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Spin-triplet pairing induced by Hund's rule coupling

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Parowanie spinowo-trypletowe zaindukowane regułą Hunda

Rozprawa doktorska
Promotor: **prof. dr hab. Józef Spałek**

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Abstract

In this Thesis we model theoretically the spin-triplet real-space superconducting pairing in orbitally degenerate narrow-band systems, induced by the intraatomic ferromagnetic exchange (known under the term *"Hund's rule"* in atomic physics). This type of pairing introduces spin-triplet superconductivity to the models analysed traditionally in the context of itinerant ferromagnetism and the orbital ordering effects. The main purpose is to discuss the feasibility of such novel pairing mechanism in a *model situation* and involves both analytic and numerical aspects of the problem in the weak-coupling limit. We consider three possible phases - B, A, and $A1$, introduced in the context of superfluid He^3. We have determined a relative stability of the phases as a function of either applied magnetic field (in the paramagnetic state) or as a function of an equilibrium magnetic moment in a weakly ferromagnetic metallic phase. Particular attention has been paid to the stability of the phases near the **Stoner threshold**, i.e. the point, at which the band ferromagnetism sets in. It has been shown that the A type of pairing induces a weak ferromagnetic moment below the Stoner threshold. Therefore, the Stoner point becomes a **hidden critical point**, here analysed in the weak-coupling limit (the combined Hartree-Fock and Bardeen-Cooper-Schriefer (HE-BCS) approximation). A detailed numerical analysis is carried out and a generalized four-dimensional formalism of Bogolyubov-Nambu-de Gennes type is developed, which makes the whole analysis more compact. Both ground-state and selected thermodynamic properties are calculated. Only spatially homogeneous state is considered.

A detailed behavior of the single Cooper pair in a two-dimensional confined system ("quantum dot") is considered in the *Supplement*, where the singlet-triplet transition is observed when the Coulomb repulsion interaction is included. Such a transition occurs also under the influence of applied magnetic field.

Keywords: spin-triplet pairing, Hund's rule exchange, exchange mediated pairing, superconducting ferromagnets.

Streszczenie

W rozprawie rozważono parowanie trypletowe elektronów w modelowych układach wąskopasmowych z degeneracją orbitalną, które jest zaindukowane wewnątrzatomowym oddziaływaniem ferromagnetycznym (znanym w fizyce atomowej jako reguła Hunda). Ten typ parowania wprowadza parowanie trypletowe do modeli używanych tradycyjnie do opisu ferromagnetyzmu i uporządkowania orbitalnego. Głównym celem ogólnym jest przedyskutowanie teoretyczne możliwości realizacji tego nowego mechanizmu parowania w sytuacji modelowej, zarówno jego aspektów analitycznych, jak i numerycznych - w granicy słabego parowania. Przebadano stabilność przestrzennie jednorodnych trzech stanów nadprzewodzących (A, B, $A1$) w polu magnetycznym, zwłaszcza w pobliżu progu Stonera - przejścia fazowego do stanu ferromagnetycznego. Wykazano, że parowanie trypletowe prowadzi do pojawienia się słabej polaryzacji spinowej w pobliżu tego kwantowego punktu krytycznego. Określono stany kwazicząstkowe w stanach skondensowanych i pokazano, że dla fazy typu B i $A1$ występuje galąź bezprzerwowa prowadząca do liniowego ciepła właściwego w stanie sparowanym. Obliczenia przeprowadzono w przybliżeniu Hartree-Focka połączonym z przybliżeniem Bardeena, Coopera i Schrieffera (BCS) w uogólnionej notacji czterowymiarowej typu Bogoliubowa, Nambu i de Gennes'a. Zarówno własności stanu podstawowego jak i wybrane wielkości termodynamiczne są uwzględnione w szczegółowej dyskusji. Uwzględniono w niej jedynie stan przestrzennie jednorodny.

W *Suplemencie* opisano zachowanie pojedynczej pary Coopera w dwuwymiarowej kropce kwantowej. Obserwuje się w niej przejście od stanu singletowego do trypletowego pary w obecności odpychającego oddziaływania kulombowskiego. Przejście takie zachodzi także pod wpływem pola magnetycznego.

Słowa kluczowe: parowanie spinowo-trypletowe, wymiana typu reguły Hunda, parowanie zaindukowane oddziaływaniem wymiany, nadprzewodzące ferromagnetyki.

