4 + \mathrm{i}\zeta_z k_y\vartheta_3 & \alpha_z + (k_x^2+k_y^2)\tau_6 + k_z^2\tau_7 \end{pmatrix} \tag{2.21}$$

The equation $\mathrm{Det}(M) = 0$ implicitly defines the transition temperature as a function of $\mathbf{k}$. The transition temperature reaches a local maximum when the magnetic state is realised. Since M is hermitian, $\mathrm{Det}(M)$ is real. Furthermore $\mathrm{Det}(M)$ contains only even powers of k_x, k_y and k_z. Using the implicit function theorem, the directional derivative of $T(\mathbf{k})$ at $\mathbf{k} = 0$ is given by

$$\mathbf{k}\cdot\nabla_{\mathbf{k}} T(\mathbf{k}) = -\frac{\sum_{i=1}^{3} \frac{\partial \mathrm{Det}(M)}{\partial k_i} k_i}{\frac{\partial \mathrm{Det}(M)}{\partial T}}. \tag{2.22}$$

2.2.1 The centrosymmetric system

In $\mathrm{Det}(M)$ there exist terms proportional to ζ_z. We can toggle the non-centrosymmetricity by choosing whether or not $\zeta_z = 0$. We shall first consider the case with the non-centrosymmetricity turned off. Our aim is to find the conditions under which the system attains a homogeneous magnetization. In doing this we assume implicitly that this is the ground state of the centrosymmetric system. We check the terms in $\mathrm{Det}(M)$ order by order in $\mathbf{k}$ for positive definiteness in both cases $T_{cz} > T_{c\perp}$ and $T_{c\perp} > T_{cz}$. The cases of interest are listed below:

- The terms in $\mathrm{Det}(M)$ which are of *highest (sixth) order* in $\mathbf{k}$ are proportional to combinations of τ-parameters only. The natural demand for stiffness $\lim_{|\mathbf{k}|\to\infty} T(\mathbf{k}) < 0$ is thus equivalent to certain

Parameter	Representation	Dimension	Basis function(s)
ζ_z	Γ_2^-	1	z
∇_z	Γ_2^-	1	z
m_z	Γ_2^+	1	z
$\nabla_{x,y}$	Γ_5^-	2	x, y
$m_{x,y}$	Γ_5^+	2	S_x, S_y

Table 2.2: Representations of parameters in tetragonal symmetry

conditions on the τ-parameters. However, conditions of sufficient simplicity cannot be found. We therefore simply assume the parameters to be such that the sixth order terms are positive definite. In any case, their coefficients do not depend on T.

- Taking into account only the *second order* terms in $\mathbf{k}$, the following condition ensures a local maximum of $T(\mathbf{k})$ at $\mathbf{k}=0$ (where $\mathbf{k}\cdot\nabla_{\mathbf{k}}T(\mathbf{k})$ is computed with (2.22))

$$0 > \lim_{|\mathbf{k}|\to 0}\frac{1}{|\mathbf{k}|^2}\mathbf{k}\cdot\nabla_{\mathbf{k}}T(\mathbf{k}) \tag{2.23}$$

- In addition, there exists the possibility that the *fourth order* terms are not positive definite – while the second order terms are – leading to local maxima of the free energy that are not included in the above condition. We need to consider the quadratic form of the forth-order coefficients, which do not need to be positive definite in $\mathbb{R}^3$, but only on the cone of vectors with positive coefficients (k_x^2, k_y^2, k_z^2).

Higher transition temperature for the z-axis $T_{cz} > T_{c\perp}$

If T_{cz} is the transition temperature, the parameters take the values $\alpha_z = 0$; $\alpha_\perp = \alpha'_\perp(T_{cz} - T_{c\perp})$ at the phase transition. The Conditions that result from the second order terms according to (2.23) are

$$\boxed{\tau_6 > 0} \quad \text{and} \quad \boxed{\tau_7 > 0}. \tag{2.24}$$

Furthermore, the positive definiteness of the fourth order terms yields

$$\boxed{\tau_1+\tau_2+\tau_3 > 0}\,, \quad \boxed{\tau_5 > 0} \quad \text{and} \quad \boxed{\tau_4^2 < \left(\sqrt{\frac{(\tau_1+\tau_2+\tau_3)\tau_7}{2}} + \sqrt{\tau_5\tau_6}\right)^2}\,. \tag{2.25}$$

In this case, **homogeneous magnetization in the z-direction** is the symmetry-broken state of the material.

Higher transition temperature for x-y-plane $T_{c\perp} > T_{cz}$

If $T_{c\perp}$ defines the transition, the parameters become $\alpha_\perp = 0$; $\alpha_z = \alpha'_z(T_{c\perp} - T_{cz})$. In this case, the second order term constraints are

$$\boxed{\tau_1+\tau_2+\tau_3 > 0} \quad \text{and} \quad \boxed{\tau_5 > 0}. \tag{2.26}$$

Additionally, the positive definite fourth order terms require

$$\boxed{\tau_2 > 0}\,, \quad \boxed{\tau_3 > 0}\,, \quad \boxed{\tau_1 > -\tau_2} \quad \text{and} \quad \boxed{\tau_1 > -\tau_3}\,. \tag{2.27}$$

The magnetically ordered state is in this case a **homogeneous magnetization in the x-y-plane**. The circular degeneracy of the orientation of $\mathbf{m}$ in the plane shall not be lifted within the scope of this discussion.

2.2.2 The effect of non-centrosymmetricity: modulated phases

Having found restrictions on the parameter ranges, we can now study the non-centrosymmetric system ($\zeta_z \neq 0$). This means that we take the MD terms with ϑ-parameters into account and perform a similar calculation. In doing so we assume that all conditions that we derived in the previous section (so as to avoid modulations with centrosymmetricity) are still valid.

Higher transition temperature for the z-axis $T_{cz} > T_{c\perp}$

If we assume that $T_{cz} > T_{c\perp}$, the second order terms yield that $T(\mathbf{k}=0) = T_{cz}$ is no longer a local maximum once ζ_z^2 exceeds the threshold value

$$\boxed{\zeta_z^2 > \frac{\tau_6 \alpha'_\perp (T_{cz} - T_{c\perp})}{\vartheta_3^2} > 0}. \tag{2.28}$$

Consequently, the magnetization becomes modulated if (2.28) holds, since the highest transition temperature no longer occurs at $\mathbf{k} = 0$.

The steepest slope of $T(\mathbf{k})$ can be found when $k_z = 0$. From this, we conclude that the modulation wavevector degenerately lies in the k_x-k_y-plane.

To lift this degeneracy, we calculate the impact of those terms proportional to $\mathbf{k}^4$ in the numerator of (2.22), which bore no influence on the limit (2.23). For $k_z = 0$ and $T = T_{cz}$ we can parametrize $k_x = k\cos\phi$ and $k_y = k\sin\phi$. Their contribution to the slope is

$$\begin{aligned} &4\zeta_z^2\vartheta_3^2\tau_2 \sin^2\phi\cos^2\phi - \zeta_z^2\vartheta_3^2\tau_3\left(\sin^2\phi - \cos^2\phi\right)^2 - \\ &\alpha'_\perp(T_{c\perp} - T_{cz})\tau_6(\tau_1+\tau_2+\tau_3)\left(\sin^2\phi + \cos^2\phi\right)^2 \end{aligned} \tag{2.29}$$

We find that this part of the slope has several maxima:

1. If $\boxed{\tau_3 > \tau_2}$, the maxima occur at $\phi = 0$ $[\pi/2]$. This corresponds to a wavevector of modulated magnetization parallel to a coordinate axis of the x-y-plane.
2. In the case that $\boxed{\tau_2 > \tau_3}$ the maxima occur at $\phi = \pi/4$ $[\pi/2]$, where the wavevector of magnetic order points along the diagonals in the x-y-plane.

We can conclude that the τ_2, τ_3-terms govern the shape of a the modulated magnetic phase. Their difference can be interpreted as an anisotropy parameter. In this derivation, we surmised that the conditions for $|\mathbf{k}| \to \infty$ apply, which we did not explicitly find. Furthermore, the structure of the $\mathbf{k}$-space surface is assumed to be sufficiently simple, such that the biggest slope points towards the local maximum.

As final step, we investigate the spatially varying magnetization vector by solving the homogeneous linear system of equations with coefficient matrix (2.21) for the two $\mathbf{k}$-vectors we obtained.

(1) Case $\tau_3 > \tau_2$
The problem is symmetric in the modes k_x and k_y. Thus, without loss of generality, we take $k_x \neq 0;\ k_y = 0;\ k_z = 0$. In this case the determinant of (2.21) defines three functions $T(k_x, 0, 0)$. However, only one of them satisfies $T(0,0,0) = T_{cz}$

$$T = \frac{T_{c\perp} + T_{cz}}{2} - k_x^2\left(\frac{\tau_1+\tau_2}{2\alpha'_\perp} + \frac{\tau_6}{2\alpha'_z}\right) + \sqrt{\left(\frac{T_{c\perp} - T_{cz}}{2} - k_x^2\left(\frac{\tau_1+\tau_2}{2\alpha'_\perp} - \frac{\tau_6}{2\alpha'_z}\right)\right)^2 + \frac{k_x^2\zeta_z^2\vartheta_3^2}{\alpha'_\perp\alpha'_z}}. \tag{2.30}$$

With the abbreviations $\varsigma_\perp = \alpha'_\perp\tau_6$ and $\varsigma_z = \alpha'_z(\tau_1+\tau_2)$ we can explicitly give the wavevector that maximizes the transition temperature

$$\boxed{k_\ominus^2 = \frac{\alpha'_\perp\alpha'_z\left\{(\varsigma_z - \varsigma_\perp)(T_{c\perp} - T_{cz}) - 2\zeta_z^2\vartheta_3^2\right\}}{(\varsigma_\perp - \varsigma_z)^2} - \frac{\sqrt{\varsigma_\perp\varsigma_z\zeta_z^2\vartheta_3^2(\varsigma_\perp + \varsigma_z)^2\left((\varsigma_z - \varsigma_\perp)(T_{cz} - T_{c\perp}) + \zeta_z^2\vartheta_3^2\right)}}{(\tau_1+\tau_2)\tau_6(\varsigma_\perp - \varsigma_z)^2}}, \tag{2.31}$$

as well as the critical temperature for the magnetic state

$$T_\ominus = \frac{\varsigma_\perp T_{c\perp} - \varsigma_z T_{cz}}{\varsigma_\perp - \varsigma_z} + \zeta_z^2 \vartheta_3^2 \frac{\varsigma_\perp + \varsigma_z}{(\varsigma_\perp - \varsigma_z)^2} + \frac{\varsigma_\perp^2 + \varsigma_z^2}{\varsigma_\perp \varsigma_z (\varsigma_\perp - \varsigma_z)^2} \sqrt{\varsigma_\perp \varsigma_z \zeta_z^2 \vartheta_3^2 \left(\zeta_z^2 \vartheta_3^2 - (\varsigma_\perp - \varsigma_z)(T_{cz} - T_{c\perp})\right)}. \quad (2.32)$$

The conditions imposed thus far are sufficient to show that $T_\ominus > T_{cz}$. The system of equations (2.21) yields $\hat{m}_y = 0$ and

$$\hat{m}_x = -\mathrm{i} \frac{\zeta_z \vartheta_3 k_\ominus}{\alpha'_\perp (T_\ominus - T_{c\perp}) + k_\ominus^2 (\tau_1 + \tau_2)} \hat{m}_z \equiv \mathrm{i} M_\ominus \hat{m}_z \quad (2.33)$$

Here we define $M_\ominus$ as the ratio of magnetization amplitudes in the z- and x-directions. In order to obtain a real magnetization, the mode $e^{-\mathrm{i}k_\ominus x}$ needs to be of the same amplitude as the mode $e^{\mathrm{i}k_\ominus x}$. Furthermore, we reach a similar result for the modes $e^{\mathrm{i}k_\ominus y}$ and $e^{-\mathrm{i}k_\ominus y}$. From this we can conclude that one of the two magnetizations spontaneously emerges

$$\boxed{\mathbf{m} = m_0 \left(\mathbf{e}_z \cos k_\ominus x + \mathbf{e}_x M_\ominus \sin k_\ominus x\right)}$$
$$\boxed{\mathbf{m} = m_0 \left(\mathbf{e}_z \cos k_\ominus y + \mathbf{e}_y M_\ominus \sin k_\ominus y\right)} \quad . \quad (2.34)$$

A spatial sketch of this vector field is given in figure 2.2.

(2) Case $\tau_2 > \tau_3$

A calculation largely similar to the one for $\tau_2 < \tau_3$ is now performed for a **k** vector pointing along the diagonal of the x-y-plane. Hence, we set $k_x = k_y \equiv k_r$ and $k_z = 0$. Solving $\mathrm{Det}(M) = 0$ for T yields the transition temperature

$$T = \frac{T_{c\perp} + T_{cz}}{2} - k_r^2 \left(\frac{\tau_1 + \tau_3}{\alpha'_\perp} + \frac{\tau_6}{\alpha'_z}\right) + \sqrt{\left(\frac{T_{c\perp} - T_{cz}}{2} - k_r^2 \left(\frac{\tau_1 + \tau_3}{\alpha'_\perp} - \frac{\tau_6}{\alpha'_z}\right)\right)^2 + 2 \frac{k_r^2 \zeta_z^2 \vartheta_3^2}{\alpha'_\perp \alpha'_z}} . \quad (2.35)$$

The maxima $k_\oslash^2$ of the function set the critical temperature $T_\oslash$ of the modulated phase. The expressions for $k_\oslash^2$ and $T_\oslash$ are the same as in (2.31) and (2.32), provided we impose the following redefined abbreviation

$$\varsigma_z = \alpha'_z (\tau_1 + \tau_3) . \quad (2.36)$$

Again, the conditions imposed thus far suffice to show that $T_\oslash > T_{cz}$, and the calculation is therefore consistent. Finally the system (2.21) yields $\hat{m}_x = \hat{m}_y$ and

$$\hat{m}_x = \mathrm{i} \frac{\left(\alpha'_\perp (T_\oslash - T_{c\perp}) + k_\oslash^2 (\tau_1 + \tau_2 + \tau_3)\right)\left(\alpha'_z (T_\oslash - T_{cz}) + 2k_\oslash^2 \tau_6\right) - (\zeta_z \vartheta_3 k_\oslash)^2}{(\zeta_z \vartheta_3 k_\oslash)\left(\alpha'_\perp (T_\oslash - T_{c\perp}) + 2k_\oslash^2 \tau_2\right)} \hat{m}_z \equiv -\mathrm{i} M_\oslash \hat{m}_z . \quad (2.37)$$

As a result, one of the two degenerate modulated magnetizations is realised spontaneously

$$\boxed{\mathbf{m} = m_0 \left[\mathbf{e}_z \cos\left(k_\oslash (x+y)\right) + \left(\mathbf{e}_x + \mathbf{e}_y\right) M_\oslash \sin\left(k_\oslash (x+y)\right)\right]}$$
$$\boxed{\mathbf{m} = m_0 \left[\mathbf{e}_z \cos\left(k_\oslash (x-y)\right) + \left(\mathbf{e}_x - \mathbf{e}_y\right) M_\oslash \sin\left(k_\oslash (x-y)\right)\right]} \quad . \quad (2.38)$$

Thus far we have only considered the second order terms in **k**. The analysis of the fourth order terms turns out to be more involved for the case in which $T_{c\perp} < T_{cz}$. A calculation yields the possibility of non-positive-definite fourth order terms only in an exotic parameter range (τ_5 would have to become large with respect to the other parameters). The result would involve k_x, k_y and k_z. However, it is questionable whether or not this indeed leads to a higher transition temperature than $T_\ominus$ and $T_\oslash$. The instability derived from the second order terms is thus believed to be the dominant one, and we spare further calculations at that point.

Higher transition temperature for x-y-plane $T_{c\perp} > T_{cz}$

In contrast to the previous considerations, for the case $T_{c\perp} > T_{cz}$ non-centrosymmetricity does not affect the magnetic state if only terms of second power in $\mathbf{k}$ are considered in $\mathrm{Det}(M)$. In fact, $T(\mathbf{k}=0) = T_{c\perp}$ would persist to be a local maximum.

This motivates us to consider terms of fourth power in **k**. We shall investigate whether they provide a local maximum greater than $T_{c\perp}$. Indeed, a modulated phase is obtained under the following combined conditions:

(1) Case $\tau_3 > \tau_2$
The system features a modulated magnetization with the propagation vector parallel to one of the coordinate axes of the x-y-plane if

$$\boxed{\zeta_z^2 > \frac{(\tau_1+\tau_2)\alpha_z'(T_{c\perp}-T_{cz})}{\vartheta_3^2} > 0}\,.$$

The solution is given by (2.34).

(2) Case $\tau_2 > \tau_3$
A modulated magnetization with the **k**-vector along the diagonals of the x-y-plane emerges if

$$\boxed{\zeta_z^2 > \frac{(\tau_1+\tau_3)\alpha_z'(T_{c\perp}-T_{cz})}{\vartheta_3^2} > 0}\,.$$

The solution is given by (2.38).

As before, the τ_2- and τ_3-terms govern the shape of the modulated phase. Under these altered conditions, we obtain the same phases from the fourth order terms as we have obtained from the second order terms in the case $T_{cz} > T_{c\perp}$. A visual summary of all the possible phases is given in the magnetic phase diagram in figure 2.1.

In total we have found four distinct magnetic phases, two homogeneous and two modulated ones. The homogeneous state with the magnetization along the z-direction is not degenerate, while the other one shows a circular degeneracy. Both phases are also present in a centrosymmetric system. The non-centrosymmetricity has no influence on the transition temperatures of the homogeneous states. The two modulated magnetic phases are twofold degenerate each. They appear only in the case of sufficiently strong non-centrosymmetricity.

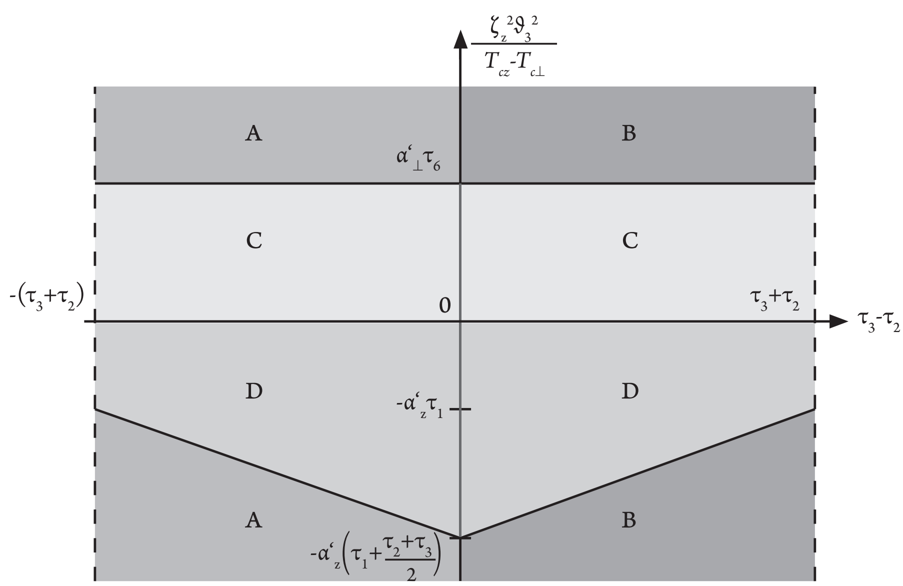

Figure 2.1: Scheme of possible magnetic phases in dependence of the anisotropy parameter $\tau_3 - \tau_2$ for fixed $\tau_1 + \tau_2$. There are four distinct phases possible: (A) a modulated magnetization along the diagonals of the x-y-plane according to (2.38); (B) a modulated magnetization along the coordinate axes of the x-y-plane according to (2.34); (C) a homogeneous magnetization in the z-direction; (D) a homogeneous magnetization in the x-y-plane. If the parameter of non-centrosymmetricity ζ_z exceeds the given thresholds, the modulated phases emerge.

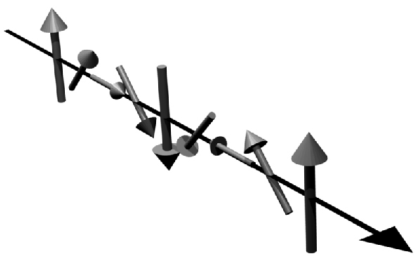

Figure 2.2: Schematic picture of the two modulated magnetic phases obtained for the tetragonal lattice. For $\tau_3 > \tau_2$, the direction of propagation (the black arrow) is either the x-axis or the y-axis, otherwise it is a diagonal in the x-y-plane. Note that the magnitude of the magnetization vector also changes in space.

2.3 Superconductivity in the homogeneous magnetic phases

In the two previous sections we have studied homogeneous superconductivity and possible magnetic phases independent of each other. We discovered four possible magnetic phases in the non-centrosymmetric tetragonal system. In this and the next section we want to develop an understanding of the emergence of superconductivity in each of the magnetic phases.

2.3.1 Coupling terms in the free energy

At first, we want to find those terms in the free energy that couple the order parameters of superconductivity η_s, η_p and the order parameter of magnetism $\mathbf{m}$ according to the already discussed symmetry requirements (tables 2.1 and 2.2). We expand the free energy up to the order "$m^2 D\eta^2$" in the order parameter and the derivative. Terms of higher order can be found in the appendix B. They are not subject to discussion here, because they do not affect the emerging phase qualitatively.

$$\begin{aligned}
f_{coupling} =& h_{s,\perp}\mathbf{m}_\perp^2 \left|\eta_s\right|^2 + h_{s,z} m_z^2 \left|\eta_s\right|^2 + h_{p,\perp}\mathbf{m}_\perp^2 \left|\eta_p\right|^2 + h_{p,z} m_z^2 \left|\eta_p\right|^2 + \\
& \upsilon_\perp \zeta_z \mathbf{m}_\perp^2 \left(\eta_s\eta_p^* + \eta_p\eta_s^*\right) + \upsilon_z\zeta_z m_z^2 \left(\eta_s\eta_p^* + \eta_p\eta_s^*\right) + \\
& \mathrm{i}\kappa_0 \left(\mathbf{e}_z \times \mathbf{m}\right)\cdot\left(\eta_s\left(\mathbf{D}_\perp\eta_p\right)^* - \eta_s^*\mathbf{D}_\perp\eta_p + \eta_p\left(\mathbf{D}_\perp\eta_s\right)^* - \eta_p^*\mathbf{D}_\perp\eta_s\right) + \\
& \mathrm{i}\kappa_s\zeta_z \left(\mathbf{e}_z \times \mathbf{m}\right)\cdot\left(\eta_s\left(\mathbf{D}_\perp\eta_s\right)^* - \eta_s^*\mathbf{D}_\perp\eta_s\right) + \mathrm{i}\kappa_p\zeta_z \left(\mathbf{e}_z \times \mathbf{m}\right)\cdot\left(\eta_p\left(\mathbf{D}_\perp\eta_p\right)^* - \eta_p^*\mathbf{D}_\perp\eta_p\right) + \\
& \nu_0 \mathbf{m}_\perp^2 \left(\eta_s D_z^*\eta_p^* + \eta_s^* D_z\eta_p\right) + \nu_p\zeta_z\mathbf{m}_\perp^2\left(\eta_p D_z^*\eta_p^* + \eta_p^* D_z\eta_p\right) + \\
& \nu_s\zeta_z\mathbf{m}_\perp^2\left(\eta_s D_z^*\eta_s^* + \eta_s^* D_z\eta_s\right) + \rho_0 m_z \mathbf{m}_\perp\left(\eta_s\mathbf{D}_\perp^*\eta_p^* + \eta_s^*\mathbf{D}_\perp\eta_p + \eta_p\mathbf{D}_\perp^*\eta_s^* + \eta_p^*\mathbf{D}_\perp\eta_s\right) + \\
& \rho_s\zeta_z m_z\mathbf{m}_\perp\left(\eta_s\mathbf{D}_\perp^*\eta_s^* + \eta_s^*\mathbf{D}_\perp\eta_s\right) + \rho_p\zeta_z m_z\mathbf{m}_\perp\left(\eta_p\mathbf{D}_\perp^*\eta_p^* + \eta_p^*\mathbf{D}_\perp\eta_p\right) + \\
& \sigma_0 m_z^2\left(\eta_s D_z^*\eta_p^* + \eta_s^* D_z\eta_p\right) + \sigma_s\zeta_z m_z^2\left(\eta_s D_z^*\eta_s^* + \eta_s^* D_z\eta_s\right) + \sigma_p\zeta_z m_z^2\left(\eta_p D_z^*\eta_p^* + \eta_p^* D_z\eta_p\right)
\end{aligned}$$

The expansion to this order already yields a wealth of coupling terms. Non-centrosymmetricity in particular allows for the terms linear in the magnetization ($\kappa_s, \kappa_p, \kappa_0$). They reflect the presence of MD spin-orbit interaction (see 1.3.3). Although the κ_0-term is not proportional to ζ_z, parity mixing is indispensable for it to subsist. The ρ_0-term has been symmetrized in the action of the derivative. The first two and the latter two summands in the bracket would each represent a valid term in the expansion on their own. The symmetrization however ensures a more symmetric result and hermitian operators from the variation equations.