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Chapter 1

Introduction

1.1 Spin-triplet pairing of fermions: A historical perspective

In this chapter we provide a brief historical survey of the spin-triplet pairing in condensed matter physics, which involves both superconducting and superfluid types of pairing. Then, in Chapter 2, our model of spin-triplet superconductivity induced by the Hund's rule coupling will be derived for a doubly degenerate narrow-band Hamiltonian. As a next step, the results for the basic electronic properties of the paired-state will be presented. Finally, after introducting the term typical for ferromagnetism appearance, the coexistence of the spin-triplet superconductivity with band ferromagnetism will be investigated.

The possibility of the spin-triplet pairing has been considered first by Layzer and Fay [1]. This mechanism of pairing induced by spin-fluctuations (in a paramagnet) was applied subsequently to explain superfluidity in liquid ^3He [2]. The spin-triplet superconductivity has also been proposed involving the same mechanism of pairing [3]. The spin triplet real space-pairing has been suggested by Baskaran as applicable to Sr_2RuO_4 [4], following the suggestion by Rice and Sigirst (1995) that Sr_2RuO_4 is similar to liquid ^3He. The importance of the Hund's rule in the pairing has been noticed even earlier [5], where it was applied to the Andersson lattice with degenerate f-level to account the properties of heavy-fermion superconductors such as UPt_3. The role of of interorbital Coulomb interactions has been also considered [6]. A number of recent papers utilize simply the BCS-like form of the pairing potential, adopted to the spin-triplet situation, and analyse the system properties without asking about the nature of

such form of attractive interaction. We consider one specific microscopic mechanism.

The current research on the spin-triplet pairing is largely based on the phenomenological models involving attractive Coulomb intra-, and/or inter-orbital interactions in real space (cf. e.g. [7], [8]). This type of models as applied to multiple-band models, started with the work of Klejnberg and Spałek (1999 and 2000). Its analytic structure has been summarized by Spałek (2001). The theoretical research on new ferromagnetic superconductors UGe_2, $URhGe$, and $ZrZn_2$ is only beginning.

1.2 Aim and scope of the Thesis

The aim of the Thesis is to introduce and discuss the local spin-triplet pairing induced by the intraatomic interorbital ferromagnetic exchange interaction (the Hund's rule) and to examine the coexistence of such paired state with the weak band ferromagnetism induced by either intraatomic Coulomb interaction (the Hubbard term) or by the two factors combined. For a detailed discussion of this mechanism of pairing we employ the simplest method of approach namely, combine the Hartree-Fock approximation for the diagonal (ferromagnetic) ordering with the off-diagonal (superconducting) paired state. The stability of different states without and in the presence of a weak applied magnetic field is discussed and the quasiparticle electronic structure is detailed. For the simplicity only a doubly-degenerate and narrow band situation is discussed in detail, as the main purpose of the Thesis is to provide an argument for feasibility of this mechanism. The application of this mechanism to concrete systems would require an incorporation of realistic band structure, which should represent the next step, unfortunately going beyond the scope of this Thesis. Also, only the spatially **homogeneous** BCS type of state is considered. The *Supplement* provides an additional argument in favour of the idea that repulsive Coulomb interaction can lead to a spin-triplet bound state of a Cooper pair. The argument presented there illustrates the old idea of Kohn and Luttinger (1965) that the repulsive interaction can lead to a nontrivial type of pairing. After all, the direct exchange interaction is a part of Coulomb repulsive interaction, selecting only the type of optimal spin configuration in a pair of orbitally distinguishable states.

Chapter 2

Two-band model of spin-triplet superconductivity

In this chapter a two-band model of spin-triplet superconductivity is formulated. As a leading pairing mechanism the direct exchange interaction in the form of the Hund's rule coupling is proposed. The Hartree-Fock-BCS approximation for the model Hamiltonian is introduced reflecting the situation in the weak-coupling regime. The obtained Hartree-Fock Hamiltonian is then rewritten in the four-dimensional notation, used subsequently to obtain a set of self-consistent equations for the parameters describing basic system properties: the ground state energy, the energy gap, the magnetic moment, and the chemical potential. Possibility of a coexistence of the spin-triplet state with a weak ferromagnetism is discussed later.

2.1 The theoretical model

The theoretical model is formulated on the basis of the results obtained in the paper of A. Klejnberg and J. Spałek [9], where the pairing mechanism together with the Hamiltonian expressing this pairing for the two-band system have been proposed and discussed within the slave-boson approach. For the needs of the investigation on the influence of ferromagnetism on the spin-triplet superconductivity and possible coexistence of both phenomena, we have considered the system in the weak coupling limit (modified Hartree-Fock-BCS approximation) to include also the averages emerging from the ferromagnetic-interaction ordering. In other words, our system will have two order parameters arising from a single interaction - the ferromagnetic exchange.

We start from an extended Hubbard model of correlated and orbitally degenerate electrons characterized by the Hamiltonian:

$$\begin{aligned}\mathcal{H} \;=\; & \underbrace{\sum_{ij(i\neq j)ll'\sigma} t_{ij}^{ll'} a_{il\sigma}^{\dagger} a_{il'\sigma}}_{(i)} + \underbrace{U \sum_{il} n_{il\uparrow} n_{il\downarrow}}_{(ii)} + \underbrace{\frac{1}{2} U' \sum_{ill'(l\neq l')\sigma\sigma'} n_{il\sigma} n_{il'\sigma'}}_{(iii)} \\ & \underbrace{- J \sum_{ill'(l\neq l')} \left(\mathbf{S}_{il} \cdot \mathbf{S}_{il'} + \frac{3}{4}\, n_{il} n_{il'} \right)}_{(iv)} + \underbrace{J \sum_{ill'(l\neq l')} a_{il\uparrow}^{\dagger} a_{il\downarrow}^{\dagger} a_{il'\downarrow} a_{il'\uparrow}}_{(v)} \; . \end{aligned} \tag{2.1}$$

The first term (i) describes electron hopping between atomic sites i and j and orbitals l, l'. The hopping integral $t_{ij}^{ll'}$ is written in the most general form and for the case of $l \neq l'$ introduces hybridization into the system. The second term (ii) describes direct Coulomb interaction between two electrons localized on the same orbital l (intra-orbital) - due to the Pauli exclusion principle both particles must have opposite spins. The third expression (iii) is responsible for the interorbital Coulomb interaction for $l \neq l'$. In that case all spin orientations are allowed. The coefficient $1/2$ at the front of (iii) prevents us from counting the same electrons' configuration twice. The fourth term (iv) introduces the Hund's rule ferromagnetic exchange between electrons localized on the same site i, but on different orbitals l and l'. This rule reflects well known fact, that electrons first choose to occupy different orbitals (on the same energy level) with the same spin orientation and then tend to fill up the remaining "spaces" according to the above mentioned Pauli exclusion principle. The fifth term (v) describes hopping of pair of the electrons between the orbitals. Note that in both (iv) and (v) Hund's coupling constant J is present but with opposite sign. The reason is that for (iv) J corresponds to the energy gained by the system from adopting to the Hund's rule, whereas in the case of (v) it describes the energy loss caused by violating that rule as the pair hopping is possible only under this circumstance.

The Hamiltonian (2.1) is very difficult to solve rigorously. In this Thesis we investigate the weak coupling limit of the model, e.g. we assume that $W > U \gg J$, with W being the bare bandwidth. Under this assumption the terms (iii) and (v) can be neglected. The term (iii) plays in that case only a minor role in comparison to the leading second one (ii) (e.g. $U' = U - \frac{5}{2}J$ for d orbitals). Therefore, it may be dropped out, as it does not differentiate between different local spin configurations at least in the weak coupling limit. The same is valid for (v), since the hopping of electron pair is automatically connected to the condition that both of them must occupy the same

orbital, but such local spin-pairing is not possible in view of the fact that $U \gg J$. Then, the simplest nontrivial Hamiltonian of the system reduces to the form

$$\mathcal{H} = \sum_{ij(i\neq j)ll'\sigma} t_{ij}^{ll'} a_{il\sigma}^{\dagger} a_{il'\sigma} + U \sum_{il} n_{il\uparrow} n_{il\downarrow} - J \sum_{ill'(l\neq l')} \left(\mathbf{S}_{il} \cdot \mathbf{S}_{il'} + \frac{3}{4}\, n_{il} n_{il'} \right) \tag{2.2}$$

Since we are interested in the qualitative aspects of the paired state, we will consider the two-band system as the least complicated one, for which all terms from the above Hamiltonian are still applicable. For the one-band system the Hund's term will not appear (the intersite exchange interaction will appear instead).