In the case of homogeneous order parameters, the h- and υ-terms couple magnetism and superconductivity. Due to the depairing mechanisms, this is unlikely to be energetically favourable. We account for that by assuming

$$h_{n,\bullet} > 0; \quad n = s, p; \; \bullet = \perp, z\,.$$

2.3.2 Magnetization $\mathbf{m} = m_z\mathbf{e}_z$

We consider a homogeneous magnetization $\mathbf{m} = m_z\mathbf{e}_z$ along the z-axis. This is one of the four magnetic states that are present in the system according to the conditions derived in 2.2. Starting point for our calculation is the free energy functional (expansion 2.2 and section 2.3.1). The variation with respect to

η_s^* and η_p^* yields

$$\begin{aligned}
0 &= a_s\eta_s + 2b_s\left|\eta_s\right|^2\eta_s + c_1\left|\eta_p\right|^2\eta_s + 2c_2\eta_p^2\eta_s^* + d\zeta_z\eta_p + \delta_0\nabla_z\eta_p + h_{s,z}m_z^2\eta_s + \sigma_0 m_z^2\nabla_z\eta_p - \\
&\quad \gamma_{s,z}\nabla_z^2\eta_s - \gamma_{0,z}\zeta_z\nabla_z^2\eta_p - \gamma_{s,\perp}\nabla_x^2\eta_s - \gamma_{0,\perp}\zeta_z\nabla_x^2\eta_p - \gamma_{s,\perp}\nabla_y^2\eta_s - \gamma_{0,\perp}\zeta_z\nabla_y^2\eta_p \\
0 &= a_p\eta_p + 2b_p\left|\eta_p\right|^2\eta_p + c_1\left|\eta_s\right|^2\eta_p + 2c_2\eta_s^2\eta_p^* + d\zeta_z\eta_s - \delta_0\nabla_z\eta_s + h_{p,z}m_z^2\eta_p + \sigma_0 m_z^2\nabla_z\eta_s - \\
&\quad \gamma_{p,z}\nabla_z^2\eta_p - \gamma_{0,z}\zeta_z\nabla_z^2\eta_s - \gamma_{p,\perp}\nabla_x^2\eta_p - \gamma_{0,\perp}\zeta_z\nabla_x^2\eta_s - \gamma_{p,\perp}\nabla_y^2\eta_p - \gamma_{0,\perp}\zeta_z\nabla_y^2\eta_s. \qquad (2.39)
\end{aligned}$$

The impact of the homogeneous magnetization is a renormalisation of the phenomenological expansion parameters. This is due to the fact that each term in f_{sc} in principle has a counterpart in $f_{coupling}$ that is in addition proportional to m^2. As we did not expand $f_{coupling}$ to higher order terms, only a few of the parameters feature this renormalisation :

$$\begin{aligned}
\bar{a}_s &= a_s + h_{s,z}m_z^2 \quad & \bar{a}_p &= a_p + h_{p,z}m_z^2 \\
\bar{d} &= d + v_z m_z^2 \quad & \bar{\delta}_0 &= \delta_0 + \sigma_0 m_z^2.
\end{aligned}$$

We neglect third-order terms in 2.39 and obtain the operators

$$\begin{aligned}
\hat{A}_s &:= \bar{a}_s + \gamma_{s,z}k_z^2 + \gamma_{s,\perp}\left(k_x^2 + k_y^2\right) \\
\hat{A}_p &:= \bar{a}_p + \gamma_{p,z}k_z^2 + \gamma_{p,\perp}\left(k_x^2 + k_y^2\right) \\
\hat{B} &:= \zeta_z\bar{d} + \mathrm{i}\bar{\delta}_0 k_z + \zeta_z\gamma_{0,z}k_z^2 + \zeta_z\gamma_{0,\perp}\left(k_x^2 + k_y^2\right). \qquad (2.40)
\end{aligned}$$

As for homogeneous superconductivity, we expect a homogeneous solution and want to avoid instabilities towards arbitrarily strong modulations of the order parameters. The only change to the operators (2.40) in the equations (2.6) is the renormalisation. As a consequence the conditions (2.9) and (2.13) are still relevant for the bared variables. If these conditions are valid for the case $m_z = 0$, they also hold in the limit of small m_z. In addition, they can set an upper bound to the magnetization, above which no stable superconductivity will emerge. Condition (2.9) for example now reads $\bar{a}_p\gamma_{s,z} > \bar{\delta}_0^2$ and is fulfilled only if

$$m_z^2 < \frac{h_{p,z}\gamma_{s,\perp} - 2\delta_0\sigma_0}{2\sigma_0^2} + \sqrt{\left(\frac{h_{p,z}\gamma_{s,\perp} - 2\delta_0\sigma_0}{2\sigma_0^2}\right)^2 + \frac{a_p\gamma_{s,z}}{\sigma_0^2}}. \qquad (2.41)$$

In conclusion, we found that a sufficiently small m_z renormalises the phenomenological parameters but other than that leads to no qualitative change of the superconducting state.

As before, we determine the mixing ratio of singlet and triplet order parameters. Depending on the sign of the round bracket, the magnetization can either reduce or enhance the parity mixing

$$\boxed{\frac{\eta_p}{\eta_s} = -\left.\frac{\hat{A}_s}{\hat{B}}\right|_{\mathbf{k}=0} \approx -\frac{a_s}{d\zeta_z}\left[1 + m_z^2\left(\frac{h_{s,z}}{a_s} - \frac{v_z}{d}\right)\right]}. \qquad (2.42)$$

However, the effect of the homogeneous magnetization on the transition temperature is unambiguous. For weak non-centrosymmetricity (small ζ_z) the expansion in ζ_z and m_z reveals that T_c is reduced:

$$\boxed{T_c = T_{cs} - m_z^2\frac{h_{s,z}}{a_s'} + \zeta_z^2\frac{d^2}{a_s'a_p'(T_{cs} - T_{cp})}\left[1 + m_z^2\frac{2v_z}{d} + m_z^2\frac{a_p'h_{s,z} - a_s'h_{p,z}}{a_s'a_p'(T_{cs} - T_{cp})}\right]}. \qquad (2.43)$$

2.3.3 Magnetization $\mathbf{m} = m_x \mathbf{e}_x$

We study the effect of the other homogeneous magnetic phase, in which the magnetic moment degenerately lies in the x-y-plane. Without loss of generality, we consider the case $\mathbf{m} = m_x \mathbf{e}_x$ and follow the same steps as in the previous section. As before, the variation equations yield a renormalisation to the phenomenological parameters

$$\begin{array}{ll} \bar{a}_s = a_s + h_{s,\perp} m_x^2 & \bar{a}_p = a_p + h_{p,\perp} m_x^2 \\ \bar{d} = d + v_\perp m_x^2 & \bar{\delta}_0 = \delta_0 + v_0 m_x^2. \end{array}$$

In addition to that, the operators in (2.6) gain new terms from the MD spin-orbit interaction

$$\begin{aligned} \hat{A}_s &:= \bar{a}_s + \gamma_{s,\perp}(k_x^2 + k_y^2) + \gamma_{s,z} k_z^2 + 2 m_x \zeta_z \kappa_s k_y \\ \hat{A}_p &:= \bar{a}_p + \gamma_{p,\perp}(k_x^2 + k_y^2) + \gamma_{p,z} k_z^2 + 2 m_x \zeta_z \kappa_p k_y \\ \hat{B} &:= \zeta_z \bar{d} + \mathrm{i}\bar{\delta}_0 k_z + \zeta_z \gamma_{0,\perp}(k_x^2 + k_y^2) + \zeta_z \gamma_{0,z} k_z^2 + 2\kappa_0 m_x k_y. \end{aligned} \tag{2.44}$$

Without the spin-orbit interaction, homogeneous superconductivity is still present in the sense of the m_z-case. The same conditions (2.9) and (2.13) for the new renormalised variables would apply. However, accounting for the spin-orbit interaction goes beyond the renormalisation. It gives rise to terms in the determinant of the system (2.6), that are linear in m_x and k_y. As a consequence, the first derivative of the transition temperature with respect to k_y does not vanish at $\mathbf{k} = 0$. This can be seen from the expansion of T_c up to first power in k_y and up to second power in the non-centrosymmetricity parameter ζ_z

$$\begin{aligned} T_c = T_{cs} - m_x^2 \frac{h_{s,\perp}}{a'_s} + \zeta_z \frac{(d + v_\perp m_x^2)^2}{a'_s a'_p (T_{cs} - T_{cp}) + m_x^2 (a'_s h_{p,\perp} - a'_p h_{s,\perp})} + \\ 2 k_y \frac{m_x \zeta_z}{a'_s} \left(\kappa_s + \frac{2 a'_s \kappa_0 (d + v_\perp m_x^2)}{a'_s a'_p (T_{cs} - T_{cp}) + m_x^2 (a'_s h_{p,\perp} - a'_p h_{s,\perp})} \right). \end{aligned} \tag{2.45}$$

As a consequence, the the maximum of the transition temperature will *always* be realised for a state of finite k_y as long as $m_x \neq 0$. This corresponds to a modulated superconductivity order parameter.

The first derivatives of the transition temperature with respect to k_x and k_z are not affected by the MD spin-orbit coupling and vanish at the origin as they did before. The corresponding phenomenological parameters are only altered by renormalisation. Hence, for sufficiently small magnetization no maximum in the transition temperature will rise at finite k_x and k_z. The conditions that avoid an instability towards infinite $\mathbf{k}$-vectors in any direction will persist to be true, because they are not altered by the spin-orbit coupling.

In conclusion, a state with $\mathbf{k} = (0, k_{y,0}, 0)$ maximizes the transition temperature. The optimal $k_{y,0}$ cannot be expressed analytically. Instead we computed an approximation that is valid to lowest order in m_x and ζ_z

$$k_{y,0} \approx -\frac{m_x \zeta_z}{\gamma_{s,\perp}} \left(\frac{2 d \kappa_0}{a'_p (T_{cs} - T_{cp})} - \kappa_s \right) \tag{2.46}$$

The mixing ratio sustains to be real in presence of the spin-orbit coupling. As a consequence, singlet and triplet phase remain in coherence. The spatial variation is a phase modulation according to

$$\boxed{\eta_n = \tilde{\eta}_n e^{\mathrm{i} k_{y,0} y} \quad n = s, p}\,.$$

We wish to once again emphasise that the $\mathbf{m}$-proportional MD spin-orbit coupling terms in $f_{coupling}$ are responsible for this behaviour. It is remarkable that states with $k_{y,0}$ and $-k_{y,0}$ are not degenerate. This could be seen as an effect of the magnetization acting differently on the charge-carriers of opposite lattice momenta. As a consequence of gauge invariance, the inhomogeneous superconducting state carries no supercurrent. The result is found to be in agreement with the one given in [23].

The effect that this modulation has on raising the transition temperature can be seen from the following expansion in ζ_z and m_z (compare to (2.43))

$$T_c = T_{cs} - m_x^2 \frac{h_{s,\perp}}{a_s'} + \zeta_z^2 \frac{d^2}{a_s' a_p' (T_{cs} - T_{cp})} \left[1 + m_x^2 \frac{2 a_p' (T_{cs} - T_{cp})}{\gamma_{s,\perp}} \left(\frac{\kappa_s}{d} - \frac{2\kappa_0}{a_p'(T_{cs} - T_{cp})} \right)^2 + m_x^2 \frac{2 v_\perp}{d} + m_x^2 \frac{a_p' h_{s,\perp} - a_s' h_{p,\perp}}{a_s' a_p' (T_{cs} - T_{cp})} \right]. \tag{2.47}$$

2.4 Superconductivity in the inhomogeneous magnetic phases

In this section we wish to address the reaction of superconductivity on the two inhomogeneous magnetic phases found in non-centrosymmetric tetragonal systems. We expect to obtain a spatial modulation of the superconductivity order parameters η_s and η_p. Let us first consider the modulation along a coordinate axis, where $k_\ominus$ and $M_\ominus$ is given by the equations (2.31) and (2.33):

$$\mathbf{m} = m_0 \cos(k_\ominus x) \mathbf{e}_z + M_\ominus m_0 \sin(k_\ominus x) \mathbf{e}_x \tag{2.48}$$

This magnetization vector is inserted in the free energy expansion $f_{cs} + f_{coupling}$. When taking the variational derivative with respect to η_s^* and η_p^*, we again neglect terms of fourth order in the superconductivity order parameters. This ensures equations that are linear in η_s and η_p. Since the magnetization solely depends on the x-coordinate, it is natural to expect a spatial variation of superconductivity only in this coordinate. For the other directions, nothing changes as compared to the calculations in the case of a homogeneous magnetization. Apart from the effect of MD spin-orbit interaction, homogeneous superconductivity persists to be favoured in y- and z-direction. For simplicity we shall *neglect* MD spin-orbit interaction at first (phenomenological parameters κ_s, κ_p and κ_0). Its effect will be separately studied in section 2.4.4.

The coupled differential equations for $\eta_s = \eta_s(x)$ and $\eta_p = \eta_p(x)$ then read

$$\begin{aligned} 0 &= \left[a_s + \frac{H_s}{2} m_0^2 \right] \eta_s + \zeta_z \left[d + \frac{V}{2} m_0^2 \right] \eta_p - \gamma_{s\perp} \nabla_x^2 \eta_s - \zeta_z \gamma_{0,\perp} \nabla_x^2 \eta_p + \\ &\quad \cos(2k_\ominus x) m_0^2 \left[\left(-\frac{H_{s-}}{2} - \zeta_z k_\ominus \rho_s M_\ominus \right) \eta_s + \left(\zeta_z \frac{V_-}{2} - k_\ominus \rho_0 M_\ominus \right) \eta_p \right] \\ 0 &= \left[a_p + \frac{H_p}{2} m_0^2 \right] \eta_p + \zeta_z \left[d + \frac{V}{2} m_0^2 \right] \eta_s - \gamma_{p\perp} \nabla_x^2 \eta_p - \zeta_z \gamma_{0,\perp} \nabla_x^2 \eta_s + \\ &\quad \cos(2k_\ominus x) m_0^2 \left[\left(-\frac{H_{p-}}{2} - \zeta_z k_\ominus \rho_p M_\ominus \right) \eta_p + \left(\zeta_z \frac{V_-}{2} - k_\ominus \rho_0 M_\ominus \right) \eta_s \right]. \end{aligned} \tag{2.49}$$

We introduced the abbreviations

$$\begin{array}{lll} V = v_\perp M_\ominus^2 + v_z & H_s = h_{s,\perp} M_\ominus^2 + h_{s,z} & H_p = h_{p,\perp} M_\ominus^2 + h_{p,z} \\ V_- = v_\perp M_\ominus^2 - v_z & H_{s-} = h_{s,\perp} M_\ominus^2 - h_{s,z} & H_{p-} = h_{p,\perp} M_\ominus^2 - h_{p,z}. \end{array} \tag{2.50}$$

In the previous cases we have performed a Fourier transformation to solve the linear variation equations. However, this system of equations features non-constant coefficients. As a result, the equations in Fourier space couple for different modes. To proceed, we have essentially two possibilities. The coefficients are periodic with periodicity $2k_\ominus$; this allows us to treat them similar to nearly free electron method for Bloch waves as introduced in section 1.5.1 (section 2.4.1). Alternatively we can solve the system in real space within suitable approximations (section 2.4.2).

2.4.1 Weak magnetization – a Bloch wave treatment

We use Bloch's theorem in order to transform equation (2.49) to **k**-space. The ansatz takes advantage of the coefficients $2k_\ominus$-periodicity and reads

$$\eta_{s,K}(x) = \sum_n s_n(k) e^{\mathrm{i}K_n x} \tag{2.51}$$

$$\eta_{p,K}(x) = \sum_n p_n(k) e^{\mathrm{i}K_n x}, \tag{2.52}$$

where $K_n = k + 2nk_\ominus$, $n \in \mathbb{Z}$ and $k \in [-k_\ominus, k_\ominus]$. The latter restriction means that k takes values in the first Brillouin zone. The variation equations are formulated as eigenvalue equations with the eigenvalue ϵ_k.

$$\begin{aligned}
0 = &\left[a_s - \epsilon_k + \frac{H_s}{2} m_0^2 + \gamma_{s,\perp} K_n^2\right] s_n + \zeta_z \left[d + \frac{V}{2} m_0^2 + \gamma_{0,\perp} K_n^2\right] p_n + \\
&\frac{1}{2}\left[\frac{H_{s-}}{2} - \zeta_z k_\ominus \rho_s M_\ominus\right] m_0^2 (s_{n-1} + s_{n+1}) + \frac{1}{2}\left[\zeta_z \frac{V_-}{2} - k_\ominus \rho_0 M_\ominus\right] m_0^2 (p_{n-1} + p_{n+1}) \\
0 = &\left[a_p - \epsilon_k + \frac{H_p}{2} m_0^2 + \gamma_{p,\perp} K_n^2\right] p_n + \zeta_z \left[d + \frac{V}{2} m_0^2 + \gamma_{0,\perp} K_n^2\right] s_n + \\
&\frac{1}{2}\left[\frac{H_{p-}}{2} - \zeta_z k_\ominus \rho_p M_\ominus\right] m_0^2 (p_{n-1} + p_{n+1}) + \frac{1}{2}\left[\zeta_z \frac{V_-}{2} - k_\ominus \rho_0 M_\ominus\right] m_0^2 (s_{n-1} + s_{n+1})
\end{aligned} \tag{2.53}$$

This represents a system of an infinite number of equations for the infinite number of unknowns s_n and p_n. In principle, it features a nontrivial solutions for certain eigenvalues ϵ_k. If the temperature dependent ϵ_k then in turn becomes zero, the original equation has a nontrivial solution. This defines the transition temperature.

To determine the eigenvalue, we proceed in two steps with the correction ansatz $\epsilon_k = \tilde{\epsilon}_k + \Delta\epsilon_k$. At first calculate an approximation $\tilde{\epsilon}_k$ by evaluating (2.53) for $n = 0$, leaving the coupling to modes $s_{\pm 1}$ and $p_{\pm 1}$ aside. The result is the eigenvalue of the homogeneously magnetized state. During the course of the calculation we have to decide on the sign of the following quantity. Without loss of generality, we assume that

$$a_p - a_s + \frac{m_0^2}{2}(H_p - H_s) + k^2(\gamma_{p,\perp} - \gamma_{s,\perp}) > 0. \tag{2.54}$$

This is motivated by the overall assumption $T_{cs} > T_{cp}$. In this approximation the eigenvalue reads

$$\tilde{\epsilon}_k = a_s + m_0^2 \frac{H_s}{2} + k^2 \gamma_{s,\perp} - \frac{\zeta_z^2 \left(d + \gamma_{0,\perp} k^2 + m_0^2 \frac{V}{2}\right)^2}{a_p - a_s + \frac{m_0^2}{2}(H_p - H_s) + k^2(\gamma_{p,\perp} - \gamma_{s,\perp})} \tag{2.55}$$

As in the case of a homogeneous magnetization, ζ_z lowers the eigenvalue, whereas a finite m_0 and k raises it. As a consequence, also the exact eigenvalue ϵ_k will become minimal at $k = 0$. This allows us to set $k = 0$ hereafter.

The mixing ratio of the superconductivity order parameters is obtained as

$$\frac{p_0}{s_0} = -\zeta_z \frac{d + m_0^2 \frac{V}{2}}{a_p - a_s + \frac{m_0^2}{2}(H_p - H_s)}. \tag{2.56}$$

As before, the triplet-phase is suppressed by ζ_z against the singlet phase.

In a second step we study the change in energy $\Delta\epsilon_k$ evoked by the modulated magnetization. This is possible by considering the modes $s_{\pm 1}$ and $p_{\pm 1}$. We evaluate the equations (2.53) for $n = 1$ and $n = -1$ with the approximate eigenvalue $\tilde{\epsilon}_0$. Higher modes (like $s_{\pm 2}$, $p_{\pm 2}$) are neglected. At this point the approximation of weak potential in analogy to the nearly free electron method kicks in: As the coupling m_0 is assumed to be small, the amplitudes s_n and p_n decrease with increasing $|n|$ and can be neglected above a certain order. The approximation of weak potential fails at points of degeneracy of the eigenvalue bands. However, as we consider only the lowest band and the center of the Brillouin zone, this is not harmful to our discussion.

We obtain expressions for $s_{\pm 1}$ and $p_{\pm 1}$ in dependence of s_0 and p_0. These can in turn be inserted in the equations for $n = 0$, thereby accounting for $\Delta\epsilon_k$. We set $\zeta_z = 0$ and obtain

$$\Delta\epsilon_0 = -m_0^4 \left(\frac{H_{s,-}^2}{32 k_\ominus^2 \gamma_{s,\perp}} + \frac{(\rho_0 k_\ominus M_\ominus)^2}{16 k_\ominus^2 \gamma_{p,\perp} + 4(a_p - a_s)} \right) \tag{2.57}$$

The results for $\tilde{\epsilon}_0$ and $\Delta\epsilon_0$ suggest to interpret terms with H_s as the general effect of the magnetization (homogeneous and inhomogeneous), while $H_{s,-}$ and ρ_0 explicitly reflect the impact of the modulation. Hence, the lowest contribution of the modulation is of order m_0^4. From $\Delta\epsilon_0 < 0$ we can conclude that the modulation acts in favour of a higher transition temperature as compared to a homogeneous magnetization of the same magnitude. The analogy in terms of a nearly free electron picture of electronic band structures is the level-repulsion.

It is questionable whether the minimal eigenvalue sustained to be at $k = 0$. An expansion of $\Delta\epsilon_k$ in k shows that there is no k-linear contribution. A quadratic term would however be overruled by the quadratic term in $\tilde{\epsilon}_0$. Hence we can assume to have the minimal eigenvalue at $k = 0$. This can be viewed as a consequence of the fact that we have chosen η_p to belong to a one-dimensional representation. Otherwise its components would correspond to spin-up and spin-down orientation, which would react differently on the magnetization by shifting the energy band minimum away from $k = 0$.

Setting $\epsilon_0 = \tilde{\epsilon}_0 + \Delta\epsilon_0 \stackrel{!}{=} 0$ allows us to deduce the shape of the critical temperature curve in dependence of the magnetization $T_c(m_0)$. We neglect all T-dependences in the denominators of (2.55) and (2.57) and set $\zeta_z = 0$. The result is a parabola in m_0^2 as shown in figure 2.3. It reveals a minimum at $m_{0,\min}^2 = \frac{H_s}{4U}$, with the abbreviation $U = \frac{H_{s,-}^2}{32 k_\ominus^2 \gamma_{s,\perp}} + \frac{\rho_0^2 k_\ominus^2 M_\ominus^2}{16 k_\ominus^2 \gamma_{p\perp}} > 0$.

$$\boxed{T_c(m_0) = T_{cs} - m_0^2 \frac{H_s}{2a_s'} + m_0^4 \frac{U}{a_s'}} \tag{2.58}$$

Finally, the spatial variation of the superconductivity order parameters in presence of the modulated magnetism shall be determined. The ratios of different modes $\frac{s_{\pm 1}}{s_0}$ and $\frac{p_{\pm 1}}{p_0}$ are obtained from the

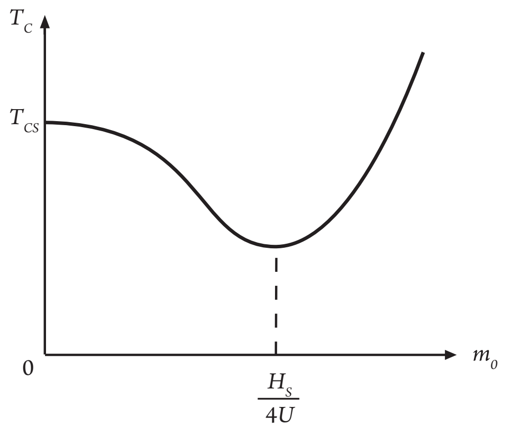

Figure 2.3: Schematic curve of the transition temperature of superconductivity in the modulated magnetic phase according to (2.58). Modulation specific parameters give rise to positive terms of fourth power in m_0.

equations for $n = \pm 1$ with the eigenvalue ϵ_0. In the limit $\zeta_z \to 0$ they become

$$\frac{s_{\pm 1}}{s_0} = \frac{m_0^2 H_{s,-}}{16\gamma_{s,\perp} k_\ominus^2}$$
$$\frac{p_{\pm 1}}{p_0} = \mathcal{O}\left(\frac{1}{\zeta_z}\right) \qquad \frac{p_{\pm 1}}{s_0} = m_0^2 \frac{\rho_0 k_\ominus M_\ominus}{2(a_p - a_s + 4\gamma_{p,\perp} k_\ominus^2)} \tag{2.59}$$

If we normalise to the homogeneous singlet contribution s_0, the singlet and triplet order parameters read in real space

$$\boxed{\eta_s(x) = s_0 \left[1 + \cos(2k_\ominus x)\frac{m_0^2 H_{s,-}}{8\gamma_{s,\perp} k_\ominus^2}\right] + \mathcal{O}(\zeta_z)}$$
$$\boxed{\eta_p(x) = s_0 \cos(2k_\ominus x) m_0^2 \frac{\rho_0 k_\ominus M_\ominus}{2(a_p - a_s + 4\gamma_{p,\perp} k_\ominus^2)} + \mathcal{O}(\zeta_z)} \quad . \tag{2.60}$$

From this result, we can draw the following conclusions. Note that they are based on the aforementioned assumption (2.54). Were they not, the singlet and triplet phases would have to be interchanged.

- At $k = 0$ we find $s_{-1} = s_{+1}$ and $p_{-1} = p_{+1}$. Hence, the modulated part of η_s and η_p will primarily follow a cosine with period $\pi / k_\ominus$.
- A substantial superconductivity modulation requires a large enough absolute value of the magnetization m_0.
- The modulated parts of both phases are suppressed by m_0^2 as compared to the homogeneous part of the singlet phase. We obtain a remarkable result; the homogeneous part of the triplet phase is suppressed by ζ_z as compared to the modulated part. Hence, the modulated magnetization creates a substantial modulated triplet phase, regardless of the strength of the non-centrosymmetricity.
- $H_{s,-}$ controls the modulation of the singlet phase and ρ_0 that of the triplet phase.

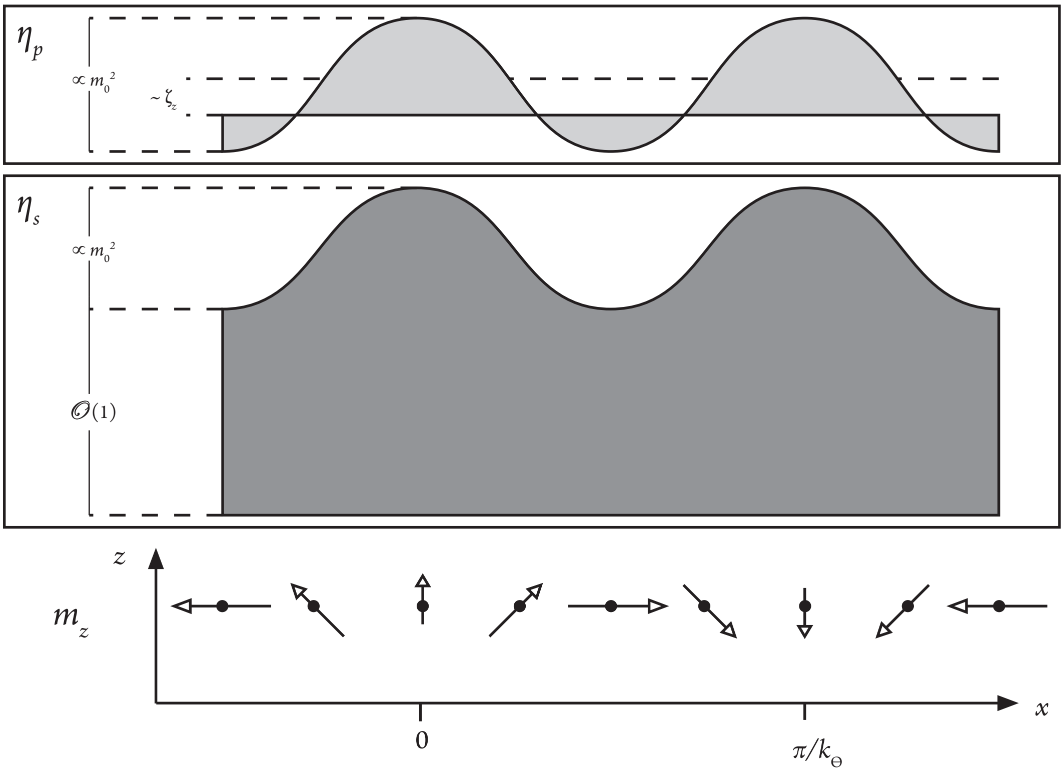

Figure 2.4: The qualitative behavior of singlet and triplet order parameters as a function of the x-coordinate. The magnitude and magnetization direction changes spatially as dictated by (2.49). The order of the modulation effects in terms of the small parameters m_0 and ζ_z is indicated on the left-hand side. The overall modulation is due to the modulated magnetization. Note that the modulation of the triplet phase is of the same order as that of the singlet phase, whereas the homogeneous part depends on non-centrosymmetricity via ζ_z.

- Intuitively we expect that superconductivity is not able to follow modulations of short wavelength of the magnetization (limit $k_\Theta \to \infty$). Our result reveals this, as the amplitude of the superconductivity modulations vanishes in this limit.

2.4.2 The coupled Mathieu equations

In this section we will present an alternative method to solve the equations (2.49). This method differs greatly from the nearly-free-electron treatment of the previous section. The results will not go beyond those we already found. Nonetheless we take this path because the quantities introduced in this section will be used in the next.

Our starting point is the following change of the unknown functions $\eta_s(x')$ and $\eta_p(x')$ to the two-vector $\mathbf{R}(x')$ with $x' = k_\Theta x$:

$$\mathbf{R}(x') = 2k_\Theta^2 \begin{pmatrix} \gamma_{s,\perp}\eta_s(x') + \gamma_{0,\perp}\zeta_z\eta_p(x') \\ \gamma_{0,\perp}\zeta_z\eta_s(x') + \gamma_{p,\perp}\eta_p(x') \end{pmatrix}. \tag{2.61}$$

This diagonalises the derivative operator and casts the equations (2.49) into a more convenient form of the following eigenvalue equation for the eigenvalue ϵ. The derivative is taken with respect to x'.

$$\boxed{\mathbf{R}'' + \left[\hat{\mathbf{T}} + m_0^2\left(\hat{\mathbf{S}} + 2\hat{\mathbf{Q}}\cos 2x'\right)\right]\mathbf{R} = \epsilon\mathbf{R}} \tag{2.62}$$

The matrices are defined as

$$\hat{\mathbf{T}} \equiv \begin{pmatrix} t_1 & t_2 \\ t_3 & t_4 \end{pmatrix} \equiv \frac{1}{k_\ominus^2\left(\gamma_{s,\perp}\gamma_{p,\perp} - \gamma_{0,\perp}^2\zeta_z^2\right)} \begin{pmatrix} d\gamma_{0,\perp}\zeta_z^2 - a_s\gamma_{p,\perp} & a_s\gamma_{0,\perp}\zeta_z - \zeta_z d\gamma_{s,\perp} \\ a_p\gamma_{0,\perp}\zeta_z - \zeta_z d\gamma_{p,\perp} & d\gamma_{0,\perp}\zeta_z^2 - a_p\gamma_{s,\perp} \end{pmatrix} \tag{2.63}$$

$$\hat{\mathbf{S}} \equiv \begin{pmatrix} s_1 & s_2 \\ s_3 & s_4 \end{pmatrix} \equiv \frac{1}{2k_\ominus^2\left(\gamma_{s,\perp}\gamma_{p,\perp} - \gamma_{0,\perp}^2\zeta_z^2\right)} \begin{pmatrix} V\gamma_{0,\perp}\zeta_z^2 - H_s\gamma_{p,\perp} & H_s\gamma_{0,\perp}\zeta_z - \zeta_z V\gamma_{s,\perp} \\ H_p\gamma_{0,\perp}\zeta_z - \zeta_z V\gamma_{p,\perp} & V\gamma_{0,\perp}\zeta_z^2 - H_p\gamma_{s,\perp} \end{pmatrix} \tag{2.64}$$

$$\begin{aligned}
\hat{\mathbf{Q}} &\equiv \begin{pmatrix} q_1 & q_2 \\ q_3 & q_4 \end{pmatrix} \\
q_1 &\equiv \frac{\gamma_{p,\perp}\left(\rho_s\zeta_z M_\ominus + \frac{H_{s-}}{2}\right) - \zeta_z\gamma_{0,\perp}\left(\rho_0 k_\ominus M_\ominus + \zeta_z\frac{V_-}{2}\right)}{2k_\ominus^2\left(\gamma_{s,\perp}\gamma_{p,\perp} - \gamma_{0,\perp}^2\zeta_z^2\right)} \\
q_2 &\equiv \frac{-\zeta_z\gamma_{0,\perp}\left(\rho_s\zeta_z M_\ominus + \frac{H_{s-}}{2}\right) + \gamma_{s,\perp}\left(\rho_0 k_\ominus M_\ominus + \zeta_z\frac{V_-}{2}\right)}{2k_\ominus^2\left(\gamma_{s,\perp}\gamma_{p,\perp} - \gamma_{0,\perp}^2\zeta_z^2\right)} \\
q_3 &\equiv \frac{-\zeta_z\gamma_{0,\perp}\left(\rho_p\zeta_z M_\ominus + \frac{H_{p-}}{2}\right) + \gamma_{p,\perp}\left(\rho_0 k_\ominus M_\ominus + \zeta_z\frac{V_-}{2}\right)}{2k_\ominus^2\left(\gamma_{s,\perp}\gamma_{p,\perp} - \gamma_{0,\perp}^2\zeta_z^2\right)} \\
q_4 &\equiv \frac{\gamma_{s,\perp}\left(\rho_p\zeta_z M_\ominus + \frac{H_{p-}}{2}\right) - \zeta_z\gamma_{0,\perp}\left(\rho_0 k_\ominus M_\ominus + \zeta_z\frac{V_-}{2}\right)}{2k_\ominus^2\left(\gamma_{s,\perp}\gamma_{p,\perp} - \gamma_{0,\perp}^2\zeta_z^2\right)}
\end{aligned} \tag{2.65}$$

Equation (2.62) is a system of two coupled Mathieu equations. This coupled system has been studied by Hansen [14]. Our understanding of the solution to the scalar Mathieu equation (section 1.5.2) provides us with little assistance in solving the vector case. Instead, we examine the effect of m_0 by regarding it as a small perturbation. The ansatz is an expansion of the smallest eigenvalue as well as the solution in even powers of m_0:

$$\epsilon = \sum_{i=0}^{\infty} m_0^{2i}\epsilon_i \qquad \mathbf{R}(x') = \sum_{i=0}^{\infty} m_0^{2i}\mathbf{R}_i(x'). \tag{2.66}$$

The equation is solved order by order in m_0^2. During the course of the calculation, we are required to make an assumption similar to but not equivalent to that of (2.54). Without loss of generality, we take

$$\frac{a_s}{\gamma_{s,\perp}} < \frac{a_p}{\gamma_{p,\perp}} \tag{2.67}$$

which is true for a higher singlet transition $T_{cs} > T_{cp}$ in the proximity of T_{cs}. Considering the limit of small non-centrosymmetricity $\zeta_z \to 0$, the solution to first order in m_0^2 is

$$\epsilon = -\frac{a_s}{k_\ominus^2\gamma_{s,\perp}}\left[1 + m_0^2\frac{H_s}{2a_s}\right] \tag{2.68}$$

$$\boxed{\mathbf{R}(x') = r_0\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} + m_0^2\frac{\cos(2x')}{\gamma_{s,\perp}}\begin{pmatrix} \frac{H_{s-}}{8k_\ominus^2} \\ \frac{\rho_0 k_\ominus M_\ominus}{4k_\ominus^2 + \left(\frac{a_p}{\gamma_{p,\perp}} - \frac{a_s}{\gamma_{s,\perp}}\right)} \end{pmatrix}\right]}\,.$$

The eigenvalue shows that a finite m_0 implies an increasing $|\epsilon|$ for $T > T_{cs}$, and thus reduces the transition temperature. This resembles the transition temperature found in equation (2.58) to order m_0^2. In addition, the spatial dependence of $\mathbf{R}(x')$ is equivalent to the findings for $\eta_s(x)$ and $\eta_p(x)$ from the nearly free electron method. This is more evident if we invert the transformation (2.61) and normalise the modulation of η_s and η_p with respect to to the homogeneous part of η_s. Comparison to the ratios of the different Fourier modes (2.69) shows that the results are similar:

$$\begin{aligned} \frac{\eta_s^{\mathrm{mod}}(x')}{\eta_s^{\mathrm{hom}}} &= m_0^2 \cos(2x') \frac{H_{s,-}}{8\gamma_{s,\perp} k_\ominus^2} \\ \frac{\eta_p^{\mathrm{mod}}(x')}{\eta_s^{\mathrm{hom}}} &= m_0^2 \cos(2x') \left(\frac{\gamma_{p,\perp}}{\gamma_{s,\perp}}\right)^2 \frac{\rho_0 k_\ominus M_\ominus}{a_p - a_s \frac{\gamma_{p,\perp}}{\gamma_{s,\perp}} + 4\gamma_{p,\perp} k_\ominus^2} \end{aligned} \tag{2.69}$$

2.4.3 Nucleation of superconductivity

The crucial assumption in the nearly-free-electron-like treatment was the weakness of the potential: Homogeneous superconductivity was assumed to be dominant over the modulations invoked by the small magnetization $\mathbf{m}(\mathbf{r})$. Our ansatz from the previous section is also capable of treating the strong potential limit. In temperatures slightly beneath the superconducting transition, the magnetization modulations will dictate where in space superconductivity is energetically favoured. This determines the nucleation of the superconductivity order parameters.

The picture is a bound state in a strong potential. As seen from (2.60) superconductivity will first nucleate at $x' = 0[\pi]$ provided $H_{s,-} > 0$. We thus treat the strong potential limit with a harmonic expansion of $\cos(2x')$ in (2.62) at $x' \approx 0$. The equation then reads

$$\mathbf{R}'' + \left[\hat{\mathbf{T}} + m_0^2\left(\hat{\mathbf{S}} + 2\hat{\mathbf{Q}}(1 - 2x'^2)\right)\right]\mathbf{R} = \epsilon \mathbf{R} \tag{2.70}$$

In the case that $\zeta_z = 0$, the matrices $\hat{\mathbf{T}}$ and $\hat{\mathbf{S}}$ are diagonal, while $\hat{\mathbf{Q}}$ has off diagonal terms $\propto \rho_0$ that couple the two equations with one another. Hence, we have the eigenvalue problem analogue to the Schrödinger equation for two coupled harmonic oscillators with different natural frequencies. This cannot be solved explicitly, but since we are interested in the ground state only, we know that the solution will behave approximately like the ansatz

$$\mathbf{R}(x') = \begin{pmatrix} 1 \\ r \end{pmatrix} e^{-\kappa x'^2} \tag{2.71}$$

with the parameters κ and r. Superconductivity thus nucleates in planes (hereafter called stripes) perpendicular to the x-axis with a distance of $\pi/k_\ominus$. Adjacent stripes have an overlap determined by κ. Since (2.71) is not the exact solution, we cannot solve for these parameters. In order to make an approximate determination of them, we take a step back, and write the functional that generates equation (2.70) in terms of $\mathbf{R}$

$$F[\mathbf{R}(x')](x') = \int_{-\infty}^{\infty} \mathrm{d}x' \frac{1}{2}\left(\mathbf{R}^{\dagger\prime}\mathbf{R}' - \mathbf{R}^\dagger\left(\hat{\mathbf{T}} + m_0^2\left(\hat{\mathbf{S}} + 2\hat{\mathbf{Q}}\right)\right)\mathbf{R} + (2x')^2 m_0^2 \mathbf{R}^\dagger \hat{\mathbf{Q}}\mathbf{R}\right). \tag{2.72}$$

We replace $\mathbf{R}$ by (2.71) and integrate out x'. The result is a function in κ and r and can be minimised with respect to them. The minimal value is determined by the two coupled equations

$$\kappa = m_0^2 \frac{\gamma_{p,\perp} H_{s,-} + 2r\rho_0 k_\ominus M_\ominus(\gamma_{s,\perp} + \gamma_{p,\perp}) + r^2 \gamma_{s,\perp} H_{p,-}}{-2a_s\gamma_{p,\perp} + m_0^2\gamma_{p,\perp}(H_{s,-} - H_s) + 2r m_0^2 \rho_0 k_\ominus M_\ominus(\gamma_{s,\perp} + \gamma_{p,\perp}) - 2r^2 a_p \gamma_{s,\perp} + r^2 m_0^2 \gamma_{s,\perp}(H_{p,-} - H_p)} \tag{2.73}$$

$$r = \frac{(2\kappa-1)m_0^2\rho_0 k_\ominus M_\ominus(\gamma_{s,\perp}+\gamma_{p,\perp})}{2\kappa\gamma_{s,\perp}(2a_p+H_p m_0^2)+4\kappa^2\gamma_{s,\perp}\gamma_{p,\perp}-m_0^2 H_{p,-}\gamma_{s,\perp}(2\kappa-1)}. \tag{2.74}$$

Since we expect triplet superconductivity to be suppressed as compared to the singlet phase, we at first neglect all r-dependent terms in (2.73), and evaluate this expression for κ at T_c according to (2.58):

$$\kappa(T_c) \approx \left.\frac{m_0^2 H_{s-}}{-2a_s+m_0^2(H_{s-}-H_s)}\right|_{T_c} = \frac{1}{1-\frac{m_0^2 H_{s-}}{16k_\ominus^2\gamma_{s,\perp}}}. \tag{2.75}$$

The divergence of the denominator of (2.75) sets an upper limit to the validity of this approximation: $m_0^2 < 16k_\ominus^2\gamma_{s,\perp}/H_{s-}$. The result shows that at the onset of superconductivity, κ is always less than 1. Furthermore, the stripes of the nucleate become more confined the larger the magnetization m_0 is. Indeed, the overlap of neighbouring stripes is initially small: For $\kappa = 1$, the relative strength of $\eta_{s,p}$ between two stripes is only $e^{-\pi^2/4} \approx 0.08 \ll 1$.

The characteristic stripe width changes with temperature as

$$\kappa^{-1/2} \propto \sqrt{\tilde{T}_c(m_0^2)-T} \tag{2.76}$$

where $\tilde{T}_c(m_0^2)$ is some magnetization-dependent temperature with $T_{cs} > \tilde{T}_c(m_0^2) > T_c(m_0^2)$.

We now want to determine an approximate value for the parameter r. If we replace κ in the equation for r by its value at the critical temperature (2.75), and assume m_0^2 to be sufficiently small such that $m_0^2 < 2k_\ominus^2\gamma_{s,\perp}/H_{s-}$, we obtain

$$r \approx m_0^2 \frac{\rho_0 k_\ominus M_\ominus(\gamma_{s,\perp}+\gamma_{p,\perp})}{\gamma_{s,\perp}\left(4a_p+m_0^2(2H_p-H_{p-})+4k_\ominus^2\gamma_{p,\perp}\right)}. \tag{2.77}$$

This result reproduces what we found out about the coupling to the triplet phase within the approximation of the previous sections: η_p is essentially proportional to m_0^2 in the proximity of T_c, and the parameter ρ_0 is responsible for the coupling to the triplet phase. This triplet phase, however, is not suppressed by ζ_z.

Our picture of the emerging superconductivity is thus Gaussian-shaped planes perpendicular to the x-direction which show simultaneous singlet and triplet superconductivity and become broader with lower temperature.

Let us now address the question of the phase-coherence of two neighbouring stripes with a relative complex phase difference $\Delta\varphi = \varphi_1 - \varphi_2$. This time, we consider the following function

$$\mathbf{R}(x') = \begin{pmatrix} 1 \\ r \end{pmatrix}\left(e^{-\kappa x'^2}e^{i\varphi_1} + e^{-\kappa(x'-\pi)^2}e^{i\varphi_2}\right) \tag{2.78}$$

to be substituted in the functional $F[\mathbf{R}]$ of equation (2.72). We restore the cosine potential at the place of the quadratic expansion. Integration over x' leaves us with the following phase-dependent terms, expressed with the entries of the matrices (2.63), (2.64) and (2.65):

$$\sqrt{\frac{\pi}{2\kappa}}e^{-\frac{\kappa\pi^2}{2}}\cos(\Delta\varphi)\tilde{F} \tag{2.79}$$

$$\tilde{F} := (1+r^2)(\kappa-\kappa^2\pi^2)-(t_1+r^2t_4)+2m_0^2(q_1+rq_2+rq_3+r^2q_4)e^{-\frac{1}{2\kappa}}. \tag{2.80}$$

The sign of the quantity $\tilde{F}$ governs the phase relation: if negative, $\Delta\varphi = 0$ is favourable, otherwise $\Delta\varphi = \pi$. We introduce the abbreviation

$$v = \sqrt{m_0^2 H_{s-}/16\gamma_{s,\perp} k_\ominus^2}$$

and evaluate $\tilde{F}$ at the transition temperature. Using κ according to (2.75) and setting $r = 0$, we obtain for sufficiently small m_0

$$\tilde{F}(v)\Big|_{T_c} \approx \frac{1-\pi^2}{1-v^2} + 8v^2 e^{v^2/2-1/2} + 8v^4 \tag{2.81}$$

This quantity is less than zero for all $0 < v < 1$. Above $v = 1$ the validity of the approximation breaks down due to the divergence in κ (see (2.75)). Hence, we conclude that neighbouring stripes are phase coherent.

The fact that these regions start to overlap reminds us of tunneling problems. We are interested in the energy gain and energy splitting associated with this overlap. In this context, a more quantum-mechanical view is helpful. We use the results of the Heitler-London theory as given in [6]. The level splitting of two neighboring bound states $|1\rangle$ and $|2\rangle$ due to a potential $\tilde{V}$ can be estimated as

$$\epsilon_V = \left| \frac{\langle 1|\tilde{V}|2\rangle\langle 1|1\rangle - \langle 1|\tilde{V}|1\rangle\langle 1|2\rangle}{|\langle 1|1\rangle|^2 - |\langle 1|2\rangle|^2} \right| \tag{2.82}$$

In our case the potential is given by $\tilde{\mathbf{V}} = 2\hat{\mathbf{Q}}\cos(2x')$. The function $\mathbf{R}(x')$ according to (2.71) corresponds to the real space projection of $|1\rangle$, while $\mathbf{R}(x'-\pi)$ is the real space projection of $|2\rangle$.

$$\langle 1|\tilde{V}|1\rangle = \sqrt{\tfrac{\pi}{2\kappa}} 2m_0^2(q_1 + rq_2 + rq_3 + r^2 q_4) e^{-\frac{1}{2\kappa}} \qquad \langle 1|1\rangle = \sqrt{\tfrac{\pi}{2\kappa}}(1+r^2)$$
$$\langle 1|\tilde{V}|2\rangle = -\sqrt{\tfrac{\pi}{2\kappa}} 2m_0^2(q_1 + rq_2 + rq_3 + r^2 q_4) e^{-\frac{1}{2\kappa}-\frac{\kappa\pi^2}{2}} \qquad \langle 1|2\rangle = \sqrt{\tfrac{\pi}{2\kappa}}(1+r^2) e^{-\frac{\kappa\pi^2}{2}}$$

The resulting energy splitting is

$$\epsilon_V = \frac{2e^{-\frac{1}{2\kappa}}}{\sinh\left(\frac{\kappa\pi^2}{2}\right)} m_0^2 \frac{H_{s-}\gamma_{p,\perp} + r\rho_0 k_\ominus M_\ominus(\gamma_{s,\perp}+\gamma_{p,\perp}) + r^2 H_{p-}\gamma_{s,\perp}}{(1+r^2)2k_\ominus^2 \gamma_{s,\perp}\gamma_{p,\perp}}. \tag{2.83}$$

We analyse this quantity for $r = 0$ at the critical temperature $T_c(m_0^2)$. ϵ_V is then proportional to m_0^2 to lowest order. Within the valid range of m_0^2 and κ, there is no point where the two energy levels degenerately cross each other (i.e. no point where $\epsilon_V = 0$). The κ-dependent part of the function features a pronounced maximum at $\kappa \approx 0.3$. This marks the point, at which the stripes melt together completely – here our approximation breaks down. From the transition till this point, an increase in ϵ_V means that a hopping of the Cooper pairs from one stripe to the next becomes more and more energetically favourable.

All the results obtained in this section indicate that the strong-potential limit at the onset of superconductivity is a consistent explanation: Stripes of superconducting condensate form in regions where this is energetically favourable. These stripes subsequently melt together coherently as temperature is lowered.

2.4.4 The effect of MD spin-orbit coupling

Thus far we have neglected the effect of the MD spin-orbit coupling introduced via the κ_s-, κ_p- and κ_0-terms in the free energy. For homogeneous magnetization their effect was phase-modulated superconductivity. As we have managed to grasp the qualitative reaction of superconductivity on the modulated magnetization, we will now take spin-orbit interaction into account.

Additionally, we must then consider the y-dependence of η_s and η_p. The further contributions to the variation equations (2.49) are

$$-\gamma_{s,\perp}\nabla_y^2\eta_s - \zeta_z\gamma_{0,\perp}\nabla_y^2\eta_p - 2\mathrm{i}\zeta_z m_0\kappa_s M_\ominus \sin(k_\ominus x)\nabla_y\eta_s + 2\mathrm{i}m_0\kappa_0 M_\ominus \sin(k_\ominus x)\nabla_y\eta_p \tag{2.84}$$

$$-\gamma_{p,\perp}\nabla_y^2\eta_p - \zeta_z\gamma_{0,\perp}\nabla_y^2\eta_s - 2\mathrm{i}\zeta_z m_0\kappa_p M_\ominus \sin(k_\ominus x)\nabla_y\eta_p + 2\mathrm{i}m_0\kappa_0 M_\ominus \sin(k_\ominus x)\nabla_y\eta_s. \tag{2.85}$$

All coefficients are periodic in x-variable, so we can again treat the equations with the NFE method in the x-direction. However, the $\sin(k_\ominus x)$-terms introduce a new periodicity, halving the Brillouin zone. We account for this by allowing n in (2.53) to *take half-integer values* as well. All parameters remain independent of y. Therefore we are able to perform a Fourier transformation in y. Since the modes do not couple, we expect one value of k_y, or a set of degenerate values, to be energetically favourable. Thus we make the ansatz $\eta_n = \tilde{\eta}_n e^{\mathrm{i}k_y y}$ $(n = s, p)$.