In the case of the two-band system, the orbital index assumes two values, $l = 1$ and 2. If the hybridization of the bands is very weak or does not appear (i.e. $t^{12} \simeq 0$), the term representing hopping of a single electron between the neighboring atomic sites can be transformed to the momentum (reciprocal) space according to the prescription

$$\sum_{ijl\sigma} t_{ij} a_{il\sigma}^{\dagger} a_{il\sigma} \longrightarrow \sum_{\mathbf{k}l\sigma} (E_{\mathbf{k}l} - \mu)\; n_{\mathbf{k}l\sigma} \;,$$

where the quantity $E_{\mathbf{k}l} \equiv E_{\mathbf{k}l} - \mu$ is the single-particle energy in the l-th band ($l = 1, 2$) and μ is the chemical potential. Hence, we can rewrite the Hamiltonian (2.2) for the canonical bands in the form

$$\begin{aligned} \mathcal{H} &= \sum_{\mathbf{k}l\sigma} (E_{\mathbf{k}l} - \mu)\; n_{\mathbf{k}l\sigma} \\ &+ U \sum_{li} n_{li\uparrow} n_{li\downarrow} - J \sum_{ll'i,(l\neq l')} \left(\mathbf{S}_{il} \cdot \mathbf{S}_{il'} + \frac{3}{4}\, n_{li} n_{l'i} \right) . \end{aligned} \tag{2.3}$$

In the new Hamiltonian hybridization of the orbitals (if exists) have been incorporated already in the single particle energies $E_{\mathbf{k}l}$; the Coulomb interaction U and the Hund's coupling parameter J are regarded then as effective parameters, which include hybridization. Such an assumption results in $\mathbf{k}$-independent U and J and in a longer run - in the isotropic gap parameter Δ.

We are interested in the spin-triplet correlations and the corresponding electron pairing. In such situation, we construct first the effective BCS Hamiltonian with the spin-triplet pairing with inclusion of the intraatomic Coulomb interaction U. We introduce the local real-space spin-triplet pairing in terms of the pairing operators $A_{i,m}$, $A_{im}^{\dagger}$ defined as follows

$$A_{im}^{\dagger} = \begin{cases} a_{i1\uparrow}^{\dagger} a_{i2\uparrow}^{\dagger} & \text{for } m = 1 \;\; (S_{tot}^{z} = 1) \\ a_{i1\downarrow}^{\dagger} a_{i2\downarrow}^{\dagger} & \text{for } m = -1 \;\; (S_{tot}^{z} = -1) \\ \frac{1}{\sqrt{2}} \left(a_{i1\uparrow}^{\dagger} a_{i2\downarrow}^{\dagger} + a_{i1\downarrow}^{\dagger} a_{i2\uparrow}^{\dagger} \right) & \text{for } m = 0 \;\; (S_{tot}^{z} = 0) \;, \end{cases} \tag{2.4}$$

with $m \equiv S^z_{tot} = S^z_{i1} + S^z_{i2}$ being the z-component of the pair spin operator. It can be shown (see Appendix A) that

$$\sum_{ll'i,(l\neq l')} \left(\mathbf{S}_{il} \cdot \mathbf{S}_{il'} + \frac{3}{4}\, n_{li} n_{l'i} \right) = 2 \sum_{i,m} A^{\dagger}_{im} A_{im} \ . \tag{2.5}$$

With help of the above relation, the Hamiltonian (2.3) can be written down in a compact form

$$\mathcal{H} = \sum_{\mathbf{k}l\sigma} (E_{\mathbf{k}l} - \mu)\ n_{\mathbf{k}l\sigma} + U \sum_{li} n_{il\uparrow} n_{il\downarrow} - 2J \sum_{i,m} A^{\dagger}_{im} A_{im} \ . \tag{2.6}$$

The physical contents of this model is as follows. The third term represents a local spin-triplet pairing correlations. The repulsive interaction of the magnitude $U > 0$, while suppressing a local spin-singlet pairing with the amplitude $\left\langle a^{\dagger}_{il\uparrow} a^{\dagger}_{il\downarrow} \right\rangle \neq 0$, is not harmful to the interband off-diagonal long-range order with the amplitudes $\left\langle A^{\dagger}_{im} \right\rangle \neq 0$, which describe the spin-triplet pairing. However, the role of the second term is highly nontrivial if a ferromagnetic ordering is taken into consideration together with the the local spin-triplet pairing. The model represented by the Hamiltonian (2.6) can describe thus a combination of the diagonal and off-diagonal types of ordering coexisting with each other. A separate question is related to the incorporation of the orbital ordering (cf. Klejnberg and Spalek, 2000; [10]).