The MD spin-orbit interaction then yields the following contributions to the equations (2.53):

$$\gamma_{s,\perp}k_y^2 s_n + \zeta_z\gamma_{0,\perp}k_y^2 p_n - \mathrm{i}\zeta_z m_0\kappa_s M_\ominus k_y(s_{n+\frac{1}{2}} - s_{n-\frac{1}{2}}) + \mathrm{i}m_0\kappa_0 M_\ominus k_y(p_{n+\frac{1}{2}} - p_{n-\frac{1}{2}}) \tag{2.86}$$

$$\gamma_{p,\perp}k_y^2 p_n + \zeta_z\gamma_{0,\perp}k_y^2 s_n - \mathrm{i}\zeta_z m_0\kappa_p M_\ominus k_y(p_{n+\frac{1}{2}} - p_{n-\frac{1}{2}}) + \mathrm{i}m_0\kappa_0 M_\ominus k_y(s_{n+\frac{1}{2}} - s_{n-\frac{1}{2}}) \tag{2.87}$$

We take (2.53) with these additional terms for $n = 0, -\frac{1}{2}, \frac{1}{2}$, resulting in 6 equations. Written as a 6×6 matrix operator acting on the vector $(s_{1/2}, p_{1/2}, s_0, p_0, s_{-1/2}, p_{-1/2})^T$ the equations take the form:

$$M = \begin{pmatrix} A_s + \gamma_{s,\perp}k_\ominus^2 & \zeta_z B + \zeta_z\gamma_{0,\perp}k_\ominus^2 & -\mathrm{i}\zeta_z E_s k_y & \mathrm{i}F k_y & C_s & D \\ \zeta_z B + \zeta_z\gamma_{0,\perp}k_\ominus^2 & A_p + \gamma_{p,\perp}k_\ominus^2 & \mathrm{i}F k_y & -\mathrm{i}\zeta_z E_p k_y & D & C_p \\ \mathrm{i}\zeta_z E_s k_y & -\mathrm{i}F k_y & A_s & \zeta_z B & -\mathrm{i}\zeta_z E_s k_y & \mathrm{i}F k_y \\ -\mathrm{i}F k_y & \mathrm{i}\zeta_z E_p k_y & \zeta_z B & A_p & \mathrm{i}F k_y & -\mathrm{i}\zeta_z E_p k_y \\ C_s & D & \mathrm{i}\zeta_z E_s k_y & -\mathrm{i}F k_y & A_s + \gamma_{s,\perp}k_\ominus^2 & \zeta_z B + \zeta_z\gamma_{0,\perp}k_\ominus^2 \\ D & C_p & -\mathrm{i}F k_y & \mathrm{i}\zeta_z E_p k_y & \zeta_z B + \zeta_z\gamma_{0,\perp}k_\ominus^2 & A_p + \gamma_{p,\perp}k_\ominus^2. \end{pmatrix} \tag{2.88}$$

Where we have introduced the abbreviations

$$\begin{aligned} A_s &= a_s'(T - T_{cs}) + \tfrac{H_s}{2}m_0^2 + \gamma_{s,\perp}k_y^2; & C_s &= \tfrac{m_0^2}{2}\left(\tfrac{H_{s-}}{2} - \zeta_z k_\ominus \rho_s M_\ominus\right) \\ A_p &= a_p'(T - T_{cp}) + \tfrac{H_p}{2}m_0^2 + \gamma_{p,\perp}k_y^2; & C_p &= \tfrac{m_0^2}{2}\left(\tfrac{H_{p-}}{2} - \zeta_z k_\ominus \rho_p M_\ominus\right) \\ B &= d + \tfrac{V}{2}m_0^2 + \gamma_{0,\perp}k_y^2; & D &= \tfrac{m_0^2}{2}\left(\tfrac{V_-}{2} - k_\ominus \rho_0 M_\ominus\right) \\ E_s &= -m_0\kappa_s M_\ominus; & E_p &= -m_0\kappa_p M_\ominus \\ F &= m_0 M_\ominus \kappa_0. \end{aligned} \tag{2.89}$$

The quantities E_s, E_p and F represent the impact of MD spin-orbit coupling.

We demand that the homogeneous linear system of equations with the given coefficient matrix has a non-trivial solution. For simplicity's sake, we set the elements $D = C_s = C_p = 0$, since they are proportional to the small quantity m_0^2, and are not connected to spin-orbit interaction. The equation $\mathrm{Det}(M) = 0$ gives an implicit function $T(k_y)$. The exact value of this function at $k_y = 0$ is

$$T_c = \frac{T_{cs} + T_{cp}}{2} - \frac{m_0^2}{4}\left(\frac{H_s}{a_s'} + \frac{H_p}{a_p'}\right) + \sqrt{\left(\frac{T_{cs} - T_{cp}}{2} + \frac{m_0^2}{4}\left(\frac{H_p}{a_p'} - \frac{H_s}{a_s'}\right)\right)^2 + \frac{\zeta_z^2\left(d + m_0^2\frac{V}{2}\right)^2}{a_s' a_p'}}. \tag{2.90}$$

The question is whether or not there exists a solution at finite k_y which shows a greater temperature than that at $k = 0$. To probe this, we determine the derivative at this point with the help the implicit function theorem. Since Det(M) depends only on k_y^2, we are allowed to take the derivative with respect to k_y^2. The result is twice the second derivative with respect to k_y. When expanded to second order in ζ_z, it reads

$$\left.\frac{\partial T}{\partial k_y}\right|_{T_c,k_y=0} = 0$$

$$\left.\frac{\partial T}{\partial k_y^2}\right|_{T_c,k_y=0} = -\frac{\gamma_{s,\perp}}{a_s'} + \frac{2F^2}{a_s' a_p' \Delta\bar{T} + a_s' \gamma_p k_\ominus^2} + \zeta_z^2 \left[\frac{2B\gamma_{0,\perp}}{a_s' a_p' \Delta\bar{T}} - \frac{B^2\left(a_s'\gamma_{p,\perp} - a_p'\gamma_{s,\perp}\right)}{a_s' a_p'^2 \Delta\bar{T}^2} + \frac{2E_s^2}{a_s'\gamma_s k_\ominus^2} + 2F^2 \frac{a_s' k_\ominus^2 \left(a_p'\gamma_{0,\perp}\Delta\bar{T} - B\gamma_{p,\perp}\right)^2 - B^2 a_p' \gamma_{s,\perp}\left(\gamma_{p,\perp}k_\ominus^2 + a_p'\Delta\bar{T}\right)}{a_s'^2 a_p' \gamma_{s,\perp}\Delta\bar{T}^2 \left(\gamma_{p,\perp}k_\ominus^2 + a_p'\Delta\bar{T}\right)} \right]. \tag{2.91}$$

Here, we have used an abbreviation for the difference in transition temperatures between the singlet and triplet states. This difference becomes renormalised by the magnetization: $\Delta\bar{T} = T_{cs} - T_{cp} + m_0^2\left(\frac{H_p}{2a_p'} - \frac{H_s}{2a_s'}\right)$.

Unlike in the case of homogeneous magnetization (2.45), the spin-orbit interaction does not bring about a k_y-linear part in $T_c(k_y)$ in this situation. The lowest term in which κ_s or κ_0 (via E_s or F) come into play is quadratic in k_y. Although the effect of the spin-orbit interaction may raise the critical temperature, it has to compete with the stiffness-term $\gamma_{s,\perp}$, which is also quadratic in k_y. If a finite k_y is favourable, the temperature bound at arbitrary big k_y-values is guaranteed by the following argument: Without the MD spin-orbit interaction, modulations are avoided by definition, according to the parameter constraints for the homogeneous phase. The spin-orbit-interaction does not however change the large-k_y expansion since there are always terms with higher powers of k_y, which are accompanied by $\gamma_{0,\perp}$, $\gamma_{s\perp}$ and $\gamma_{p\perp}$.

A state with finite k_y is favoured if $\frac{\partial T}{\partial k_y^2}(k_y = 0)$ as given by (2.91) is positive. The condition for that to be true would involve the variables that control the coupling to the triplet phase (d, $\gamma_{0,\perp}$, V, κ_0). To keep it simple, we will neglect these terms for the further discussion in this section, and consider the singlet phase alone:

$$V = d = \gamma_{0,\perp} = \kappa_0 = 0$$

The condition for an additional modulation induced from spin-orbit interaction becomes:

$$\boxed{1 < \mu := \frac{2\zeta_z^2 m_0^2 \kappa_s^2 M_\ominus^2}{\gamma_{s,\perp}^2 k_\ominus^2}} \tag{2.92}$$

Let us now turn to the question of how the MD spin-orbit coupling changes the modulation of the superconductivity phase. The coefficient matrix (2.88) yields $s_{-1} = -s_1$ and $p_{-1} = -p_1$. These are all purely imaginary numbers. Thus we can conclude that spin-orbit coupling will not destroy the coherence of the singlet and triplet phases. Rather, it will coherently induce an additional modulation to the phases and will also change the mixing ratio. In the simplified calculation without the triplet phase, Det(M) = 0 can be solved with respect to T exactly:

$$T_c(k_y) = T_{cs} - m_0^2\frac{H_s}{2a_s'} - \frac{\gamma_{s,\perp}}{2a_s'}(k_\ominus^2 + 2k_y^2) + \frac{1}{2\gamma_{s,\perp}}\sqrt{\gamma_{s,\perp}^2 k_\ominus^2 + 16\zeta_z^2 m_0^2 \kappa_s^2 M_\ominus^2 k_y^2} \tag{2.93}$$

This function has two degenerate maxima at

$$k_{y,0} = \pm\frac{k_\ominus}{2}\sqrt{\mu - \frac{1}{\mu}}. \tag{2.94}$$

We see that the enhancement of the critical temperature via a the rising k-vector is strong yet continuous as the condition becomes true. Thus the phase transition between the homogeneous and inhomogeneous states is of second order. We have to assume that m_0 and ζ_z are small quantities. So as to maintain the validity of our derivation, the k_y-modulated state can occur *only* if the spin-orbit coupling κ_s is strong against the superconducting condensate stiffness parameter $\gamma_{s,\perp}$ and the wavelength of the magnetic modulations is rather long.

We can now calculate the spatial dependence of the singlet phase more explicitly, given condition (2.92). This is performed by adding the modulation from the spin-orbit coupling to the already computed modulated phase according to (2.69):

$$\boxed{\eta_s = s_0 \exp\left[\pm \mathrm{i} y \frac{k_\ominus}{2}\sqrt{\mu - \frac{1}{\mu}}\right]\left[1 \pm \sqrt{2\frac{\mu-1}{\mu+1}}\sin(k_\ominus x) + m_0^2 \frac{H_{s,-}}{8\gamma_{s,\perp}k_\ominus^2}\cos(2k_\ominus x)\right]}. \tag{2.95}$$

The impact of spin-orbit coupling is twofold: firstly we obtain an additional modulation of the absolute value of η_s proportional to $\sin 2k_\ominus$, and secondly an overall phase modulation perpendicular to the plane containing the modulated magnetic moments. Both effects are tied together.

We have not discussed the relative strength of the modulations from the spin-orbit interaction, but it is clear that the $\cos(2k_\ominus x)$-component would also be influenced by the spin-orbit interaction, had we included one order higher in the coefficients ($s_{\pm 1}$ and $p_{\pm 1}$). Again, we want to mention that the triplet phase will feature the same modulation as (2.95). The impact of spin-orbit coupling on the ratio η_s/η_p was not studied.

2.4.5 The London penetration depth

A measure for the strength of superconductivity is the London penetration depth λ, or in our case the penetration depth tensor $\lambda_{i,j}^{-2}$ $(i, j \in x, y, z)$. It is a natural length-scale given by the Ginzburg-Landau equations that describes the supercurrent shielding of magnetic fields penetrating a superconductor. A large penetration depth reveals weak superconductivity. In the London gauge ($\nabla\mathbf{A} = 0$), the London equation for the magnetic field

$$\Delta\mathbf{B} = \hat{\lambda}^{-2}\mathbf{B}$$

is equivalent to an equation for the vector potential

$$\Delta\mathbf{A} - \hat{\lambda}^{-2}\mathbf{A} = \frac{4\pi}{c}\mathbf{j}_d. \tag{2.96}$$

The latter is obtained from the variation of the free energy functional of the form (1.6) with respect to $\mathbf{A}$:

$$\mathbf{j} = -c\frac{\delta F}{\delta\mathbf{A}} = \mathbf{j}_d + \frac{c}{4\pi}(\hat{\lambda}^{-2} - \Delta)\mathbf{A} \stackrel{!}{=} 0$$

From the form of the free energy and coupling terms, neglecting terms with second-order derivatives, we get:

$$
\begin{aligned}
j_x &= -\mathrm{i}4\pi e\Big[\gamma_{s,\perp}\eta_s^* D_x\eta_s + \gamma_{p,\perp}\eta_p^* D_x\eta_p + \zeta_z\gamma_{0,\perp}\left(\eta_s^* D_x\eta_p + \eta_p^* D_x\eta_s\right) + \\
&\quad \mathrm{i}\left(\mathbf{e}_z\times\mathbf{m}\right)_x\left(\zeta_z\kappa_s|\eta_s|^2 + \zeta_z\kappa_p|\eta_p|^2 + 2\kappa_0|\eta_s\eta_p|\right) + \rho_0 m_x m_z(\eta_s\eta_p^* + \eta_s^*\eta_p) - \mathrm{c.c.}\Big] \\
j_y &= -\mathrm{i}4\pi e\Big[\gamma_{s,\perp}\eta_s^* D_y\eta_s + \gamma_{p,\perp}\eta_p^* D_y\eta_p + \zeta_z\gamma_{0,\perp}\left(\eta_s^* D_y\eta_p + \eta_p^* D_y\eta_s\right) + \\
&\quad \mathrm{i}\left(\mathbf{e}_z\times\mathbf{m}\right)_y\zeta_z\left(\kappa_s|\eta_s|^2 + \kappa_p|\eta_p|^2 + 2\kappa_0|\eta_s\eta_p|\right) + \rho_0 m_y m_z(\eta_s\eta_p^* + \eta_s^*\eta_p) - \mathrm{c.c.}\Big] \\
j_z &= -\mathrm{i}4\pi e\Big[\delta_0\eta_s\eta_p^* + \gamma_{s,z}\eta_s^* D_z\eta_s + \gamma_{p,z}\eta_p^* D_z\eta_p + \zeta_z\gamma_{0,\perp}\left(\eta_s^* D_z\eta_p + \eta_p^* D_z\eta_s\right) + \\
&\quad \nu_0(m_x^2 + m_y^2)\eta_s\eta_p^* + \sigma_0 m_z^2\eta_s\eta_p^* - \mathrm{c.c.}\Big]
\end{aligned}
\tag{2.97}
$$

This leads to a diagonal penetration depth tensor. Off-diagonal elements would show up had we used a higher order expansion in the coupling terms to magnetism (see appendix).

$$
\lambda^{-2} = \begin{pmatrix} \lambda_\perp^{-2} & 0 & 0 \\ 0 & \lambda_\perp^{-2} & 0 \\ 0 & 0 & \lambda_z^{-2} \end{pmatrix}
\tag{2.98}
$$

The components are given by

$$
\begin{aligned}
\lambda_\perp^{-2} &= \frac{32\pi^2 e^2}{c^2}\left(\gamma_{s,\perp}|\eta_s|^2 + \gamma_{p,\perp}|\eta_p|^2 + 2\zeta_z\gamma_{0,\perp}\left|\eta_s^*\eta_p\right|\right) \\
\lambda_z^{-2} &= \frac{32\pi^2 e^2}{c^2}\left(\gamma_{s,z}|\eta_s|^2 + \gamma_{p,z}|\eta_p|^2 + 2\zeta_z\gamma_{0,z}\left|\eta_s^*\eta_p\right|\right).
\end{aligned}
$$

As a result of the modulation of the order parameters, the London penetration depth changes periodically in the x−direction. For $\zeta_z = 0$ and weak spin-orbit coupling we can use the results from (2.60) and obtain contributions for two wavelengths

$$
\lambda_\perp^{-2} = \frac{32\pi^2 e^2}{c^2}|s_0|^2\left[\gamma_{s,\perp} + \cos(2k_\ominus x)m_0^2\frac{H_{s,-}}{8k_\ominus^2} + \cos^2(2k_\ominus x)\frac{m_0^4}{4}\left(\frac{H_{s,-}^2}{64k_\ominus^4\gamma_{s,\perp}} + \frac{\rho_0^2 k_\ominus^2 M_\ominus^2\gamma_{p,\perp}}{a_p - a_s\frac{\gamma_{s,\perp}}{\gamma_{p,\perp}} + 4\gamma_{p,\perp}k_\ominus^2}\right)\right]
\tag{2.99}
$$

For small m_0 the dominant contribution to the modulation comes from the singlet channel. Furthermore we can draw an intuitively clear conclusion: We assume $h_{s,\perp} \approx h_{s,z}$ and take without loss of generality $M_\ominus > 1$. Superconductivity is then most pronounced when the magnetization is along the z-direction where it is smaller in magnitude than in the x-y-plane. Thus superconductivity is favoured in regions with smaller absolute value of the magnetization, as we have already seen in the section on nucleation of the superconductivity condensate. Note that this is a result of the non-constancy of $|\mathbf{m}|$ in this magnetic phase, which is in turn due to the non-degenerate z-axis in tetragonal symmetry.

Let us finally study the magnetic field induced by the modulated order parameters. For a modulated penetration depth, the London equation (2.96) becomes difficult to treat. To avoid difficulties we restrict ourselves to the lowest order modulation effect. We consider only the homogeneous part of $\lambda_\perp^{-2}$, denoted by $\tilde{\lambda}_\perp^{-2}$, and let the inhomogeneity $\mathbf{j}_d$ be spatially modulated.

The problem is addressed with the inclusion of the effect of the MD spin-obit interaction for both cases: when the condition (2.92) is satisfied and when it is violated. In case of the weak spin-orbit interaction, superconductivity did not gain an additional phase modulation. The **B**-field gains its leading modulation from the magnetization via the spin-orbit coupling terms. If we neglect the triplet phase, this reads

$$B_z = \cos(k_\ominus x)|s_0|^2 \frac{8\pi e\kappa_s\zeta_z m_0 M_\ominus}{c} \frac{k_\ominus}{k_\ominus^2 + \tilde{\lambda}_\perp^{-2}}.$$

This is in phase with the z-component of the given magnetization and shows the largest response if $\lambda_\perp^{-2} \approx k_\ominus^2$. However, if the wavelength of the magnetic modulation is smaller than the London penetration depth, the induced magnetic field is suppressed. The situation is illustrated in figure 2.5.

If on the other hand the MD spin-orbit interaction is strong enough to invoke a modulation of the complex phase of the order parameters, the situation is different. We calculate the magnetic field by taking η_s as given by (2.95), and again neglect the triplet phase $\eta_p = 0$. The modulation of the absolute value of η_s however has two contributions, one from the MD spin-orbit coupling ($\propto \cos(k_\ominus x)$), and one from the other coupling terms ($\propto \sin(2k_\ominus x)$). Not necessarily assuming that either is dominant, we include both to lowest order. The resulting **B** again shows an x-dependent z-component:

$$B_z = \cos(k_\ominus x)\frac{4\pi e k_\ominus^3 \gamma_{s,\perp}^2 |s_0|^2}{\zeta_z c m_0 \kappa_s M_\ominus (k_\ominus^2 + \tilde{\lambda}_\perp^{-2})} + \sin(2k_\ominus x)\sqrt{\mu - \frac{1}{\mu}}\frac{\pi e m_0^2 H_{s,-}|s_0|^2}{c(4k_\ominus^2 + \tilde{\lambda}_\perp^{-2})}$$

In this case however, we cannot simply consider the limits of $k_\ominus$ as compared to the London penetration depth, because it controls the modulation of superconductivity and magnetization at the same time.

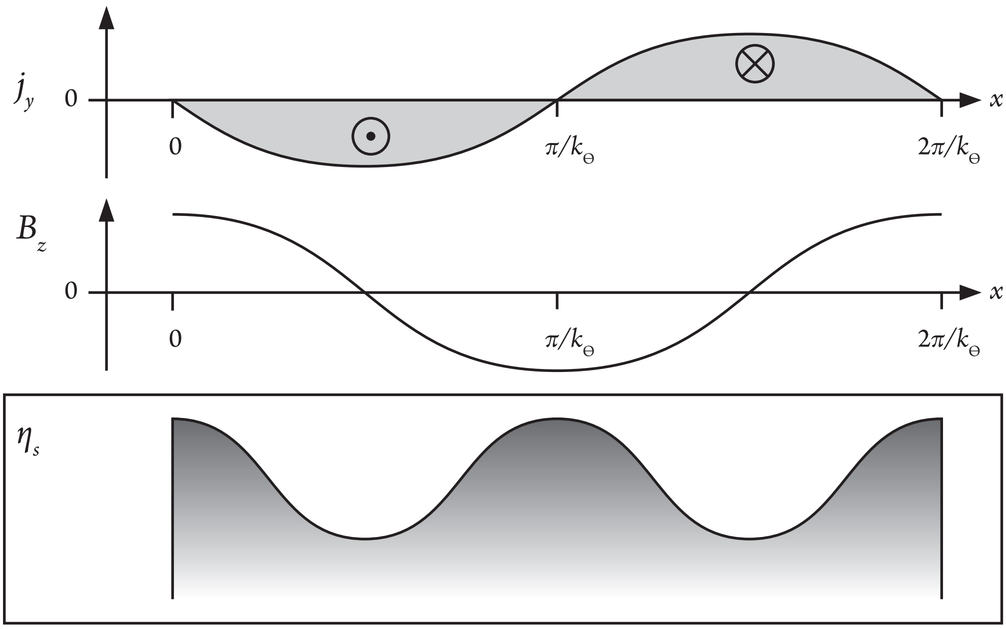

Figure 2.5: In case of the modulated magnetic phase in tetragonal symmetry, an inhomogeneous superconducting state emerges (compare 2.4). The graph qualitatively shows the induced magnetic field B_z and supercurrent j_y for the case of a weak spin-orbit interaction ($\mu < 1$).

2.4.6 The modulated magnetization in the diagonal direction

Thus far we were only concerned with one of the two modulated magnetic states that were obtained in 2.2. The other phase featured a wavevector along a x-y-plane diagonal. One of its two degenerate forms is:

$$\mathbf{m} = m_0 \left[\mathbf{e}_z \cos\left(k_\oslash (x+y)\right) + \left(\mathbf{e}_x + \mathbf{e}_y\right) M_\oslash \sin\left(k_\oslash (x+y)\right)\right]$$

Instead of performing the calculations also for this magnetic phase, we can show that both problems are equivalent under a suitable coordinate transformation. The variation equations (2.49) have the same form in the new coordinates $\tilde{x}$ and $\tilde{y}$, if we

- change the coordinates by $\tilde{x} = x + y$ and $\tilde{y} = x - y$,
- replace the parameters of the magnetic state $k_\ominus$ and $M_\ominus$ by $k_\oslash$ and $M_\oslash$, and
- multiply the parameters $h_{s,\perp}$, $h_{p,\perp}$, $v_\perp$, $\gamma_{s,\perp}$, $\gamma_{p,\perp}$, $\gamma_{0,\perp}$, ρ_s and ρ_0 by two.

With this transformation applied, we can translate all former results to this situation. The final modulation of singlet and triplet phase without spin-orbit coupling now reads according to (2.60)

$$\boxed{\eta_s(x,y) = \tilde{\eta}_s \left[1 + \cos\left(2k_\oslash (x+y)\right) \frac{m_0^2 H_{s,-}}{8\gamma_{s,\perp} k_\oslash^2}\right] + \mathcal{O}(\zeta_z)}$$
$$\boxed{\eta_p(x,y) = \tilde{\eta}_s \cos\left(2k_\oslash (x+y)\right) m_0^2 \frac{\rho_0 k_\oslash M_\oslash}{a_p - a_s + 8\gamma_{p,\perp} k_\oslash^2} + \mathcal{O}(\zeta_z)} \quad . \tag{2.100}$$

2.5 Summary of chapter 2: Tetragonal crystal structure

Homogeneous superconductivity: Parity mixing energetically favourable. No superconductivity in presence of strong non-centrosymmetricity.

Magnetic states:

- homogeneous

  (1) in z-direction

  (2) in x-y-plane (circular degeneracy)

- inhomogeneous: If non-centrosymmetricity exceeds a threshold. Magnetic moment spins around an axis perpendicular to the propagation direction and periodically changes its magnitude.

  (3) propagation parallel to the x- or y-axis (2-fold degenerate)

  (4) propagation parallel to either of the two diagonals in the x-y-plane (2-fold degenerate)

Superconductivity in each of the magnetic states:

- in homogeneous magnetic phases

  (1): Renormalisation of the parameters. Transition temperature reduced by depairing mechanisms.

  (2): Additional coherent *phase modulation* of the order parameters of superconductivity originating from the MD spin-orbit interaction. Propagation vector of the modulation in the x-y-plane, perpendicular to the magnetization.

- in inhomogeneous magnetic phases

  (3) and (4): Reaction of superconductivity on both modulated magnetic states equivalent.

  Strength of the *MD spin-orbit coupling* and the *wavelength of the magnetization* decide:

  small: Coherent modulation in the absolute values of the superconductivity order parameters. Parallel propagation vector with half the wavelength of the magnetic modulation. Modulated portion of singlet and triplet phase are of the same order of magnitude. Supercurrent induction by magnetization via MD spin-orbit coupling.

  large: Additional coherent phase modulation of the superconductivity order parameters; propagation vector of the modulation in the x-y-plane, perpendicular to the one of the magnetization. Additional contributions to the supercurrent.

  Superconductivity emerging in stripe-like state close to transition temperature. Superconductivity favoured where in space the absolute value of magnetization is the smallest. Phase coherence of adjacent stripes.

CHAPTER 3

Cubic crystal symmetry

In this chapter we perform the same analysis for a crystal lattice with cubic symmetry as done in the previous one for tetragonal symmetry. The space group under consideration is O_h. While the z-axis was thus far not degenerate with x- and y-axes, all three axes are now degenerate. As we shall see, this leads to qualitative differences.