The simplest solution of the model is to execute the Hartree-Fock approximation combined with the BCS approximation [11]. This approach is justified qualitatively by the circumstance that the single-particle excitations contribute to the temperature dependence of magnetization $M \sim T^2$, where T is the temperature; this contribution is markedly visible in the temperature dependence of the magnetization for $URhGe$ [12]. A simultaneous implementation of the BCS approximation is justified a posteriori, since the Curie (i.e. magnetic transition) temperature $T_{\mathrm{C}} \sim J/10$ turns out to be substantially larger than the superconducting temperature $T_{\mathrm{S}} \sim T^*_{\mathrm{F}} \exp\left(-\frac{1}{J\rho}\right)$, where T^*_{F} is the effective Fermi temperature. Hence, it is proper to consider the BCS approach to the pairing part [13], [14].

In the next Section the combined Hartree-Fock-BCS approximation will be presented in detail taking the Hamiltonian (2.6) as a starting point for further investigations.

2.2 The combined Hartree-Fock-BCS approximation

Following Hartree-Fock-BCS approximation, we make decomposition of pair-electron operators (the second and the third terms in (2.6)) according to the rule

$$AB \longrightarrow A < B > + < A > B - < A >< B > \ . \tag{2.7}$$

The rule above is actually the consequence of Wick's theorem. The BCS approximation is introduced by the assumption that averages of the type $< a_{il\sigma} a_{il'\sigma'} >$, which normally should vanish, assume nonzero values and are calculated self-consistently, whenever such a state is stable against the normal state.

Following the combined Hartree-Fock-BSC approximation we can rewrite second (Hubbard) term of effective Hamiltonian (2.6) in the approximate form

$$U \sum_{il} n_{il\uparrow} n_{il\downarrow} \longrightarrow U \sum_{il} \left\{ \langle n_{il\uparrow} \rangle \, n_{il\downarrow} + \langle n_{il\downarrow} \rangle \, n_{il\uparrow} - \langle n_{il\uparrow} \rangle \, \langle n_{il\downarrow} \rangle \right\} \ , \tag{2.8}$$

as we neglect the spin siglet pairing. For l-th orbital on i-th atomic site the following relations are fulfilled

$$\begin{cases} n_{il} = \frac{1}{2} \left(n_{il\uparrow} + n_{il\downarrow} \right) \\ S^z_{il} = \frac{1}{2} \left(n_{il\uparrow} - n_{il\downarrow} \right) \end{cases} \ , \tag{2.9}$$

from which expression for $n_{il\sigma}$ can be extracted. Combining both equations we have

$$n_{il\sigma} = \frac{n_{il}}{2} + \sigma S^z_{il} \ . \tag{2.10}$$

Substituting this result to the decomposed Hubbard term (2.8), we obtain

$$\begin{aligned} U \sum_{il} \ n_{il\uparrow} n_{il\downarrow} \ &\longrightarrow \\ U \textstyle\sum_{il} \ &\left\{ \frac{< n_l >}{2} \sum_{\sigma} n_{il\sigma} - < S^z_l > \sum_{\sigma} \sigma n_{il\sigma} + < S^z_l >^2 - \frac{< n_l >^2}{4} \right\} \ . \end{aligned} \tag{2.11}$$

The first and the last terms are constant (no charge ordering is assumed) and thus can be neglected. The first one can be included into the band energy and the last is constant, since number of electrons in the system is fixed. Thus, both terms lead only to shift of the reference point of the system energy. In effect, we retain only the nontrivial terms, i.e.

$$U \sum_{il} n_{il\uparrow} n_{il\downarrow} \longrightarrow -U \sum_{il} \left(< S^z_l > \sum_{\sigma} \sigma n_{il\sigma} \right) + 2NU < S^z_l >^2 \ , \tag{2.12}$$

where $N = \sum_i 1$ is the number of atomic states. For the two-band system, we have two possible values of l ($l = 1, 2$) and therefore $\sum_{il} 1 = 2N$.