Furthermore, we introduce non-centrosymmetricity differently. Instead of one distinct axis that violates parity, we assume that parity is violated isotropically in all spatial directions. Our ansatz for the gap function reflects this:

$$\mathbf{g}_{\mathbf{k}} = \mathbf{k}.$$

Apart form parity, the real lattice order-parameter ζ_1 must have full point group symmetry. Thus it exhibits the symmetry properties of the irreducible representation Γ_1^-. As before, the magnitude measures the strength of non-centrosymmetricity.

3.1 Homogeneous superconductivity

As a primer, we investigate the properties of homogeneous superconductivity in the absence of both a magnetic order and a magnetic field.

Parameter	Representation	Dimension	Basis function
η_s	Γ_1^+	1	$x^2 + y^2 + z^2$
η_p	Γ_1^-	1	
ζ_1	Γ_1^-	1	
D_x, D_y, D_z	Γ_4^-	3	x, y, z

Table 3.1: Representations of parameters in cubic symmetry

For the sake of simplicity, we once again fix the superconductivity order parameters η_s and η_p such that they belong to a one-dimensional representation. The expansion of the free energy to the same order as in the case of tetragonal structure is given by:

$$\begin{aligned} f_{sc} \quad = \quad & a_s\left|\eta_s\right|^2+a_p\left|\eta_p\right|^2+b_s\left|\eta_s\right|^4+b_p\left|\eta_p\right|^4+c_1\left|\eta_s\right|^2\left|\eta_p\right|^2+c_2\left(\eta_s^{*2}\eta_p^2+\eta_s^2\eta_p^{*2}\right)+ \\ & d\zeta_1\left(\eta_s^*\eta_p+\eta_s\eta_p^*\right)+\gamma_s\left|\mathbf{D}\eta_s\right|^2+\gamma_p\left|\mathbf{D}\eta_p\right|^2+\gamma_0\zeta_1\left(\mathbf{D}^*\eta_s^*\mathbf{D}\eta_p+\mathbf{D}\eta_s\mathbf{D}^*\eta_p^*\right). \end{aligned} \tag{3.1}$$

This functional is rather similar to the one considered in tetragonal symmetry. The physical meaning of all expansion parameters is the same as in the previous case. Since all axes are degenerate, we can drop the subscripts $\perp$ and z that were present in tetragonal symmetry. Note that due to the symmetry requirements, no first order derivative terms are allowed in this case (formerly proportional to $\delta_{s,p,0}$). Neglecting all fourth order terms first, the variation equations read in Fourier space:

$$\begin{aligned} \hat{A}_s\hat{\eta}_s+\hat{B}\hat{\eta}_p &= 0 \\ \hat{A}_p\hat{\eta}_p+\hat{B}\hat{\eta}_s &= 0, \end{aligned} \tag{3.2}$$

with the simple form of the operators:

$$\hat{A}_s := a_s+\gamma_s\mathbf{k}^2; \quad \hat{A}_p := a_p+\gamma_p\mathbf{k}^2; \quad \hat{B} := \zeta_1 d+\zeta_1\gamma_0\mathbf{k}^2. \tag{3.3}$$

Using the same linear temperature expansion for a_s and a_p as before (equation (2.3)), we determine the transition temperature from the zero of the determinant of (3.2)

$$T_c = \frac{T_{cs}+T_{cp}}{2}-\mathbf{k}^2\gamma_+ + \sqrt{\left[\frac{T_{cs}-T_{cp}}{2}-\mathbf{k}^2\gamma_-\right]^2+\frac{\zeta_1^2}{a_s'a_p'}\left(d^2+2d\gamma_0\mathbf{k}^2+\gamma_0^2\mathbf{k}^4\right)}, \tag{3.4}$$

where we defined

$$\gamma_\pm = \frac{\gamma_s}{2a_s'}\pm\frac{\gamma_p}{2a_p'} \tag{3.5}$$

Again we look for constraints to the phenomenological constants, such that homogeneous superconductivity ($\mathbf{k}=0$) has the highest transition temperature. Without loss of generality, we again assume that $T_{cs} > T_{cp}$. In addition to the positiveness of the stiffness coefficients $\gamma_s > 0$ and $\gamma_p > 0$, we deduce the following conditions from (2.12)

$$\boxed{2\gamma_s\frac{a_p'(T_{cs}-T_{cp})}{d\gamma_0-\frac{4\gamma_+d^2}{T_{cs}-T_{cp}}} > \zeta_1^2} \qquad \boxed{\gamma_s\gamma_p > \gamma_0^2\zeta_1^2}. \tag{3.6}$$

Expanded in the small quantity ζ_1, the transition temperature of the homogeneous state is obtained as:

$$\boxed{T = T_{cs}+\zeta_1^2\frac{d^2}{a_s'a_p'(T_{cs}-T_{cp})}}. \tag{3.7}$$

This again shows that strong non-centrosymmetricity could be harmful to the stability of superconductivity. Analogous to the case of tetragonal symmetry, we determine the mixing ratio as

$$\boxed{\frac{\eta_p}{\eta_s} = -\left.\frac{\hat{B}}{\hat{A}_p}\right|_{\mathbf{k}=0} = -\frac{\zeta_1 d}{a_p'(T_{cs}-T_{cp})}}. \tag{3.8}$$

The whole discussion on the effect of fourth order terms (section 2.1.3) is one to one applicable to the cubic case, since all terms without derivatives of order parameters are exactly the same for cubic and tetragonal symmetry (under the replacement $\zeta_z \longrightarrow \zeta_1$). Therefore we briefly recall the result: The singlet and the triplet phase are in phase for $d\zeta_1 < 0$, and have a relative minus sign if $d\zeta_1 > 0$.

3.2 Magnetic phases

The aim of this section is to determine all possible magnetic states in a non-centrosymmetric cubic system.

Parameter	Representation	Dimension	Basis function
ζ_1	Γ_1^-	1	
$\nabla_x, \nabla_y, \nabla_z$	Γ_4^-	3	x, y, z
m_x, m_y, m_z	Γ_4^+	3	S_x, S_y, S_z

Table 3.2: Representations of parameters in cubic symmetry

To keep the expansions simple, it is convenient to introduce a notation for two new products. The first one produces a vector belonging to the irreducible representation Γ_4, provided **a** and **b** also belong to Γ_4. The result of the second product is a vector of the two-dimensional representation Γ_3, provided **a** and **b** belong to Γ_4.

$$\mathbf{a} \star \mathbf{b} \equiv \left(a_y b_z + a_z b_y, a_x b_z + a_z b_x, a_x b_y + a_y b_x\right)$$

$$\mathbf{a} \mathbin{\bullet} \mathbf{b} \equiv \left(\sqrt{3}(a_x b_x - a_y b_y), 3a_z b_z - \mathbf{a}\cdot\mathbf{b}\right)$$

Finally, the usual vector product of two Γ_4-vectors is a vector in the irreducible representation Γ_5. With this in mind, the expansion of the free energy density in the magnetic order parameter **m** takes the following compact form:

$$\begin{aligned} f_{mag} \quad = \quad & \alpha \mathbf{m}^2 + \beta_1 (\mathbf{m}\cdot\mathbf{m})^2 + \beta_2 (\mathbf{m}\star\mathbf{m})^2 + \beta_3 (\mathbf{m}\mathbin{\bullet}\mathbf{m})^2 + \vartheta\zeta_1 \mathbf{m}\cdot(\nabla\times\mathbf{m}) + \\ & \tau_1 (\nabla\times\mathbf{m})^2 + \tau_2 (\nabla\star\mathbf{m})^2 + \tau_3 (\nabla\cdot\mathbf{m})^2 + \tau_4 (\nabla\mathbin{\bullet}\mathbf{m})^2 \end{aligned} \tag{3.9}$$

We want to find all stable magnetic phases and in particular study the effect of non-centrosymmetricity via the term proportional to ζ_1. This term reflects the effect of the MD spin-orbit interaction. The only temperature dependent coefficient is

$$\alpha(T) = \alpha'(T - T_c). \tag{3.10}$$

The variational derivatives of $\int \mathrm{d}^3 r\, f_{mag}$ with respect to m_x, m_y and m_z yield a system of three linear homogeneous equations. When transformed to Fourier space, the coefficient matrix takes the form

$$M = \begin{pmatrix} \alpha + (k_y^2 + k_z^2)\tau_+ + k_x^2\tilde{\tau} & -k_x k_y \tau^* - \mathrm{i}k_z\vartheta\zeta_1 & -k_x k_z \tau^* + \mathrm{i}k_y\vartheta\zeta_1 \\ -k_x k_y \tau^* + \mathrm{i}k_z\vartheta\zeta_1 & \alpha + (k_x^2 + k_z^2)\tau_+ + k_y^2\tilde{\tau} & -k_y k_z \tau^* - \mathrm{i}k_x\vartheta\zeta_1 \\ -k_x k_z \tau^* - \mathrm{i}k_y\vartheta\zeta_1 & -k_y k_z \tau^* + \mathrm{i}k_x\vartheta\zeta_1 & \alpha + (k_x^2 + k_y^2)\tau_+ + k_z^2\tilde{\tau} \end{pmatrix}. \tag{3.11}$$

Because the τ-parameters only come in three combinations, by introducing the following shorthand notation we explicitly reduce the number of independent parameters by one:

$$\begin{aligned}\tau_+ &= \tau_1 + \tau_2 \\ \tilde{\tau} &= \tau_3 + 4\tau_4 \\ \tau^* &= \tau_1 - \tau_2 + 2\tau_4. \end{aligned} \tag{3.12}$$

Once more, the equation $\mathrm{Det}(M) = 0$ implicitly defines the **k**-dependence of the critical temperature $T(\mathbf{k})$. The maxima of this function determine the wavevector of the realised magnetic phase.

$$\begin{aligned} 0 &= \mathrm{Det}(M) \\ &= \alpha^3 + \left(k_x^2 + k_y^2 + k_z^2\right)\left[\alpha^2\left(2\tau_+ + \tilde{\tau}\right) - \alpha\vartheta^2\zeta_1^2\right] + \left(k_x^4 + k_y^4 + k_z^4\right)\left[\alpha\tau_+\left(\tau_+ + 2\tilde{\tau}\right) - \tilde{\tau}\vartheta^2\zeta_1^2\right] + \\ &\quad \left(k_x^2k_y^2 + k_y^2k_z^2 + k_x^2k_z^2\right)\left[\alpha\left(3\tau_+^2 + 2\tau_+\tilde{\tau} + \tilde{\tau}^2 - \tau^{*2}\right) - \left(\tau_+ - \tau^*\right)\vartheta^2\zeta_1^2\right] \\ &\quad \left(k_x^4k_y^2 + k_x^2k_y^4 + k_y^4k_z^2 + k_y^2k_z^4 + k_x^4k_z^2 + k_x^2k_z^4\right)\left(\tau_+^3 - \tau_+\tau^{*2} + \tau_+^2\tilde{\tau} + \tau_+\tilde{\tau}^2\right) + \\ &\quad k_x^2k_y^2k_z^2\left(2\tau_+^3 - 2\tau^{*3} + 3\tau_+^2\tilde{\tau} - 3\tau^{*2}\tilde{\tau} + \tilde{\tau}^3\right) + \left(k_x^6 + k_y^6 + k_z^6\right)\tau_+^2\tilde{\tau} \end{aligned} \tag{3.13}$$

3.2.1 The centrosymmetric system

Before we further analyse $T(\mathbf{k})$, we study the system in the absence of non-centrosymmetricity ($\zeta_1 = 0$). In this case, homogeneous magnetization must be the ground state rather than any modulated magnetization. This in particular excludes instabilities for arbitrary large **k**-values. As a result, we shall obtain restrictions to the parameters in f_{mag}. To ensure a homogeneous magnetization, we demand that the terms $\propto k^2$, $\propto k^4$ and $\propto k^6$ in $\mathrm{Det}(M)$ are positive definite.

The *second-order terms* in (3.13) are positive definite, if and only if

$$2\tau_+ + \tilde{\tau} > 0.$$

From the *fourth order terms*,

$$\left(2\tau_+ + \tilde{\tau}\right)^2 > \tau^{*2} \quad \text{and} \quad \tau_+\left(\tau_+ + 2\tilde{\tau}\right) > 0$$

arise as additional constraints. The *sixth-order terms* in **k** are analysed by parametrising in spherical coordinates

$$\mathbf{k} = k\left(\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta)\right)^T. \tag{3.14}$$

There are at most three extremal points

$$\mathbf{k} = k\mathbf{e}_i, \quad \mathbf{k} = k\left(\mathbf{e}_i + \mathbf{e}_j\right) \quad \text{and} \quad \mathbf{k} = k\left(\mathbf{e}_x + \mathbf{e}_y + \mathbf{e}_z\right) \quad \text{with} \quad i, j \in \{x, y, z\}, i \neq j,$$

amongst which we must find the absolute minimum. We obtain further conditions by demanding that the sixth-order terms are positive in all these local minima. If we merge them with the constraints from the other orders, the final conditions are

$$\boxed{\tau_+ > 0} \quad \boxed{-\sqrt{\tau_+^2 + \tilde{\tau}^2 + \frac{3}{2}\tau_+\tilde{\tau}} < \tau^* < \tau_+ + \frac{\tilde{\tau}}{2}} \quad \boxed{\tilde{\tau} > 0}. \tag{3.15}$$

3.2.2 The effect of non-centrosymmetricity: modulated phases

Let us now turn to the case with non-centrosymmetricity ($\zeta_1 \neq 0$). Here we expect to have a modulated magnetic phase. In tetragonal symmetry, we obtained homogeneous magnetic phases until non-centrosymmetricity overcomes a certain threshold. In contrast to this, non-centrosymmetric cubic symmetry never shows a homogeneous phase. Since the fourth order terms become negative *promptly* for temperatures below T_c ($\alpha < 0$), an inhomogeneous magnetization will be present for arbitrary small ζ_1 (see equation (3.13)). Our goal is to determine the **k**-vector which maximises the transition temperature, and to determine the corresponding spatial dependence of the magnetization.

We directly see that the second-order terms are rotationally symmetric and thus do not lift the spherical degeneracy of the energetically favourable direction in **k**-space. To proceed, we solve equation (3.13) with respect to T. Using the parametrization (3.14), the three rather cumbersome solutions are expanded in k up to order k^2. The first solution features a negative prefactor of k, the second one shows a positive prefactor, and the third solution has no k-linear term. All their k^2 terms are negative definite. To obtain a maximum in the transition temperature, only the second solution comes into question. Its expansion reads:

$$T = T_c + \frac{|k\vartheta\zeta_1|}{\alpha'} - \frac{k^2}{3\alpha'}\Big[2\tau_+ + \tilde{\tau} + \cos^4(\theta)\,(\tau_+ - \tilde{\tau}) - \sin^2(\theta)\cos^2(\theta)\left(\tau_+ - 3\tau^* - \tilde{\tau}\right) + \frac{\sin^4(\theta)}{8}\left(5\tau_+ + 3\tau^* - 5\tilde{\tau} + 3\cos(4\phi)\left(\tau_+ - \tau^* - \tilde{\tau}\right)\right)\Big] \tag{3.16}$$

Since the k-linear term is isotropic, the direction (ϕ, θ) that minimises the (positive) term in square brackets will maximise the transition temperature. This term possesses the same three types of stationary points as those obtained in 3.2.1:

- **k** pointing along a coordinate axis (transition temperature $T_\oplus$, 6-fold degenerate),
- **k** pointing along a face diagonal (T_f, 8-fold degenerate), and
- **k** pointing along a body diagonal ($T_\otimes$, 8-fold degenerate).

To maximise the temperature, the following conditions are obtained if (3.16) is evaluated for these **k**-vectors:

- $T_\oplus > T_\otimes$ if $\tau_+ < \tilde{\tau} + \tau^*$
- $T_\oplus > T_f$ if $\tau_+ < \tilde{\tau} + \tau^*$
- $T_\otimes > T_f$ if $\tau_+ > \tilde{\tau} + \tau^*$

From this we can conclude that only two different magnetic phases are realised, since T_f never maximises the transition temperature. For further discussion we pick the following examples out of degenerate **k**-vectors:

- $\mathbf{k} = k\mathbf{e}_z$ in the case $\tau_+ < \tilde{\tau} + \tau^*$
- $\mathbf{k} = k\left(\mathbf{e}_x + \mathbf{e}_y + \mathbf{e}_z\right)$ in the case $\tau_+ > \tilde{\tau} + \tau^*$

Case $\mathbf{k} = k\mathbf{e}_z$

Let us without loss of generality look at $\mathbf{k} = k\mathbf{e}_z$ and determine the optimal value of k, the transition temperature and the corresponding magnetization $\mathbf{m}(x, y, z)$. It results that, in this case, (3.16) is coincidentally the exact solution of equation (3.13)

$$T = T_c + \frac{|k\vartheta\zeta_1|}{\alpha'} - \frac{k^2\tau_+}{\alpha'}. \tag{3.17}$$

The value of k that maximises this is

$$k_\oplus = \frac{|\vartheta\zeta_1|}{2\tau_+} \tag{3.18}$$

and the transition temperature is obtained as

$$\boxed{T_\oplus = T_c + \frac{(\vartheta\zeta_1)^2}{4\alpha'\tau_+}}. \tag{3.19}$$

In this case, the equation $M(\hat{m}_x, \hat{m}_y, \hat{m}_z)^T = 0$ with M from (3.11) is easily solved, resulting in $\hat{m}_z = 0$ and $\hat{m}_x = -\mathrm{i}\hat{m}_y$. Thus the real magnetization is a helix along z-direction:

$$\boxed{\mathbf{m} = m_0\left(\sin(k_\oplus z)\mathbf{e}_x + \cos(k_\oplus z)\mathbf{e}_y\right)} \tag{3.20}$$

The overall amplitude m_0 is undetermined.

Case $\mathbf{k} = k\left(\mathbf{e}_x + \mathbf{e}_y + \mathbf{e}_z\right)$

In this case, an exact treatment of (3.13) leads to unwieldily results. Instead, we use the expansion (3.16) to determine the value of $k_\otimes$ that maximises the transition temperature:

$$k_\otimes \approx \frac{3|\vartheta\zeta_1|}{2(2\tau_+ + \tilde{\tau} + \tau^*)} \tag{3.21}$$

$$\boxed{T_\otimes \approx T_c + \frac{3(\vartheta\zeta_1)^2}{4\alpha'(2\tau_+ + \tilde{\tau} + \tau^*)}} \tag{3.22}$$

Without knowing the exact values of these quantities, it is not trivial to determine the solution of the homogeneous linear system of equations $(\hat{m}_x, \hat{m}_y, \hat{m}_z)^T$. However, the coefficient matrix takes a highly symmetric form (with some f, g):

$$M = \begin{pmatrix} f & g & g^* \\ g^* & f & g \\ g & g^* & f \end{pmatrix}. \tag{3.23}$$

Note that the three equations are equivalent under cyclic or anticyclic permutations of the x-, y- and z-components of $\mathbf{m}$. Furthermore, f and g must satisfy

$$\mathrm{Det}(M) = 0 \quad \Longleftrightarrow \quad f^3 + g^3 - 3fgg^* + g^{*3} = 0 \tag{3.24}$$

which has three solutions. The first corresponds to $\hat{m}_x = \hat{m}_y = \hat{m}_z$ and leads to a lower transition temperature than T_c. The other two solutions are degenerate and differ in cyclic and anticyclic permutation of the indices. For these solutions the non-trivial null-space of M is one-dimensional with

$$\hat{m}_x = e^{\pm\mathrm{i}\frac{2}{3}\pi}\hat{m}_y = e^{\pm\mathrm{i}\frac{4}{3}\pi}\hat{m}_z$$

Hence, the real magnetization has a spatial modulation of

$$\boxed{\mathbf{m} = m_0 \left[\sin\left(k_\otimes (x+y+z)\right)\mathbf{e}_x + \sin\left(k_\otimes (x+y+z) \pm \frac{2}{3}\pi\right)\mathbf{e}_y + \sin\left(k_\otimes (x+y+z) \pm \frac{4}{3}\pi\right)\mathbf{e}_z\right]} \tag{3.25}$$

This helical phase seems to be more bulky than the one discussed in the previous section. However, it turns out that apart from the direction of propagation (which is the body diagonal instead of a coordinate axis) the structure is the same.

In conclusion, we have found two magnetically ordered ground states, each of which is helically modulated and eight-fold degenerate. This result is qualitatively different from the case of tetragonal symmetry.

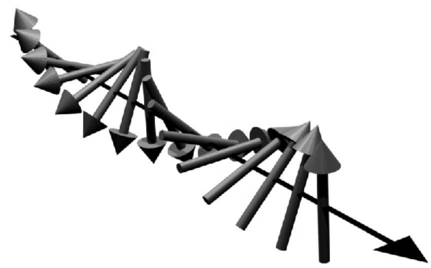

Figure 3.1: Schematic picture of the two helical magnetic phases obtained for cubic lattice. For $\tau_+ < \tilde{\tau} + \tau^*$, the direction of propagation (the black arrow) is a coordinate axis. For $\tau_+ > \tilde{\tau} + \tau^*$, the helix propagates along the body diagonal. The magnitude of the magnetization vector is the same at every point in space.

3.3 Superconductivity in the inhomogeneous magnetic phases

In 3.2 we found two magnetic phases in a non-centrosymmetric cubic material. This section will be dedicated to study the impact of these helical magnetizations on superconductivity.

3.3.1 Coupling terms in the free energy

The expansion terms of the free energy that are allowed by symmetry restrictions which couple magnetic order with superconductivity are given below. As in section 2.3 we account for terms up to order "$m^2 D\eta^2$".

$$\begin{aligned} f_{coupling} &= h_s (\mathbf{m})^2 |\eta_s|^2 + h_p (\mathbf{m})^2 |\eta_p|^2 + v\zeta_1 (\mathbf{m})^2 \left(\eta_s \eta_p^* + \eta_p \eta_s^*\right) + \\ &\quad \mathrm{i}\kappa_s \zeta_1 \mathbf{m}\cdot\left(\eta_s \mathbf{D}^* \eta_s^* - \eta_s^* \mathbf{D}\eta_s\right) + \mathrm{i}\kappa_p \zeta_1 \mathbf{m}\cdot\left(\eta_p \mathbf{D}^* \eta_p^* - \eta_p^* \mathbf{D}\eta_p\right) + \\ &\quad \mathrm{i}\kappa_0 \mathbf{m}\cdot\left(\eta_s \mathbf{D}^* \eta_p^* - \eta_s^* \mathbf{D}\eta_p + \eta_p \mathbf{D}^* \eta_s^* - \eta_p^* \mathbf{D}\eta_s\right) \end{aligned}$$

It is worth mentioning that there are no terms of the form "$m^2 D\eta^2$". This is easily explained. The only Γ_1-quantity that can be constructed from any three quantities belonging to the irreducible representation Γ_4 (like $\mathbf{m}$ and $\mathbf{D}$) is the triple product. However, since $\mathbf{m}$ appears twice, the triple product vanishes.

The parameters κ_s, κ_p and κ_0 once again display the effect of the MD spin-orbit interaction. The depairing terms h_s and h_p are assumed to be positive.

3.3.2 Helical magnetic phase along a coordinate axis

Let us begin by considering the helical magnetic order as given by (3.20) and study the response of superconductivity. Taking the variational derivative yields additional terms in the operators (3.26) which become:

$$\begin{aligned} A_s &:= a_s + h_s m_0^2 - \gamma_s \nabla^2 + \mathrm{i}2\kappa_s \zeta_1 m_0 \left(\sin(k_1 z)\nabla_x + \cos(k_1 z)\nabla_y\right) \\ A_p &:= a_p + h_p m_0^2 - \gamma_p \nabla^2 + \mathrm{i}2\kappa_p \zeta_1 m_0 \left(\sin(k_1 z)\nabla_x + \cos(k_1 z)\nabla_y\right) \\ B &:= \zeta_1 d + \zeta_1 v m_0^2 - \zeta_1 \gamma_0 \nabla^2 + \mathrm{i}2\kappa_0 m_0 \left(\sin(k_1 z)\nabla_x + \cos(k_1 z)\nabla_y\right) \end{aligned} \tag{3.26}$$

An important consequence of this result is that the equations look as though they describe a homogeneous magnetization – save for the terms that originate from the MD spin-orbit interaction. In this case the expansion parameters become renormalised as pointed out in our analysis of homogeneous magnetization in tetragonal symmetry. Difficulties may arise if the conditions (3.6), rewritten in terms of the renormalised parameters, are violated.