The Hund's coupling part of the Hamiltonian requires a more careful treatment. Due to the relation

$$\sum_{ll'i,(l\neq l')} \left(\mathbf{S}_{il} \cdot \mathbf{S}_{il'} + \frac{3}{4}\, n_{li} n_{l'i} \right) = 2 \sum_{i,m} A^{\dagger}_{im} A_{im}$$

derived in Appendix A, both representations (the spin and the pair-operator) of that term must be taken into account while making Hartree-Fock-type decomposition with nonzero anomalous averages. Explicitly, we make a decomposition of the Wick type

$$\begin{aligned} \sum_{i,m} A^{\dagger}_{i,m} A_{i,m} \;\longrightarrow\; & \sum_{i,m} \left\{ \left\langle A^{\dagger}_{i,m} \right\rangle A_{i,m} + A^{\dagger}_{i,m} \left\langle A_{i,m} \right\rangle - \left\langle A^{\dagger}_{i,m} \right\rangle \left\langle A_{i,m} \right\rangle \right\} \\ + & \sum_{ill'(l\neq l')} \left\{ \bar{S^z}_l S^z_{l'i} + \bar{S^z}_{l'} S^z_{li} - \bar{S^z}_l \bar{S^z}_{l'} \right\} \\ + & \frac{3}{4} \sum_{ill'(l\neq l')} \left\{ \left\langle n_{li} \right\rangle n_{l'i} + \left\langle n_{l'i} \right\rangle n_{li} - \left\langle n_{li} \right\rangle \left\langle n_{l'i} \right\rangle \right\} \; . \end{aligned} \tag{2.13}$$

The above expression contains both the diagonal and the off-diagonal averages. As before, the terms proportional to average number of particles - $\langle n_{li} \rangle$, can be neglected. We assume additionally, that the energy bands are equivalent and put $\bar{S^z}_l = \bar{S^z}$. In what follows, the Hund's-rule coupling part of the Hamiltonian (2.6) can be cast into the form

$$\begin{aligned} -2J \sum_{i,m} A^{\dagger}_{i,m} A_{i,m} \;\longrightarrow\; & -\sum_{i,m} \left\{ \Delta^{*}_{i,m} A_{i,m} + A^{\dagger}_{i,m} \Delta_{i,m} \right\} \\ & - (2J)\; 2\bar{S^z} \sum_{il} S^z_{li} \\ & + N \sum_{m} \frac{|\Delta_{i,m}|^2}{2J} + (2J) 2N \bar{S^z}^2 \; , \end{aligned} \tag{2.14}$$

where we have introduced the *gap parameter* as

$$\Delta_{i,m} = 2J \left\langle A_{i,m} \right\rangle \; . \tag{2.15}$$

Finally, with the help of (2.12) and (2.14), we can write down the whole Hamiltonian in the Hartree-Fock-BCS approximation for the system in the form

$$\begin{aligned} \mathcal{H}_{HF} \;=\; & \sum_{\mathbf{k}l\sigma} (E_{\mathbf{k}l} - \mu)\, n_{\mathbf{k}l\sigma} \\ & - \sum_{i,m} \left\{ \Delta^{*}_{i,m} A_{i,m} + A^{\dagger}_{i,m} \Delta_{i,m} \right\} - 2I\bar{S^z} \sum_{il} S^z_{li} \\ & + N \left\{ \sum_{m} \frac{|\Delta_{i,m}|^2}{2J} + 2I \bar{S^z}^2 \right\} \; , \end{aligned} \tag{2.16}$$

where the parameter $I = U + 2J$ can be identified as the effective magnetic coupling constant. As one can see, the effective Hamiltonian contains the term responsible for an appearance of the ferromagnetic polarization, as well as the term describing the local spin-triplet pairing. Therefore, we may expect ferromagnetism coexisting with spin-triplet paired phase if both $\bar{S}^z$ and at least one of the gap parameters Δ_m ($m = +1, 0, -1$) are nonzero simultaneously for the case of an energetically stable solution. Furthermore, the paired state may have up to three independent superconducting gaps, each of which being a complex number.

In the following sections the real-space Hamiltonian (2.16) will be transformed to the momentum space, which is followed by the presentation of the method of determining its solutions.