To explore the effect of the MD terms, we recall the line of arguments presented in 2.4.4. All the coefficients of the differential equation are independent of the x- and y-coordinates. In the z-variable, the equation's coefficients are periodic. This once again motivates the cutting of the Fourier space in k_z-direction into Brillouin zones and to perform a NFE-like treatment as was done in 2.4.1. The ansatz thus reads with $K_n = k + nk_\oplus,\ n \in \mathbb{Z},\ k \in \left[-\frac{k_\oplus}{2}, \frac{k_\oplus}{2}\right]$

$$\eta_s(x,y,z) = e^{\mathrm{i}(k_x x + k_y y)} \sum_n s_n(k) e^{\mathrm{i}K_n z} \tag{3.27}$$

$$\eta_p(x,y,z) = e^{\mathrm{i}(k_x x + k_y y)} \sum_n p_n(k) e^{\mathrm{i}K_n z}. \tag{3.28}$$

Since the modulation in the z-direction is uninfluenced by the spin-orbit interaction for the given magnetization, we assume maximal transition temperature at $k = 0$. The equations then read

$$\begin{aligned} &\left(a_s + h_s m_0^2 + \gamma_s (2nk_\oplus)^2 + \gamma_s (k_x^2 + k_y^2)\right) s_n + \zeta_1 \left(d + v m_0^2 + \gamma_0 (2nk_\oplus)^2 + \gamma_0 (k_x^2 + k_y^2)\right) p_n + \\ &\qquad m_0 \kappa_s \zeta_1 \left\{(k_x \mathrm{i} - k_y) s_{n-1} - (k_x \mathrm{i} + k_y) s_{n+1}\right\} = 0 \\ &\left(a_p + h_p m_0^2 + \gamma_p (2nk_\oplus)^2 + \gamma_p (k_x^2 + k_y^2)\right) p_n + \zeta_1 \left(d + v m_0^2 + \gamma_0 (2nk_\oplus)^2 + \gamma_0 (k_x^2 + k_y^2)\right) s_n + \\ &\qquad m_0 \kappa_p \zeta_1 \left\{(k_x \mathrm{i} - k_y) p_{n-1} - (k_x \mathrm{i} + k_y) p_{n+1}\right\} = 0. \end{aligned} \tag{3.29}$$

As in previous discussions, we confine the calculations to three Fourier amplitudes by taking care of s_0, p_0, $s_{\pm 1}$ and $p_{\pm 1}$. The equations for $n = -1, 0, 1$ represent a homogeneous linear system of six equations for these six unknowns and have a coefficient matrix similar to M from (2.88). Main differences are that the coupling to next-next neighbouring modes (C_s,C_p and D in section 2.4.4) are not present and that both k_x and k_y appear explicitly.

A finite k_x or k_y would lead to modulated superconductivity, both in the phase and in the absolute value of the order parameters. The question is whether or not this would enhance the transition temperature.

The points at which the determinant of the coefficient matrix vanishes define an implicit function $T(k_x, k_y)$. The exact solution at $k_x = k_y = 0$ is given by

$$T = \frac{T_{cs} + T_{cp}}{2} - m_0^2 \left(\frac{h_s}{a'_s} + \frac{h_p}{a'_p} \right) + \sqrt{\left(\frac{T_{cs} - T_{cp}}{2} + m_0^2 \left(\frac{h_p}{a'_p} - \frac{h_s}{a'_s} \right) \right)^2 + \frac{\zeta_1^2 \left(d + m_0^2 v\right)^2}{a'_s a'_p}} \tag{3.30}$$

With the implicit function theorem we determine the directional derivatives. Because the implicit function depends only on k_x^2 and k_y^2, we may also use the implicit function theorem to calculate the second derivatives. These are the derivative with respect to the variable squared divided by two.

$$\begin{aligned} \left.\frac{\partial T}{\partial k_x}\right|_{T_c, k_x=0, k_y=0} &= \left.\frac{\partial T}{\partial k_y}\right|_{T_c, k_x=0, k_y=0} = 0 \\ \left.\frac{\partial T}{\partial k_x^2}\right|_{T_c, k_x=0, k_y=0} &= \left.\frac{\partial T}{\partial k_y^2}\right|_{T_c, k_x=0, k_y=0} \neq 0 \\ \left.\frac{\partial T}{\partial k_x k_y}\right|_{T_c, k_x=0, k_y=0} &= 0 \end{aligned} \tag{3.31}$$

As in 2.4.4, there are no k-linear contributions to the temperature.

The derivative with respect to k_x^2 and k_y^2 results in a rather bulky expression. This expression depends on γ_s, the variables that couple the singlet and the triplet phases (d, v, γ_0), and the spin-orbit interaction (κ_s, κ_p, κ_0). Its sign decides whether a finite **k**-vector is favoured or whether homogeneous superconductivity persists despite the modulated magnetization. If we neglect all terms that couple singlet and triplet phase ($\gamma_0 = 0$, $v = 0$, $\kappa_0 = 0$ and $d = 0$), this condition simplifies to a form familiar from tetragonal symmetry. Modulated superconductivity is favoured if the spin-orbit coupling is sufficiently strong as opposed to the stiffness parameter γ_s

$$\boxed{1 < \mu \equiv \frac{2\zeta_1^2 m_0^2 \kappa_s^2}{\gamma_s^2 k_\oplus^2}}. \tag{3.32}$$

We can furthermore interpret this threshold in the light of the parameters m_0 and $k_\oplus$ that originate from the given magnetic state. Superconductivity is forced to follow the modulation of the magnetic state if the magnetization is great and the wavelength of the modulation sufficiently long.

From the symmetry of the equations with respect to the singlet and the triplet phase we can conclude that both order parameters are in coherence even when modulated. Thus, the only qualitative information we lose when neglecting the triplet phase is the impact of the spin-orbit coupling on the mixing ratio.

Homogeneous superconductivity

If condition (3.32) is not satisfied, the superconducting condensate stays homogeneous despite the modulated magnetic background. From our expansion of $f_{coupling}$ we can determine the following renormalisation of the phenomenological expansion parameters:

$$\begin{aligned} \bar{a}_s &= a_s + h_s m_0^2 \\ \bar{a}_p &= a_p + h_p m_0^2 \\ \bar{d} &= d + v m_0^2. \end{aligned} \tag{3.33}$$

The exact transition temperature is given by (3.30). From the expansion in ζ_1, we see that the magnetization lowers the transition temperature:

$$\boxed{T_c = T_{cs} - m_0^2 \frac{h_s}{a_s'} + \zeta_1^2 \frac{d^2}{a_s' a_p' (T_{cs} - T_{cp})} \left[1 + m_0^2 \frac{2v}{d} + m_0^2 \frac{a_p' h_s - a_s' h_p}{a_s' a_p' (T_{cs} - T_{cp})} \right]}. \tag{3.34}$$

In principle we would also have to check whether the conditions on phenomenological parameters that avoid arbitrary strong modulations are still satisfied (see (3.6)). The first condition ensures a local maximum at $\mathbf{k} = 0$. This problem has meanwhile been reformulated in the form of equation (3.31) and is therefore already satisfied if homogeneous superconductivity is present. The second inequality remains unaltered because we do not consider a renormalisation of the parameters γ_s, γ_p and γ_0.

Inhomogeneous superconductivity

If condition (3.32) holds, an inhomogeneous superconductivity phase would be present. We analyse the six coupled NFE equations to extract more information on it.

To begin, we find a circular degeneracy for the $\mathbf{k}$-vector in the x-y-plane. Without loss of generality we from here on out choose $k_x \neq 0$, $k_y = 0$. Again, we neglect the triplet phase by setting

$$\kappa_0 = 0; \quad \gamma_0 = 0; \quad v = 0 \quad \text{and} \quad d = 0. \tag{3.35}$$

The favoured value of k_x is then given in terms of the parameter introduced in (3.32)

$$k_x \approx \pm \frac{k_\oplus}{2} \sqrt{\mu - \frac{1}{\mu}}. \tag{3.36}$$

Correspondingly the critical temperature as given in equation (3.34) is raised due to the modulation by an amount

$$\boxed{\Delta T_c = \frac{k_\oplus^2 \gamma_s}{4 a_s'} \frac{\mu + 1}{\mu} (\mu - 1)^2}. \tag{3.37}$$

The coefficients $s_{\pm 1}$ and $p_{\pm 1}$ are purely imaginary numbers. They fulfill

$$s_1 = -s_{-1} \quad \text{and} \quad p_1 = -p_{-1}, \tag{3.38}$$

giving rise to a coherent modulation of the singlet and the triplet phase as $\sin(k_\oplus z)$. Because we neglected the triplet phase, the result for the singlet order parameter is

$$\boxed{\eta_s(x,y,z) \approx s_0 e^{\pm \mathrm{i} \frac{k_\oplus}{2} \sqrt{\mu - \mu^{-1}} x} \left[1 \pm \sqrt{2 \frac{\mu - 1}{\mu + 1}} \sin k_\oplus z \right]}. \tag{3.39}$$

Since μ must satisfy (3.32), the term in square brackets is unlikely to become negative. At the point at which μ exceeds the threshold (3.32), modulations appear in a continuous way. Provided the values of μ are not too large, the homogeneous part of η_s will still dominate. This justifies our earlier neglection of higher order modes $s_{\pm n}, n \geq 2$. These would be further suppressed.

According to (3.38), we expect the triplet phase to show a similar modulation. The relative magnitude as compared to the singlet phase is however not easily determined. It will depend on the parameters γ_0,

v and d and their relative magnitude with respect to the parameters of spin-orbit coupling κ_s, κ_p, and κ_0. Thus we will not address this issue any further.

In conclusion, we find the coherent modulation of the singlet and the triplet order parameters in absolute magnitude in the z-direction and a periodic phase-change in some direction perpendicular to that. Either both modulations are present or neither. These modulations need a sufficiently strong spin-orbit interaction to be present.

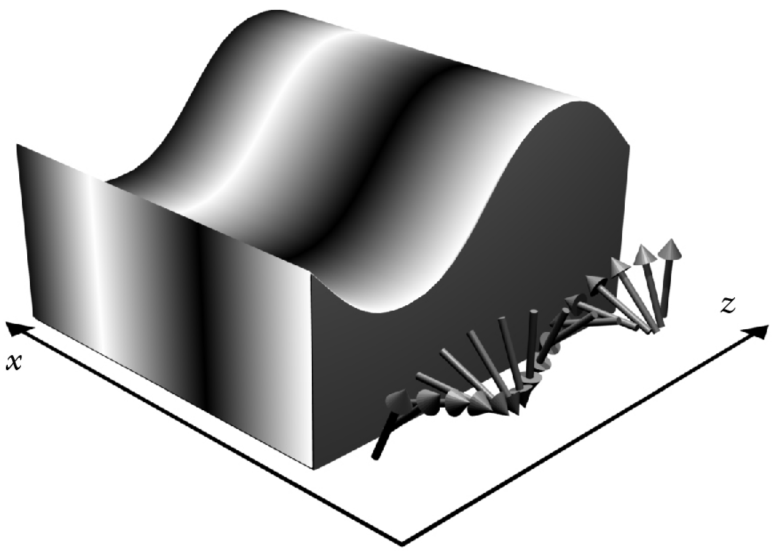

Figure 3.2: Schematic picture of the superconductivity order parameters according to equation (3.39). In the regime of strong spin-orbit coupling the reaction of superconductivity to the modulated magnetic phases obtained for cubic lattice is twofold: The order parameter exhibits an amplitude modulation in the z-direction, and in addition to that features a phase modulation perpendicular to the z-direction (depicted by the colour gradient). The wavelengths of the modulations are different from each other.

3.3.3 Helical magnetic phase along a body diagonal

In section 3.2 we found a second magnetically ordered phase. The discussion is more convenient if the direction of propagation is along one of the coordinate axes. Thus we perform a shift of coordinates from x, y, z to a tilted orthonormal system $\tilde{x}, \tilde{y}, \tilde{z}$ defined by its unit vectors

$$\begin{aligned}
\mathbf{e}_{\tilde{x}} &= \sqrt{\frac{2}{3}}\left(\mathbf{e}_x - \frac{\mathbf{e}_y}{2} - \frac{\mathbf{e}_z}{2}\right)\\
\mathbf{e}_{\tilde{y}} &= \frac{1}{\sqrt{2}}\left(\mathbf{e}_y + \mathbf{e}_z\right)\\
\mathbf{e}_{\tilde{z}} &= \frac{1}{\sqrt{3}}\left(\mathbf{e}_x + \mathbf{e}_y + \mathbf{e}_z\right)
\end{aligned} \tag{3.40}$$

In these coordinates, the magnetization vector (3.25) becomes

$$\boxed{\mathbf{m} = m_0\sqrt{\frac{3}{2}}\left(\sin\left(\sqrt{3}k_\otimes \tilde{z}\right)\mathbf{e}_{\tilde{x}} + \cos\left(\sqrt{3}k_\otimes \tilde{z}\right)\mathbf{e}_{\tilde{y}}\right)} \tag{3.41}$$

The variation equations are also written in the new coordinates, taking into account that orthonormality and the affinity of the transformation prevents the alteration of the Laplacian $\nabla^2 = \tilde{\nabla}^2$. The operators become:

$$\begin{aligned} A_s &:= a_s + h_s m_0^2 - \gamma_s \tilde{\nabla}^2 + \mathrm{i}\sqrt{6}\kappa_s \zeta_1 m_0 \left(\sin\left(\sqrt{3}k_\otimes \tilde{z}\right)\nabla_{\tilde{x}} + \cos\left(\sqrt{3}k_\otimes \tilde{z}\right)\nabla_{\tilde{y}}\right) \\ A_p &:= a_p + h_p m_0^2 - \gamma_p \tilde{\nabla}^2 + \mathrm{i}\sqrt{6}\kappa_p \zeta_1 m_0 \left(\sin\left(\sqrt{3}k_\otimes \tilde{z}\right)\nabla_{\tilde{x}} + \cos\left(\sqrt{3}k_\otimes \tilde{z}\right)\nabla_{\tilde{y}}\right) \\ B &:= \zeta_1 d + \zeta_1 v m_0^2 - \zeta_1 \gamma_0 \tilde{\nabla}^2 + \mathrm{i}\sqrt{6}\kappa_0 m_0 \left(\sin\left(\sqrt{3}k_\otimes \tilde{z}\right)\nabla_{\tilde{x}} + \cos\left(\sqrt{3}k_\otimes \tilde{z}\right)\nabla_{\tilde{y}}\right). \end{aligned} \tag{3.42}$$

These operators have the same form as (3.26) and the calculation is unaltered if we replace

$$\begin{aligned} (x,y,z) &\longrightarrow (\tilde{x},\tilde{y},\tilde{z}) \\ \kappa_i &\longrightarrow \sqrt{\frac{3}{2}}\kappa_i \quad i = s,p,0 \\ k_\oplus &\longrightarrow \sqrt{3}k_\otimes. \end{aligned} \tag{3.43}$$

Similarly we can retain all results of the previous section with these replacements. As before, we have homogeneous superconductivity that becomes renormalised in the same way as for the other magnetization, provided spin-orbit coupling dominates over the stiffness parameter. The condition for a modulated superconducting phase now reads:

$$\boxed{1 < \tilde{\mu} \equiv \frac{\zeta_1^2 m_0^2 \kappa_s^2}{\gamma_s^2 k_\otimes^2}} \tag{3.44}$$

If we neglect the triplet phase, the modulation of singlet superconductivity reads in the original coordinates

$$\boxed{\eta_s(x,y,z) \approx s_0 \exp\left[\pm\mathrm{i}\frac{k_\otimes}{\sqrt{2}}\sqrt{\tilde{\mu}^2 - \tilde{\mu}^{-2}}\left(x - \frac{y}{2} - \frac{z}{2}\right)\right]\left\{1 \pm \sqrt{2\frac{\tilde{\mu}-1}{\tilde{\mu}+1}}\sin\left(k_\otimes(x+y+z)\right)\right\}} \tag{3.45}$$

We again obtain a circular degeneracy for the direction of phase modulation. Here the phase modulation direction was taken to be $\mathbf{e}_{\tilde{x}}$.

It is worth noting that as in the case of tetragonal symmetry, both modulated magnetizations are equivalent in their impact on superconductivity.

3.3.4 The London penetration depth

In closing this chapter, we complete our picture of the superconducting states by considering the London equations for the state with inhomogeneous magnetization according to the results from section 3.3.2. Taking into account considerations for the case of tetragonal symmetry (section 2.4.5), we take the variational derivative of (1.6) with respect to the vector potential $\mathbf{A}$. The London equation in the London gauge is

$$\Delta\mathbf{A} - \lambda^{-2}\mathbf{A} = \frac{4\pi}{c}\mathbf{j}_d.$$

For cubic symmetry and the free energy expansion up to the order considered in this chapter, the London penetration depth tensor reduces to a scalar:

$$\lambda^{-2} = \frac{32\pi^2 e^2}{c^2}\left(\gamma_s|\eta_s|^2 + \gamma_p|\eta_p|^2 + 2\gamma_0|\eta_s\eta_p|\right). \tag{3.46}$$

Homogeneous superconductivity in a modulated magnetization

Let us first consider the state of homogeneous superconductivity in the modulated magnetization $\mathbf{m}(\mathbf{r})$ as given by (3.20). This was derived under the assumption of a weak spin-orbit interaction. The London penetration depth is spatially constant in this case. However, the current gains the modulation of the magnetization via the spin-orbit interaction and reads

$$\mathbf{j}_d(\mathbf{r}) = -\frac{8\pi e}{c}\mathbf{m}(\mathbf{r})\left(\zeta_1\kappa_s|\eta_s|^2 + \zeta_1\kappa_p|\eta_p|^2 + 2\kappa_0|\eta_s\eta_p|\right). \tag{3.47}$$

Via this current, superconductivity screens the magnetization (Meissner-Ochsenfeld effect). It invokes a magnetic field which is also in phase with the magnetization

$$\mathbf{B} = -\frac{4\pi}{c}\mathbf{j}_d(\mathbf{r})\frac{k_\oplus}{k_\oplus^2 + \lambda^{-2}}. \tag{3.48}$$

This most efficiently suppresses the modulated magnetization provided the wavelength of magnetic order is the same as London penetration depth $k_\oplus^2 \approx \lambda^{-2}$.

Inhomogeneous superconductivity

An important consequence of the state of inhomogeneous superconductivity is the modulated London penetration depth (3.46). We consider the modulation of η_s only, neglecting η_p as we did in section 3.3.2. The modulation of λ^{-2} has the same period of $2\pi/k_\oplus$ as the modulated magnetization. The positions of maxima and minima are degenerate due to the circular degeneracy of the k_x-k_y-components of the modulated superconductivity wavevector.

As we did in the consideration of tetragonal symmetry, we can only account for the lowest order modulations. These alone provide a sufficiently clear qualitative picture of currents and fields. When $\eta_p = 0$, the current reads

$$\mathbf{j}_d = \frac{4\pi \mathrm{i} e}{c}\gamma_s\left(\eta_s^*\nabla\eta_s - \eta_s\nabla\eta_s^*\right) - \frac{8\pi\zeta_1 e}{c}\kappa_s\mathbf{m}|\eta_s|^2.$$

We use the result (3.39) and obtain the following magnetic field

$$\mathbf{B} = \frac{k_\oplus}{k_\oplus^2 + \tilde{\lambda}^{-2}}\,\frac{\tilde{\lambda}^{-2}}{e}\left[\mathbf{e}_y\cos(k_\oplus z)\sqrt{\frac{2}{\mu}}k_\oplus(\mu-1) - \mathbf{m}(\mathbf{r})\frac{\zeta_1\kappa_s}{\gamma_s}\right],$$

where $\tilde{\lambda}^{-2}$ denotes the homogeneous part of the London penetration depth. The second terms contribution in the square brackets is identical to the homogeneous superconductivity magnetic field (3.48). The additional spin-orbit coupling contribution at lowest modulation order is perpendicular to the modulation of the complex phase in x-direction.

3.4 Summary of chapter 3: Cubic crystal structure

Homogeneous superconductivity: Parity mixing energetically favourable as in tetragonal structure.

Magnetic states:

- *no* homogeneous magnetized phases already for arbitrarily small non-centrosymmetricity.
- inhomogeneous: Magnetic moment spins along a helix, being constant in magnitude.
  - **(1)** propagation parallel to one of the coordinate axes (6-fold degenerate)
  - **(2)** propagation parallel to one of the body diagonals (8-fold degenerate)

Superconductivity in each of the magnetic states:

(1) and (2): Reaction of superconductivity on both inhomogeneous magnetic states equivalent.

Strength of the *MD spin-orbit coupling* and the *wavelength of the magnetization* decide:

small: Homogeneous superconductivity with renormalised parameters. Transition temperature reduced by depairing terms. Supercurrent proportional to the magnetization evoked by MD spin-orbit-coupling terms.

large: Coherent modulation of the phase and the absolute value of the superconductivity order parameters. Phase modulation perpendicular to the propagation direction of the helical magnetization; circular degeneracy. Modulation in absolute value in the propagation direction of the helix with the same wavelength as the magnetization. Additional contributions to the supercurrent from the modulation of the superconductivity order parameter.

CHAPTER 4

Comparison and conclusion of results with a minimal model

In this final chapter we wish to summarize our results. Before doing so, we give a short overview on experimental results for two materials, $CeRhSi_3$ and UIr. Both of them do not entirely fit into the categories of systems that were subject to the analysis in this work. Thus far, a non-centrosymmetric material with cubic or tetragonal structure that shows the coexistence of superconductivity with ferromagnetic order has not been discovered.

Furthermore, we give a minimal model that is capable of mimicking the response of superconductivity on the inhomogeneous magnetic phases as obtained in the previous two chapters. This finally leads us to a comparison of the situations in tetragonal and cubic symmetry, which concludes this work.

4.1 The experimental examples

4.1.1 Tetragonal non-centrosymmetric $CeRhSi_3$

This work dealt with ferromagnetic materials, in a sense that a homogeneous magnetization is the magnetic state of the centrosymmetric system ($\mathbf{k} = 0$). As a consequence of non-centrosymmetricity, we have seen that the ground state is shifted (the cubic case) or might be shifted (the tetragonal case) to finite values of $\mathbf{k}$. Since we determined the ground state from an expansion around $\mathbf{k} = 0$, we still call the modulated states ferromagnetic. Would the expansion had been carried out starting from an antiferromagnetic wavevector (e.g. $\mathbf{k} = (\pi,\pi,\pi)$) a deviating extremum would correspond to an incommensurately antiferromagnetic phase.

Such a magnetic state is found in tetragonal non-centrosymmetric $CeRhSi_3$ [5]. The material has a $BaNiSn_3$-type crystal structure, lacking a mirror plane normal to the c-axis (z-axis in our former coordinate system). Kimura et al. report pressure-induced superconductivity of an anisotropic nature in this material [17]. In the c-axis direction, the ambient pressure alone suffices for superconductivity, whereas for the a-axis superconductivity sets in at 12 kbar [18]. The superconductivity persists up to the highest pressure achieved in the experiments (23 kbar) with increasing critical temperature of up to 1 K. The incommensurate magnetic order already exists at ambient pressure with $T_N = 1.61$ K. T_N increases with pressure up to up to 7.5 kbar and then decreases with increasing pressure. At 22 kbar the magnetic order vanishes, and it seems that T_N and T_c coincide at this point. Up to this pressure the emergence of superconductivity in the magnetically ordered phase is observed ($T_c < T_N$).

The the vector of the magnetization $\mathbf{k} = (\pm 0.215, 0, 0.5)$ is incommensurable along the a-axis only. Neglecting the antiferromagnetism in c-direction, this is the situation that we studied in section 2.4. (Where the crystallographic a-direction coincides with the x-axis.) Our results within the picture of superconductivity nucleation developed in section 2.4.3 might provide us with an understanding of the anisotropy in the onset of superconductivity. In the z-direction, the onset of superconductivity is related to the total loss of resistance, since the Cooper pairs are extended along the stripes as discussed. In the x-direction, however, there is still a finite resistance below T_c, because the Cooper pairs must tunnel between adjacent superconducting stripes. As the stripes melt together and the homogeneous part of the superconductivity order parameter prevails, resistivity also drops in x-direction.

Another outstanding effect observed in $CeRhSi_3$ is a highly anisotropic upper critical field H_{c2} as reported in [16]. Under the case of fields along the a-axis, H_{c2} is moderate. Along the c-axis however, $H_{c2}(T = 0\text{K})$ exceeds values of 30 T within a certain pressure range. Moreover, the $H_{c2}(T)$ curve features a positive curvature in the case of the latter. This can qualitatively be understood from the absence or suppression of paramagnetic limiting in non-centrosymmetric superconductors for fields $H||c$ and $H\perp c$ respectively [12].

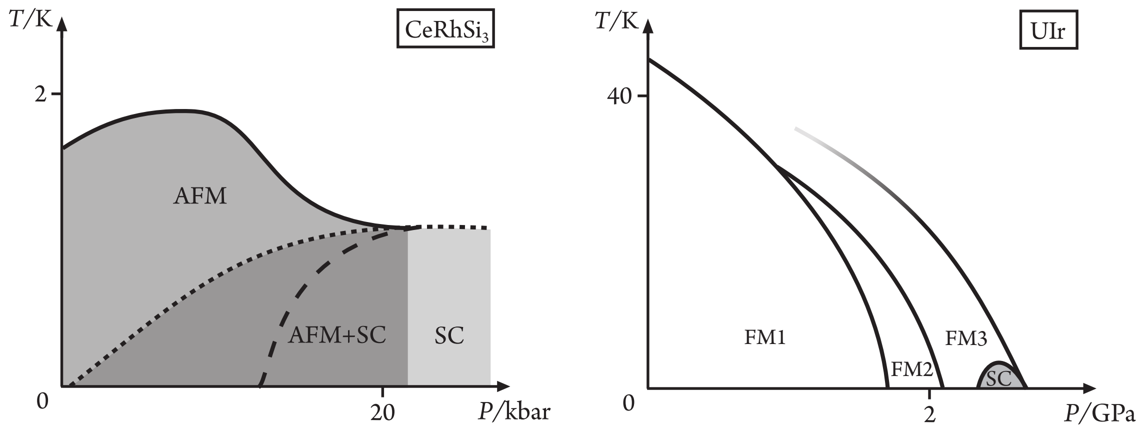

Figure 4.1: Schematic pressure-temperature phase diagrams of $CeRhSi_3$ and UIr based on [18] and [2]. Left: Superconductivity in the phase of incommensurable antiferromagnetism in $CeRhSi_3$ is anisotropic. The critical temperature along the crystallographic c-axis is higher (the dotted line) than the transition temperature along the a-axis (the dashed line). At the pressure where T_c and T_N meet, the antiferromagnetic order vanishes and superconductivity persists. Right: Three distinct ferromagnetic phases are observed in UIr. FM3 fully contains a region of superconductivity next to the quantum-critical point (The value of T_c has been magnified).

4.1.2 Monoclinic non-centrosymmetric UIr

UIr is the sole example of non-centrosymmetric crystal structure in which a coexistence of superconductivity and ferromagnetism was observed [2]. At ambient pressure, the ground state is a truly ferromagnetic phase FM1 with a Curie temperature of $T_{c1} = 46$ K. The itinerant magnetic moments originate from the $5f$-shell of the Uranium and order along the $[10\bar{1}]$ direction. Via the application of pressure, two further ferromagnetic phases, FM2 and FM3, can be induced. FM3 breaks down at a ferromagnetic quantum critical point at a pressure of 2.8 GPa. The phase fully contains a region where the material becomes superconducting with a critical temperature always less than 1 K. While the quantum critical point features a first-order phase transition, the transition between the phases FM1 and FM2 is of first order and is accompanied by a strong drop in the magnetic moment.
Not much is known about the superconducting phase so far. Despite from the fact that the crystal symmetry is a different one, we thus cannot draw parallels to the results of our calculations.

4.2 A minimal model

In this section we discuss a toy model to study the influence of the magnetic states on superconductivity. This model should be capable of illustrating the shape of the superconductivity phase correctly, and at the same time involve fewer parameters than those in our strictly derived description.

We recall that the order parameters of superconductivity η_s and η_p are related to the spin-singlet and spin-triplet configuration of the Cooper pairs. As pointed out in the introduction 1.3.3, non-centrosymmetricity is accompanied by the meaninglessness of this classification. Accordingly, we could think of one order parameter $\eta = \eta_s + \eta_p$. This quantity can however not be used in an Ginzburg-Landau expansion of the free energy since it has no defined parity. Thus we so far used two parameters η_s and η_p with defined (positive and negative) parity.

In order to simplify the calculation we shall now use a single order parameter η with mixed symmetry. Consequently, we have to allow for terms of both symmetries in the free energy. The variables ζ_z and ζ_1 were introduced so as to aid in the balancing of negative parity terms and are no longer needed in this case. Because η can be split up into a term belonging to Γ_2^- and one of Γ_1^+ in tetragonal systems, we have to allow for terms of mixed Γ_1^+-Γ_2^--symmetry. For cubic crystals we permit for mixed Γ_1^+-Γ_1^--symmetry. With this simplification we lose the the information on the mixing ratio of both symmetry parts. This is not a critical loss, as all our calculations showed that η_s and η_p share coherent behaviour.

4.2.1 Tetragonal symmetry

With our mixed order parameter the expansion of the free energy functional takes the form (as before, a vector with index $\perp$ has only x and y component):

$$\begin{aligned} f_{sc} + f_{coupling} =& a|\eta|^2 + b|\eta|^4 + \gamma_\perp |\mathbf{D}_\perp \eta|^2 + \gamma_z |D_z\eta|^2 + \delta(\eta D_z^* \eta^* + \eta^* D_z \eta) \\ & h_\perp \mathbf{m}_\perp^2 |\eta|^2 + h_z m_z^2 |\eta|^2 + \mathrm{i}\kappa (\mathbf{e}_z \times \mathbf{m}) \cdot (\eta \mathbf{D}_\perp^* \eta^* + \eta^* \mathbf{D}_\perp \eta) + \nu \mathbf{m}_\perp^2 (\eta D_z^* \eta^* + \eta^* D_z \eta) + \\ & \rho m_z \mathbf{m}_\perp \cdot (\eta \mathbf{D}_\perp^* \eta^* + \eta^* \mathbf{D}_\perp \eta) + \sigma m_z^2 (\eta D_z^* \eta^* + \eta^* D_z \eta) \end{aligned} \tag{4.1}$$

With $a = a'(T - T_c)$, where T_c is the transition temperature of homogeneous superconductivity in the absence of a magnetically ordered state. In absence of a magnetic field, the variational derivative of the free energy is

$$\begin{aligned}0 =& a\eta + 2b\eta^*\eta^2 - \gamma_\perp\nabla_\perp^2\eta - \gamma_z\nabla_z^2\eta + h_\perp\mathbf{m}_\perp^2\eta + h_z m_z^2\eta - \\ & \mathrm{i}\kappa\left((\mathbf{e}_z\times\mathbf{m})\cdot\nabla_\perp\eta + \nabla_\perp\cdot(\mathbf{e}_z\times\mathbf{m})\eta\right) - \nu\eta\nabla_z\mathbf{m}_\perp^2 - \rho\eta\nabla_\perp\cdot\mathbf{m}_\perp m_z - \sigma\eta\nabla_z m_z^2.\end{aligned} \tag{4.2}$$

We are now only interested in the impact of one of the two equivalent modulated magnetic phases of the material:

$$\mathbf{m} = m_0\left(\mathbf{e}_z\cos k_\ominus x + \mathbf{e}_x M_\ominus \sin k_\ominus x\right) \tag{4.3}$$

We neglect spin-orbit interaction ($\kappa = 0$) and assume that there will be no modulations in neither the y- nor the z-direction. With this magnetization inserted, the variation equation becomes a differential equation for $\eta(x')$ in the variable $x' = k_\ominus x$:

$$\boxed{0 = \eta'' + \bar{a}\eta + 2w\cos(2x')\eta} \tag{4.4}$$

Where we defined

$$\bar{a} = -\frac{a + m_0^2\left(\frac{h_\perp M_\ominus^2}{2} + \frac{h_z}{2}\right)}{\gamma_\perp k_\ominus^2} \qquad w = \frac{m_0^2}{2\gamma_\perp k_\ominus^2}\left(\rho k_\ominus M_\ominus + \frac{h_\perp M_\ominus^2}{2} - \frac{h_z}{2}\right) \tag{4.5}$$

Equation (4.4) is Mathieu's differential equation which was already discussed in the introductory chapter 1.5.2 and mentioned in chapter 2. The general solution is a linear combination of Mathieu-Sine S and Mathieu-Cosine C. However, Mathieu's differential equation does not have stable (i.e. bounded) solutions for all values of $\bar{a}$ and w. We numerically calculated a stability diagram shown in figure 4.2. For fixed magnetization, w is *not* temperature dependent and the system follows a straight line parallel to the $\bar{a}$-axis as temperature decreases. The first intersection of this line with the region of stability defines the superconductivity transition temperature T^*. It is at the boundary of the stability region, where $\bar{a}$ and w take characteristic values, and the solution is periodic (see 1.5.2). We can use the expansions given by (1.13) and (1.14) to determine the transition temperature and the approximate solution:

$$T^* = T_c - \frac{m_0^2}{2a'}\left(h_\perp M_\ominus^2 + h_z\right) + \frac{m_0^4}{8\gamma_\perp k_\ominus^2 a'}\left(\rho k_\ominus M_\ominus + \frac{h_\perp M_\ominus^2}{2} - \frac{h_z}{2}\right)^2 \tag{4.6}$$

$$\eta(x) = \eta_0\left[1 + \frac{m_0^2}{4\gamma_\perp k_\ominus^2}\left(\rho k_\ominus M_\ominus + \frac{h_\perp M_\ominus^2}{2} - \frac{h_z}{2}\right)\cos(2k_\ominus x)\right] \tag{4.7}$$

We recover the temperature dependence with negative m_0^2- and positive m_0^4-term as calculated in 2.4.1 and sketched in figure 2.3. The superconductivity order parameter has the same spatial modulation as $\eta_s + \eta_p$ according to (2.69). Compared to the result from the previous scenario of chapter 2, the fact that parity information is lost is clearly visible at this point. Apart from this, we obtain modulated superconductivity in strong agreement with the results from the full description model.

4.2.2 Cubic symmetry

Let us further apply the toy model to the case of cubic symmetry. Here we are required to take the MD spin-orbit interaction into account in order to correctly describe the reaction of superconductivity to the modulated magnetization. The simplified expansion of the free energy functional reads:

$$f_{sc} + f_{coupling} = a|\eta|^2 + b|\eta|^4 + \gamma|\mathbf{D}\eta|^2 + h\mathbf{m}^2|\eta|^2 + \mathrm{i}\kappa\left(\eta^*\mathbf{m}\cdot\mathbf{D}\eta - \eta\mathbf{m}\cdot\mathbf{D}^*\eta^*\right) \tag{4.8}$$

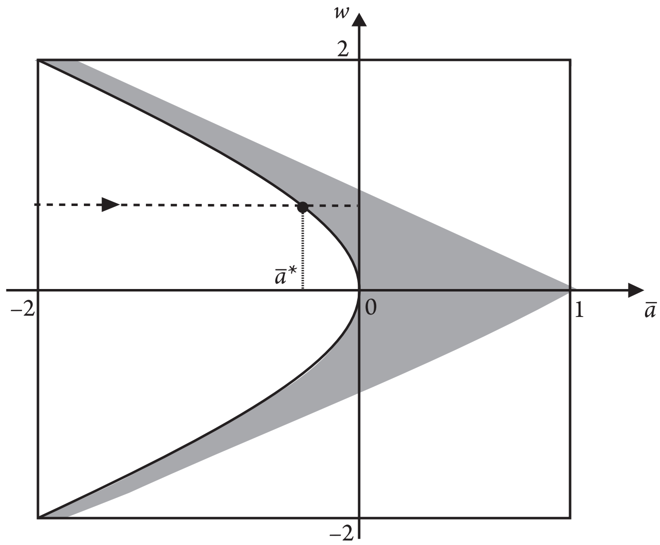

Figure 4.2: Zoomed-in portion of the zeroth order stability region of Mathieu's equation. The parameter w is essentially proportional to the magnetization, while $\bar{a}$ is an affine function of temperature. In the case of tetragonal symmetry, the diagram allows for the following interpretation: As the temperature is lowered, a system with fixed magnetization evolves along a line parallel to the $\bar{a}$-axis, as indicated by the dashed line. The critical temperature T^* is defined by the value $\bar{a}^*$, at the point where this line first hits the region of stability (dot): $T^* = T_c - \gamma_\perp k_\ominus^2 \frac{\bar{a}^*}{a'} - \frac{m_0^2}{a'}\left(\frac{h_\perp M_\ominus^2}{2} + \frac{h_z}{2}\right)$

Correspondingly, the variation equations are in absence of an external magnetic field (neglecting the fourth order term):

$$0 = a\eta + h\mathbf{m}^2\eta - \gamma\nabla^2\eta + 2\mathrm{i}\kappa\mathbf{m}\cdot\nabla\eta. \tag{4.9}$$

We wish to study superconductivity in presence of one of the two equivalent magnetizations we found for cubic symmetry:

$$\mathbf{m} = m_0\left(\sin(k_\oplus z)\mathbf{e}_x + \cos(k_\oplus z)\mathbf{e}_y\right) \tag{4.10}$$

If we Fourier transform the equation with this magnetization in the x- and y-direction, the resulting differential equation is

$$\boxed{0 = \nabla_{z'}^2\eta(k_x,k_y,z') + \bar{a}\eta(k_x,k_y,z') + 2w\cos\left(2z'\right)\eta(k_x,k_y,z')}\,. \tag{4.11}$$

We also transformed the z-coordinate, and introduced the following abbreviations:

$$\bar{a} = -4\frac{a + hm_0^2 + \gamma(k_x^2+k_y^2)}{\gamma k_\oplus^2} \qquad w = \frac{4\kappa m_0}{\gamma k_\oplus^2}\sqrt{k_x^2+k_y^2}$$

$$z' = \frac{k_\oplus z}{2} - \frac{1}{2}\arctan\frac{k_y}{k_x} - \frac{\pi}{4} \tag{4.12}$$

This is once again the canonical from of Mathieu's equation in the variable z'. Contrary to the example of tetragonal symmetry discussed in the previous section, $\bar{a}$ and w are not independent from one another. Rather, both depend on $k \equiv \sqrt{k_x^2 + k_y^2}$. Thus we have a circular degeneracy in the k_x-k_y-plane and a parametric function $\bar{a}(w)$ is defined, corresponding to a parabola in the stability diagram, which is characteristic for every temperature:

$$\bar{a}(w) = -\left(\frac{\gamma k_\oplus w}{2\kappa m_0}\right)^2 - 4\frac{a'(T - T_c) + hm_0^2}{\gamma k_\oplus^2} \tag{4.13}$$

To calculate which value of k and which transition temperature is favoured we compare this parabola with the shape of the stability region in diagram 4.3. As temperature is lowered, the parabola (4.13) approaches the zeroth order branch of the stability region from the left. Since the asymptotic behaviour of $a_0(w)$ is linear while $\bar{a}(w)$ is a quadratic function, there will always be a temperature at which the two curves touch. This defines the superconductivity transition temperature. There are two possible cases:

- If the quadratic expansion of $a_0(w)$ has a *smaller* coefficient than that of $\bar{a}(w)$, the transition will occur at $w = 0$. Because $k = 0$, this will correspond to a homogeneous superconducting state with a transition temperature $T^* = T_c - hm_0^2/a'$. The parameter value k that belongs to the contact point determines the x-y-modulation of the state.

- If on the other hand a touching point at $w \neq 0$ exists, an inhomogeneous state has a higher transition temperature.

From the expansion (1.13) of the stability region we obtained the following threshold as a condition for this:

$$\boxed{1 < \mu \equiv \frac{2\kappa^2 m_0^2}{\gamma^2 k_\oplus^2}} \tag{4.14}$$

This result is in good agreement with (3.32). We can now use the expansions (1.13) and (1.14) to calculate the transition temperature and the spatial modulation of superconductivity. The favoured value of k is

$$k = \frac{2k_\oplus}{\sqrt{7}}\sqrt{\frac{1}{\mu} - \frac{1}{\mu^2}} \tag{4.15}$$

To lift the degeneracy we choose without loss of generality $k_x = k$ and $k_y = 0$. Then

$$\begin{aligned} T &= T_c - \frac{m_0^2 h}{2a'} + \frac{2\gamma k_\oplus}{7a'}\left(1 - \frac{1}{\mu}\right)^2 = T_c - \frac{m_0^2 h}{2a'} + \frac{\gamma^2 k_\oplus^4}{14a'\kappa^4 m_0^4}\left(\gamma^2 k_\oplus^2 - 2\kappa^2 m_0^2\right) \\ \eta(x,z) &= \eta_0 \exp\left[\mathrm{i}\frac{2k_\oplus}{\sqrt{7}}\sqrt{\frac{1}{\mu} - \frac{1}{\mu^2}}\,x\right]\left\{1 + \frac{4}{\sqrt{14}}\sqrt{1 - \frac{1}{\mu}}\sin(k_\oplus z)\right\} \end{aligned} \tag{4.16}$$

This result strongly resembles our previous findings (3.39): It shows an amplitude modulation in the z-direction and a phase-modulation perpendicular to the z-direction. The slight change in the μ-dependence does not affect the lowest order expansion in μ around 1.

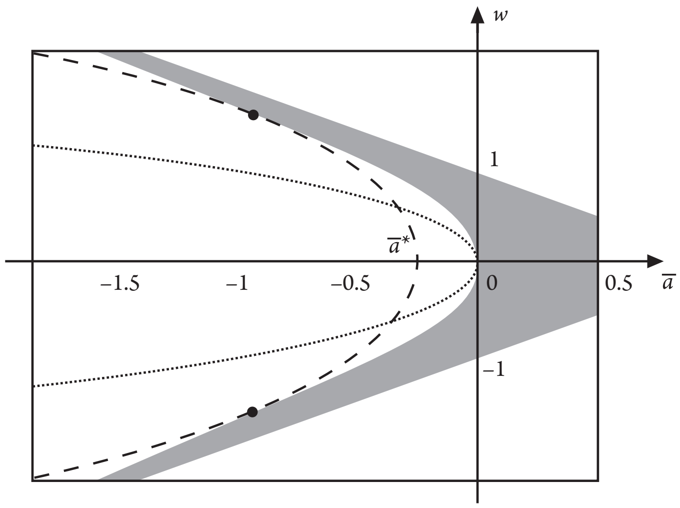

Figure 4.3: Zoomed-in region of the stability diagram of Mathieu's equation. Equation (4.12) defines a parabola $\bar{a}(w)$ which is parametrised by k. The curvature of this curve is given by the magnetization and the temperature-independent phenomenological parameters. As temperature decreases, the parabola migrates from left to right. The transition temperature is reached when the parabola touches the region of stability (dots on dashed curve) and defined by the intersection of this parabola with the $\bar{a}$-axis, $\bar{a}^*$. The k-value of the state is given by the position of the contact point (dot). If the curvature of the parabola at $k = 0$ is larger than that of the stability region (dotted line), there will be no contact with the region of stability until the transition to the homogeneous state $\bar{a} = 0$, $k = 0$.

4.3 Comparison of results from tetragonal and cubic symmetry

Naively one could think that the case of cubic symmetry is just a special case of tetragonal systems, where certain parameters are identified with one another (e.g. $T_{c1} = T_{c2}$ for magnetism). Thus one might not expect qualitative differences in the results. We nevertheless studied both cases independently because of the quite different way we introduced non-centrosymmetricity. In tetragonal symmetry, parity is violated in z-direction only. For cubic systems we assumed to find parity violation in all spatial directions isotropically.

At first, we determined the conditions under which homogeneous superconductivity can exist. They are very similar in both cases. The consequence of non-centrosymmetricity is parity mixing: Since the mixed state has a higher transition temperature, it is impossible to have either pure singlet or pure triplet superconductivity. Both order parameters are either in phase or have a phase-shift of π with respect to one another. Furthermore, we found indications for an upper bound to the strength of non-centrosymmetricity if we require to have a stable superconducting state.

We then determined the magnetic states of both systems. In tetragonal structure, there are four distinct magnetic phases to be found, two of which are homogeneous (z-direction or degenerate in x-y-plane) and two of which are modulated. The latter are such that the magnetization is always parallel to a plane which contains the modulation wavevector. The non-centrosymmetric cubic system on the other hand shows no homogeneous magnetic phase, but shows two modulated ones. Both are helical states, the first with propagation direction along a coordinate axis and the second with propagation direction along a body diagonal. In each of the systems the two modulated magnetic phases are equivalent under a suitable coordinate transformation.

The final step was to study how superconductivity develops, given one of these magnetic phases. The primary impact of homogeneous phases is a renormalisation of the phenomenological expansion parameters. In consequence, these homogeneous phases reduce the transition temperature and alter the mixing ratio. A more important repercussion is the action of the spin-orbit coupling in tetragonal symmetry for a homogeneous magnetization in the x-y-plane. This leads to inhomogeneous superconductivity with phase modulation in the x-y-plane perpendicular to the magnetization.

The inhomogeneous magnetic phases lead to qualitatively different responses: In cubic symmetry, the impact is either renormalised homogeneous superconductivity or a modulation both in the phase and the absolute value of the order parameter. The strength of the MD spin-orbit coupling and the wavelength of the magnetic modulations decide which of these states is realised. In tetragonal systems with the according modulated magnetic state, superconductivity always turns to an inhomogeneous state, where the absolute magnitude of the order parameter changes in space. Additionally, a modulation of the complex phase is obtained for a sufficiently strong spin-orbit coupling. Consequently, the London penetration depth is also modulated in these systems. Directly below T_c, the superconducting phase is expected to emerge in a stripe-like shape.

The expansions of the free energy were symmetric in the order parameter of singlet and triplet states. In all calculations, we assumed that the transition temperature of singlet superconductivity is higher than the one of triplet superconductivity. If this is not the case, all results remain valid if the subscripts s and p are interchanged.

Finally, we considered a simplified model that well resembled the reaction of superconductivity to modulated magnetic states. The price we pay in allowing for symmetry-mixed terms in the free energy expansion is the loss of parity mixing information.

A prospective line of study in this field is the analysis of the interplay of superconductivity and antiferromagnetic magnetic order. We do not recommend taking multidimensional representations of the order parameters η_s and η_p into account, as this would promote the complexity of the equations to an unacceptable level. However, in the framework of the simplified model a multidimensional order parameter η of mixed parity might clear the way for the exploration of diverse superconductivity phases.

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APPENDIX A

Higher dimensional superconductivity order parameters

In the course of this work, we also considered to analyse superconductivity in non-centrosymmetric cubic and tetragonal systems with order parameters out of a higher than one-dimensional irreducible representation of the point group. The expansion of the free energy is given below for some examples, without the coupling terms to a magnetic field or given magnetization. However, they were no subject to further investigation.

A.1 Tetragonal crystal symmetry: Two-dimensional order parameters $\vec{\eta}_s(\Gamma_5^+)$ and $\vec{\eta}_p(\Gamma_5^-)$

$$
\begin{aligned}
f_{sc} \quad = \quad & a_s\left|\vec{\eta}_s\right|^2 + a_p\left|\vec{\eta}_p\right|^2 + \\
& b_{s,1}\left|\vec{\eta}_s\right|^4 + b_{s,2}\left|\eta_{s,x}\eta^*_{s,y} + \eta_{s,y}\eta^*_{s,x}\right|^2 + b_{s,3}\left|\eta_{s,x}\eta^*_{s,x} - \eta_{s,y}\eta^*_{s,y}\right|^2 + \\
& b_{p,1}\left|\vec{\eta}_p\right|^4 + b_{p,2}\left|\eta_{p,x}\eta^*_{p,y} + \eta_{p,y}\eta^*_{p,x}\right|^2 + b_{p,3}\left|\eta_{p,x}\eta^*_{p,x} - \eta_{p,y}\eta^*_{p,y}\right|^2 + \\
& c_1\left|\vec{\eta}_s\right|^2\left|\vec{\eta}_p\right|^2 + c_2\left(\vec{\eta}_s{}^{*2}\vec{\eta}_p{}^2 + \vec{\eta}_s{}^2\vec{\eta}_p{}^{*2}\right) + c_3\left|\vec{\eta}_s\cdot\vec{\eta}_p{}^*\right|^2 + \\
& c_4\left(\eta_{s,x}\eta^*_{s,x} - \eta_{s,y}\eta^*_{s,y}\right)\left(\eta_{p,x}\eta^*_{p,x} - \eta_{p,y}\eta^*_{p,y}\right) + c_5\left|\eta^*_{s,x}\eta_{p,y} - \eta^*_{s,y}\eta_{p,x}\right|^2 + \\
& d\zeta_z\left(\eta^*_{s,x}\eta_{p,y} - \eta^*_{s,y}\eta_{p,x} + \eta_{s,x}\eta^*_{p,y} - \eta_{s,y}\eta^*_{p,x}\right) + \\
& \gamma_{s,1}\left(D_x\vec{\eta}_s\left(D_x\vec{\eta}_s\right)^* + D_y\vec{\eta}_s\left(D_y\vec{\eta}_s\right)^*\right) + \gamma_{s,2}D_z\vec{\eta}_s\left(D_z\vec{\eta}_s\right)^* + \gamma_{s,3}\left|D^*_x\eta_{s,x} + D^*_y\eta_{s,y}\right|^2 + \\
& \gamma_{s,4}\left(D_x\eta_{s,x}D^*_x\eta^*_{s,x} - D_x\eta_{s,y}D^*_x\eta^*_{s,y} + D_y\eta_{s,x}D^*_y\eta^*_{s,x} - D_y\eta_{s,y}D^*_y\eta^*_{s,y}\right) + \\
& \gamma_{s,5}\left|D^*_y\eta_{s,x} - D^*_x\eta_{s,y}\right|^2 + \\
& \gamma_{p,1}\left(D_x\vec{\eta}_p\left(D_x\vec{\eta}_p\right)^* + D_y\vec{\eta}_p\left(D_y\vec{\eta}_p\right)^*\right) + \gamma_{p,2}D_z\vec{\eta}_p\left(D_z\vec{\eta}_p\right)^* + \gamma_{p,3}\left|D^*_x\eta_{p,x} + D^*_y\eta_{p,y}\right|^2 + \\
& \gamma_{p,4}\left(D_x\eta_{p,x}D^*_x\eta^*_{p,x} - D_x\eta_{p,y}D^*_x\eta^*_{p,y} + D_y\eta_{p,x}D^*_y\eta^*_{p,x} - D_y\eta_{p,y}D^*_y\eta^*_{p,y}\right) + \\
& \gamma_{p,5}\left|D^*_y\eta_{p,x} - D^*_x\eta_{p,y}\right|^2 + \\
& \delta_1\zeta_z\left(D^*_x\eta^*_{s,x}D_x\eta_{p,y} - D^*_x\eta^*_{s,y}D_x\eta_{p,x} + D_x\eta_{s,x}D^*_x\eta^*_{p,y} - D_x\eta_{s,y}D^*_x\eta^*_{p,x} + \right. \\
& \quad \left. D^*_y\eta^*_{s,x}D_y\eta_{p,y} - D^*_y\eta^*_{s,y}D_y\eta_{p,x} + D_y\eta_{s,x}D^*_y\eta^*_{p,y} - D_y\eta_{s,y}D^*_y\eta^*_{p,x}\right) + \\
& \delta_2\zeta_z\left(D^*_z\eta^*_{s,x}D_z\eta_{p,y} - D^*_z\eta^*_{s,y}D_z\eta_{p,x} + D_z\eta_{s,x}D^*_z\eta^*_{p,y} - D_z\eta_{s,y}D^*_z\eta^*_{p,x}\right)
\end{aligned}
$$

A.2 Cubic crystal symmetry: Two-dimensional order parameters $\vec{\eta}_s(\Gamma_3^+)$ and $\vec{\eta}_p(\Gamma_3^-)$

$$
\begin{aligned}
f_{hom} = \; & a_s\left|\vec{\eta}_s\right|^2 + a_p\left|\vec{\eta}_p\right|^2 + \\
& b_{s,1}\left|\vec{\eta}_s\right|^4 + b_{s,2}\left|\eta_{s,x}\eta^*_{s,y} - \eta_{s,y}\eta^*_{s,x}\right|^2 + b_{p,1}\left|\vec{\eta}_p\right|^4 + b_{p,2}\left|\eta_{p,x}\eta^*_{p,y} - \eta_{p,y}\eta^*_{p,x}\right|^2 + \\
& c_1\left|\vec{\eta}_s\right|^2\left|\vec{\eta}_p\right|^2 + c_2\left(\vec{\eta}_s^{\,*2}\vec{\eta}_p^{\,2} + \vec{\eta}_s^{\,2}\vec{\eta}_p^{\,*2}\right) + c_3\left|\vec{\eta}_s\cdot\vec{\eta}_p^{\,*}\right|^2 + \\
& c_4\left(\left(\eta_{s,x}\eta^*_{s,x} - \eta_{s,y}\eta^*_{s,y}\right)\left(\eta_{p,x}\eta^*_{p,x} - \eta_{p,y}\eta^*_{p,y}\right) + \left(\eta^*_{s,x}\eta_{s,y} + \eta^*_{s,y}\eta_{s,x}\right)\left(\eta^*_{p,x}\eta_{p,y} + \eta^*_{p,y}\eta_{p,x}\right)\right) + \\
& d\zeta_1\left(\eta_{s,x}\eta^*_{p,x} + \eta_{s,y}\eta^*_{p,y} + \eta^*_{s,x}\eta_{p,x} + \eta^*_{s,y}\eta_{p,y}\right) + \\
& \gamma_{s,1}\left|\vec{\eta}_s\right|^2\left|\vec{D}\right|^2 + \gamma_{s,2}\left(\left|\left(\sqrt{3}\eta_{s,y} - \eta_{s,x}\right)D_x\right|^2 + \left|\left(\sqrt{3}\eta_{s,y} + \eta_{s,x}\right)D_y\right|^2 + \left|2\eta_{s,x}D_z\right|^2\right) + \\
& \gamma_{s,3}\left[\left(|D_z|^2 - \frac{1}{2}|D_x|^2 - \frac{1}{2}\left|D_y\right|^2\right)\left(\left|\eta_{s,y}\right|^2 - \left|\eta_{s,x}\right|^2\right) + \right. \\
& \left. \frac{2}{\sqrt{3}}\left(|D_x|^2 + \left|D_y\right|^2\right)\left(\eta_{s,x}\eta^*_{s,y} + \eta^*_{s,x}\eta_{s,y}\right)\right] + \\
& \gamma_{p,1}\left|\vec{\eta}_p\right|^2\left|\vec{D}\right|^2 + \gamma_{p,2}\left(\left|\left(\sqrt{3}\eta_{p,y} - \eta_{p,x}\right)D_x\right|^2 + \left|\left(\sqrt{3}\eta_{p,y} + \eta_{p,x}\right)D_y\right|^2 + \left|2\eta_{p,x}D_z\right|^2\right) + \\
& \gamma_{p,3}\left[\left(|D_z|^2 - \frac{1}{2}|D_x|^2 - \frac{1}{2}\left|D_y\right|^2\right)\left(\left|\eta_{p,y}\right|^2 - \left|\eta_{p,x}\right|^2\right) + \right. \\
& \left. \frac{2}{\sqrt{3}}\left(|D_x|^2 + \left|D_y\right|^2\right)\left(\eta_{p,x}\eta^*_{p,y} + \eta^*_{p,x}\eta_{p,y}\right)\right] + \\
& \delta_1\zeta_1\left(\eta_{s,x}\eta^*_{p,x} + \eta_{s,y}\eta^*_{p,y} + \eta^*_{s,x}\eta_{p,x} + \eta^*_{s,y}\eta_{p,y}\right)\left|\vec{D}\right|^2 + \\
& \delta_2\zeta_1\left[\left(\left(\sqrt{3}\eta_{s,y} - \eta_{s,x}\right)\left(\sqrt{3}\eta^*_{p,y} - \eta^*_{p,x}\right)|D_x|^2 + \right.\right. \\
& \left.\left. \left(\sqrt{3}\eta_{s,y} + \eta_{s,x}\right)\left(\sqrt{3}\eta^*_{p,y} + \eta^*_{p,x}\right)\left|D_y\right|^2 + 4\eta_{s,x}\eta^*_{p,x}|D_z|^2\right) + \text{c.c.}\right] + \\
& \delta_3\zeta_1\left[\left(|D_z|^2 - \frac{1}{2}|D_x|^2 - \frac{1}{2}\left|D_y\right|^2\right)\left(\eta_{s,y}\eta^*_{p,y} - \eta_{s,x}\eta^*_{p,x} + \eta^*_{s,y}\eta_{p,y} - \eta^*_{s,x}\eta_{p,x}\right) + \right. \\
& \left. \frac{2}{\sqrt{3}}\left(|D_x|^2 + \left|D_y\right|^2\right)\left(\eta_{s,x}\eta^*_{p,y} + \eta^*_{p,x}\eta_{s,y} + \eta^*_{s,x}\eta_{p,y} + \eta_{p,x}\eta^*_{s,y}\right)\right]
\end{aligned}
$$

A.3 Cubic crystal symmetry: Three-dimensional order parameters $\vec{\eta}_s(\Gamma_5^+)$ and $\vec{\eta}_p(\Gamma_5^-)$

$$
\begin{aligned}
f_{hom} \;=\;& a_s \left|\vec{\eta}_s\right|^2 + a_p \left|\vec{\eta}_p\right|^2 + \\
& b_{s,1} \left|\vec{\eta}_s\right|^4 + b_{s,2} \left|\vec{\eta}_s{}^2\right|^2 + b_{s,3} \left(\left|\eta_{s,x}\right|^2 \left|\eta_{s,y}\right|^2 + \left|\eta_{s,y}\right|^2 \left|\eta_{s,z}\right|^2 + \left|\eta_{s,z}\right|^2 \left|\eta_{s,x}\right|^2 \right) + \\
& b_{p,1} \left|\vec{\eta}_p\right|^4 + b_{p,2} \left|\vec{\eta}_p{}^2\right|^2 + b_{p,3} \left(\left|\eta_{p,x}\right|^2 \left|\eta_{p,y}\right|^2 + \left|\eta_{p,y}\right|^2 \left|\eta_{p,z}\right|^2 + \left|\eta_{p,z}\right|^2 \left|\eta_{p,x}\right|^2 \right) + \\
& c_1 \left|\vec{\eta}_s\right|^2 \left|\vec{\eta}_p\right|^2 + c_2 \left(\vec{\eta}_s{}^{*2} \vec{\eta}_p{}^2 + \vec{\eta}_s{}^2 \vec{\eta}_p{}^{*2} \right) + c_3 \left|\vec{\eta}_s \times \vec{\eta}_p\right|^2 + \\
& c_4 \left|\vec{\eta}_s \cdot \vec{\eta}_p\right|^2 + c_5 \left|\vec{\eta}_s \star \vec{\eta}_p\right|^2 d\zeta_1 \left(\vec{\eta}_s{}^* \cdot \vec{\eta}_p + \vec{\eta}_s \cdot \vec{\eta}_p{}^* \right) + \\
& \gamma_{s,1} \sum_{i,j=1}^{3} D_i^* \eta_{s,j}^* D_i \eta_{s,j} + \gamma_{s,2} \left|\vec{D} \cdot \vec{\eta}_s\right|^2 + \gamma_{s,3} \left|\vec{D} \star \vec{\eta}_s\right|^2 + \gamma_{s,4} \left|\vec{D} \times \vec{\eta}_s\right|^2 + \gamma_{s,5} \left|\vec{D} \mathbin{\scriptstyle\blacksquare} \vec{\eta}_s\right|^2 + \\
& \gamma_{p,1} \sum_{i,j=1}^{3} D_i^* \eta_{p,j}^* D_i \eta_{p,j} + \gamma_{p,2} \left|\vec{D} \cdot \vec{\eta}_p\right|^2 + \gamma_{p,3} \left|\vec{D} \star \vec{\eta}_p\right|^2 + \gamma_{p,4} \left|\vec{D} \times \vec{\eta}_p\right|^2 + \gamma_{p,5} \left|\vec{D} \mathbin{\scriptstyle\blacksquare} \vec{\eta}_p\right|^2 + \\
& \delta_1 \zeta_1 \sum_{i,j=1}^{3} \left(D_i^* \eta_{s,j}^* D_i \eta_{p,j} + D_i \eta_{s,j} D_i^* \eta_{p,j}^* \right) + \\
& \delta_2 \zeta_1 \left(\left(\vec{D} \cdot \vec{\eta}_s\right) \left(\vec{D} \cdot \vec{\eta}_p\right)^* + \left(\vec{D} \cdot \vec{\eta}_s\right)^* \left(\vec{D} \cdot \vec{\eta}_p\right) \right) + \\
& \delta_3 \zeta_1 \left(\left(\vec{D} \star \vec{\eta}_s\right) \cdot \left(\vec{D} \star \vec{\eta}_p\right)^* + \left(\vec{D} \star \vec{\eta}_s\right)^* \cdot \left(\vec{D} \star \vec{\eta}_p\right) \right) + \\
& \delta_4 \zeta_1 \left(\left(\vec{D} \times \vec{\eta}_s\right) \cdot \left(\vec{D} \times \vec{\eta}_p\right)^* + \left(\vec{D} \times \vec{\eta}_s\right)^* \cdot \left(\vec{D} \times \vec{\eta}_p\right) \right) + \\
& \delta_5 \zeta_1 \left(\left(\vec{D} \mathbin{\scriptstyle\blacksquare} \vec{\eta}_s\right) \cdot \left(\vec{D} \mathbin{\scriptstyle\blacksquare} \vec{\eta}_p\right)^* + \left(\vec{D} \mathbin{\scriptstyle\blacksquare} \vec{\eta}_s\right)^* \cdot \left(\vec{D} \mathbin{\scriptstyle\blacksquare} \vec{\eta}_p\right) \right)
\end{aligned}
$$

APPENDIX B

Coupling of superconductivity and magnetic order

The calculations of chapters 2 and 3 are based on expansions of $f_{coupling}$ up to the order "$m^2 D\eta^2$". Higher order terms have been derived, but were not used in the calculations because they do not give rise to qualitatively different behavior and further complicate the equations. For homogeneously magnetized states, their impact is a renormalization of other parameters.
The expansions are only given for the one-dimensional representations of the order parameters η_s and η_p used in this work.

B.1 Tetragonal crystal symmetry

$$
\begin{aligned}
f_{coupling} \;=\;& h_{s,\perp}\mathbf{m}_\perp^2\left|\eta_s\right|^2 + h_{s,z}m_z^2\left|\eta_s\right|^2 + h_{p,\perp}\mathbf{m}_\perp^2\left|\eta_p\right|^2 + h_{p,z}m_z^2\left|\eta_p\right|^2 + \\
& \nu_\perp\zeta_z\mathbf{m}_\perp^2\left(\eta_s\eta_p^* + \eta_p\eta_s^*\right) + \nu_z\zeta_z m_z^2\left(\eta_s\eta_p^* + \eta_p\eta_s^*\right) + \\
& \mathrm{i}\kappa_s\zeta_z\left(\mathbf{e}_z\times\mathbf{m}\right)\cdot\left(\eta_s\left(\mathbf{D}_\perp\eta_s\right)^* - \eta_s^*\mathbf{D}_\perp\eta_s\right) + \mathrm{i}\kappa_p\zeta_z\left(\mathbf{e}_z\times\mathbf{m}\right)\cdot\left(\eta_p\left(\mathbf{D}_\perp\eta_p\right)^* - \eta_p^*\mathbf{D}_\perp\eta_p\right) + \\
& \mathrm{i}\kappa_0\left(\mathbf{e}_z\times\mathbf{m}\right)\cdot\left(\eta_s\left(\mathbf{D}_\perp\eta_p\right)^* - \eta_s^*\mathbf{D}_\perp\eta_p + \eta_p\left(\mathbf{D}_\perp\eta_s\right)^* - \eta_p^*\mathbf{D}_\perp\eta_s\right) + \\
& \nu_0\mathbf{m}_\perp^2\left(\eta_s D_z^*\eta_p^* + \eta_s^* D_z\eta_p\right) + \nu_p\zeta_z\mathbf{m}_\perp^2\left(\eta_p D_z^*\eta_p^* + \eta_p^* D_z\eta_p\right) + \\
& \nu_s\zeta_z\mathbf{m}_\perp^2\left(\eta_s D_z^*\eta_s^* + \eta_s^* D_z\eta_s\right) + \rho_0 m_z\mathbf{m}_\perp\left(\eta_s\mathbf{D}_\perp^*\eta_p^* + \eta_s^*\mathbf{D}_\perp\eta_p + \eta_p\mathbf{D}_\perp^*\eta_s^* + \eta_p^*\mathbf{D}_\perp\eta_s\right) + \\
& \rho_s\zeta_z m_z\mathbf{m}_\perp\left(\eta_s\mathbf{D}_\perp^*\eta_s^* + \eta_s^*\mathbf{D}_\perp\eta_s\right) + \rho_p\zeta_z m_z\mathbf{m}_\perp\left(\eta_p\mathbf{D}_\perp^*\eta_p^* + \eta_p^*\mathbf{D}_\perp\eta_p\right) + \\
& \sigma_0 m_z^2\left(\eta_s D_z^*\eta_p^* + \eta_s^* D_z\eta_p\right) + \sigma_s\zeta_z m_z^2\left(\eta_s D_z^*\eta_s^* + \eta_s^* D_z\eta_s\right) + \sigma_p\zeta_z m_z^2\left(\eta_p D_z^*\eta_p^* + \eta_p^* D_z\eta_p\right) \\
& u_1 m_z^2\left|D_z\eta_s\right|^2 + u_2 m_z^2\left|D_z\eta_p\right|^2 + u_3\zeta_z m_z^2\left(D_z\eta_s D_z^*\eta_p^* + D_z^*\eta_s^* D_z\eta_p\right) + \\
& u_4\left(m_x^2 + m_y^2\right)\left|D_z\eta_s\right|^2 + u_5\left(m_x^2 + m_y^2\right)\left|D_z\eta_p\right|^2 + \\
& u_6\zeta_z\left(m_x^2 + m_y^2\right)\left(D_z^*\eta_s^* D_z\eta_p + D_z\eta_s D_z^*\eta_p^*\right) + \\
& u_7 m_z^2\left|\mathbf{D}_\perp\eta_s\right|^2 + u_8 m_z^2\left|\mathbf{D}_\perp\eta_p\right|^2 + u_9\zeta_z m_z^2\left(\mathbf{D}_\perp\eta_s\cdot\mathbf{D}_\perp^*\eta_p^* + \mathbf{D}_\perp^*\eta_s^*\cdot\mathbf{D}_\perp\eta_p\right) + \\
& u_{10}\zeta_z\left(m_x m_z\left(D_z\eta_s D_x\eta_p^* + D_z^*\eta_s^* D_x^*\eta_p\right) + m_y m_z\left(D_z\eta_s D_y\eta_p^* + D_z^*\eta_s^* D_y^*\eta_p\right)\right) + \\
& u_{11}\left(m_x m_z\left(D_z\eta_s D_x\eta_s^* + D_z^*\eta_s^* D_x^*\eta_s\right) + m_y m_z\left(D_z\eta_s D_y\eta_s^* + D_z^*\eta_s^* D_y^*\eta_s\right)\right) + \\
& u_{12}\left(m_x m_z\left(D_z\eta_p D_x\eta_p^* + D_z^*\eta_p^* D_x^*\eta_p\right) + m_y m_z\left(D_z\eta_p D_y\eta_p^* + D_z^*\eta_p^* D_y^*\eta_p\right)\right) + \\
& u_{13}\left(m_x^2 + m_y^2\right)\left(D_x\eta_s D_x^*\eta_s^* + D_y\eta_s D_y^*\eta_s^*\right) + u_{14}\left(m_x^2 + m_y^2\right)\left(D_x\eta_s D_x^*\eta_s^* - D_y\eta_s D_y^*\eta_s^*\right) + \\
& u_{15} m_x m_y\left(D_x\eta_s D_y^*\eta_s^* + D_y\eta_s D_x^*\eta_s^*\right) + u_{16}\left(m_x^2 + m_y^2\right)\left(D_x\eta_p D_x^*\eta_p^* + D_y\eta_p D_y^*\eta_p^*\right) + \\
& u_{17}\left(m_x^2 + m_y^2\right)\left(D_x\eta_p D_x^*\eta_p^* - D_y\eta_p D_y^*\eta_p^*\right) + u_{18} m_x m_y\left(D_x\eta_p D_y^*\eta_p^* + D_y\eta_p D_x^*\eta_p^*\right) + \\
& u_{19}\zeta_z\left(m_x^2 + m_y^2\right)\left(D_x\eta_s D_x^*\eta_p^* + D_y\eta_s D_y^*\eta_p^* + D_x^*\eta_s^* D_x\eta_p + D_y^*\eta_s^* D_y\eta_p\right) + \\
& u_{20}\zeta_z\left(m_x^2 + m_y^2\right)\left(D_x\eta_s D_x^*\eta_p^* - D_y\eta_s D_y^*\eta_p^* + D_x^*\eta_s^* D_x\eta_p - D_y^*\eta_s^* D_y\eta_p\right) + \\
& u_{21}\zeta_z m_x m_y\left(D_x\eta_s D_y^*\eta_p^* + D_y\eta_s D_x^*\eta_p^* + D_x^*\eta_s^* D_y\eta_p + D_y^*\eta_s^* D_x\eta_p\right)
\end{aligned}
$$

B.2 Cubic crystal symmetry

In the following we use the two products **.** and $\star$ as they were introduced in section 3.2.

$$
\begin{aligned}
f_{coupling} \quad = \quad & h_s (\mathbf{m})^2 \left|\eta_s\right|^2 + h_p (\mathbf{m})^2 \left|\eta_p\right|^2 + v\zeta_1 (\mathbf{m})^2 \left(\eta_s \eta_p^* + \eta_p \eta_s^*\right) + \\
& \mathrm{i}\kappa_s \zeta_1 \mathbf{m} \cdot \left(\eta_s \mathbf{D}^* \eta_s^* - \eta_s^* \mathbf{D} \eta_s\right) + \mathrm{i}\kappa_p \zeta_1 \mathbf{m} \cdot \left(\eta_p \mathbf{D}^* \eta_p^* - \eta_p^* \mathbf{D} \eta_p\right) + \\
& \mathrm{i}\kappa_0 \mathbf{m} \cdot \left(\eta_s \mathbf{D}^* \eta_p^* - \eta_s^* \mathbf{D} \eta_p + \eta_p \mathbf{D}^* \eta_s^* - \eta_p^* \mathbf{D} \eta_s\right) \\
& \mathrm{i}\nu\zeta_1 \left(\mathbf{m} \cdot \left(\mathbf{D}\eta_s \times \mathbf{D}^* \eta_p^*\right) - \mathbf{m} \cdot \left(\mathbf{D}^* \eta_s^* \times \mathbf{D}\eta_p\right)\right) \\
& u_1 \left|\mathbf{m} \cdot \mathbf{D}\eta_s\right|^2 + u_2 \left|\mathbf{m} \cdot \mathbf{D}\eta_p\right|^2 + \\
& u_3 \zeta_1 \left(\left(\mathbf{m} \cdot \mathbf{D}\eta_s\right)\left(\mathbf{m} \cdot \mathbf{D}\eta_p\right)^* + \left(\mathbf{m} \cdot \mathbf{D}\eta_s\right)^* \left(\mathbf{m} \cdot \mathbf{D}\eta_p\right)\right) + \\
& u_4 \zeta_1 \left(\left(\mathbf{m} \,\mathbf{.}\, \mathbf{D}\eta_s\right)\left(\mathbf{m} \,\mathbf{.}\, \mathbf{D}\eta_p\right)^* + \left(\mathbf{m} \,\mathbf{.}\, \mathbf{D}\eta_s\right)^* \left(\mathbf{m} \,\mathbf{.}\, \mathbf{D}\eta_p\right)\right) + \\
& u_5 \left|\mathbf{m} \star \mathbf{D}\eta_s\right|^2 + u_6 \left|\mathbf{m} \star \mathbf{D}\eta_p\right|^2 + \\
& u_7 \zeta_1 \left(\left(\mathbf{m} \star \mathbf{D}\eta_s\right)\left(\mathbf{m} \star \mathbf{D}\eta_p\right)^* + \left(\mathbf{m} \star \mathbf{D}\eta_s\right)^* \left(\mathbf{m} \star \mathbf{D}\eta_p\right)\right) + \\
& u_8 \left|\mathbf{m} \times \mathbf{D}\eta_s\right|^2 + u_9 \left|\mathbf{m} \times \mathbf{D}\eta_p\right|^2 + \\
& u_{10} \zeta_1 \left(\left(\mathbf{m} \times \mathbf{D}\eta_s\right)\left(\mathbf{m} \times \mathbf{D}\eta_p\right)^* + \left(\mathbf{m} \times \mathbf{D}\eta_s\right)^* \left(\mathbf{m} \times \mathbf{D}\eta_p\right)\right)
\end{aligned}
$$

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Index

Overview of expansion parameters in f_{sc} and $f_{coupling}$

Parameter indices denote: $s\ldots$ singlet term $p\ldots$ triplet term $0\ldots$ mixed term

Physical meaning	**Restrictions**	**Tetragonal**	**Toy tetra**	**Cubic**	**Toy cubic**
Only temperature dependent parameter, drives phase transition	$\propto (T - T_c)$	a_s, a_p	a	a_s, a_p	a
Fourth order terms bound free energy towards arbitrary strong η		b_s, b_p, c_1, c_2	b	b_s, b_p, c_1, c_2	b
Stiffness terms avoid arbitrary modulations of η	> 0	$\gamma_{s,\perp}, \gamma_{p,\perp}, \gamma_{0,\perp}$, $\gamma_{s,z}, \gamma_{p,z}, \gamma_{0,z}$	$\gamma_\perp, \gamma_z$	$\gamma_s, \gamma_p, \gamma_0$	γ
Controls mixing of singlet and triplet phase, spin-orbit interaction		d		d	
		$\delta_\perp, \delta_z, \delta_0$	δ		
Suppresses superconductivity in presence of (homogeneous) magnetization	> 0	$h_{s,\perp}, h_{p,\perp}$, $h_{s,z}, h_{p,z}$	$h_\perp, h_z$	h_s, h_p	h
Suppresses mixed superconductivity in presence of magnetization		$v_\perp, v_z$		v	
MD spin-orbit interaction allowed by non-centrosymmetricity		$\kappa_s, \kappa_p, \kappa_0$	κ	$\kappa_s, \kappa_p, \kappa_0$	κ
Terms via which a modulated magnetization evokes modulated η		ν_s, ν_p, ν_0, ρ_s, ρ_p, ρ_0, $\sigma_s, \sigma_p, \sigma_0$	ν, ρ, σ		

List of variables and abbreviations used in more than one section

ζ_z, ζ_1	non-centrosymmetricity order parameters in tetragonal and cubic symmetry
η_s, η_p	order parameter of singlet and triplet superconductivity
$\mathbf{m}$	order parameter of magnetism/magnetization
$k_\ominus$	wave vector of tetragonal modulated magnetism along coordinate axes
$M_\ominus$	ratio of m_x and m_z amplitudes for this magnetic state
$k_\oslash$	wave vector of tetragonal modulated magnetism along diagonals
$M_\oslash$	ratio of $m_{x,y}$ and m_z amplitudes for this magnetic state
$k_\oplus$	wave vector of cubic modulated magnetism along coordinate axes
$k_\otimes$	wave vector of cubic modulated magnetism along body diagonal
$x' = k_\ominus x$	change of coordinates for tetragonal superconductivity
$z' = \frac{k_\oplus z}{2} - \frac{1}{2}\arctan\frac{k_y}{k_x} - \frac{\pi}{4}$	change of coordinates in cubic toy model
$\mu,\ \tilde{\mu}$	relative strength of spin-orbit interaction and stiffness, slightly different definition in tetragonal symmetry, cubic symmetry and cubic toy model
$s_n,\ p_n$	coefficients of n^{th} mode in NFE method for singlet and triplet phase
$T_{cs},\ T_{cp}$	transition temperature of singlet and triplet phase of superconductivity
$\hat{\mathbf{Q}}, \hat{\mathbf{T}}, \hat{\mathbf{S}}$	coefficient matrices of coupled Mathieu equations in tetragonal symmetry
$q_i,\ t_i,\ s_i;\ i = 1\ldots4$	entries of coefficient matrices $\hat{\mathbf{Q}}, \hat{\mathbf{T}}, \hat{\mathbf{S}}$ enumerated row by row
$\mathbf{R}(\xi)$	two-vector representing the order parameters η_p and η_s after linear transformation that casts the equation in the form of coupled Mathieu equations

$H_s = h_{s,\perp} M_\ominus^2 + h_{s,z}$

$H_{s-} = h_{s,\perp} M_\ominus^2 - h_{s,z}$

$H_p = h_{p,\perp} M_\ominus^2 + h_{p,z}$

$H_{p-} = h_{p,\perp} M_\ominus^2 - h_{p,z}$

$V = v_\perp M_\ominus^2 + v_z$

$V_- = v_\perp M_\ominus^2 - v_z$