2.3 Transformation of the effective Hamiltonian to momentum space

Before we can proceed further, i.e. introduce the method used for resolving the eigenvalues and the eigenstates of the effective Hamiltonian, it is convenient to transform it to the reciprocal (momentum) space. The transformation is carried out with help of relations between the particle annihilation and creation operators $a_{il\sigma}$, $a^{\dagger}_{il\sigma}$ used for description of the model in the real space and the corresponding operators defined in the momentum space. These relations have the following form in the lattice case

$$a_{il\sigma} = \frac{1}{\sqrt{N}} \sum_{k} e^{-i\mathbf{k}\mathbf{R}_i} a_{\mathbf{k}l\sigma} \qquad \text{and} \qquad a^{\dagger}_{il\sigma} = \frac{1}{\sqrt{N}} \sum_{k} e^{i\mathbf{k}\mathbf{R}_i} a^{\dagger}_{\mathbf{k}l\sigma} \; . \tag{2.17}$$

Substitiuting (2.17) into the real-space effective Hamiltonian (2.16), we will obtain the expression

$$\begin{aligned}
\mathcal{H}_{HF} \;=\; & \sum_{\mathbf{k}l\sigma} (E_{\mathbf{k}l} - \mu - \sigma I \bar{S}^z)\, n_{\mathbf{k}l\sigma} \\
& - \frac{2J}{N} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \delta_{\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4} \Big\{ \Big\langle a^{\dagger}_{\mathbf{k}_1 1\uparrow} a^{\dagger}_{\mathbf{k}_2 2\uparrow} \Big\rangle a_{\mathbf{k}_4 2\uparrow} a_{\mathbf{k}_3 1\uparrow} + \Big\langle a^{\dagger}_{\mathbf{k}_1 1\downarrow} a^{\dagger}_{\mathbf{k}_2 2\downarrow} \Big\rangle a_{\mathbf{k}_4 2\downarrow} a_{\mathbf{k}_3 1\downarrow} \\
& \qquad + \frac{1}{2} \Big\langle a^{\dagger}_{\mathbf{k}_1 1\uparrow} a^{\dagger}_{\mathbf{k}_2 2\downarrow} + a^{\dagger}_{\mathbf{k}_1 1\downarrow} a^{\dagger}_{\mathbf{k}_2 2\uparrow} \Big\rangle (a_{\mathbf{k}_4 2\downarrow} a_{\mathbf{k}_3 1\uparrow} + a_{\mathbf{k}_4 2\uparrow} a_{\mathbf{k}_3 1\downarrow}) + HC \Big\} \\
& + \frac{2J}{N} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \delta_{\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4} \Big\{ \Big\langle a^{\dagger}_{\mathbf{k}_1 1\uparrow} a^{\dagger}_{\mathbf{k}_2 2\uparrow} \Big\rangle \langle a_{\mathbf{k}_4 2\uparrow} a_{\mathbf{k}_3 1\uparrow} \rangle + \Big\langle a^{\dagger}_{\mathbf{k}_1 1\downarrow} a^{\dagger}_{\mathbf{k}_2 2\downarrow} \Big\rangle \langle a_{\mathbf{k}_4 2\downarrow} a_{\mathbf{k}_3 1\downarrow} \rangle \\
& \qquad + \frac{1}{2} \Big\langle a^{\dagger}_{\mathbf{k}_1 1\uparrow} a^{\dagger}_{\mathbf{k}_2 2\downarrow} + a^{\dagger}_{\mathbf{k}_1 1\downarrow} a^{\dagger}_{\mathbf{k}_2 2\uparrow} \Big\rangle \langle a_{\mathbf{k}_4 2\uparrow} a_{\mathbf{k}_3 1\downarrow} + a_{\mathbf{k}_4 2\downarrow} a_{\mathbf{k}_3 1\uparrow} \rangle \Big\}
\end{aligned}$$

$$+ \quad 2NI\bar{S}^{z\,2} \,,$$

where $\delta_{\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4}$ is a *Kronecker delta* defined by the identity

$$\delta_{\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4} = \frac{1}{N}\sum_i e^{-i(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)\mathbf{R}_i} \,. \tag{2.18}$$

Averages $\left\langle a^\dagger_{\mathbf{k}l\sigma} a^\dagger_{\mathbf{k}'l'\sigma'}\right\rangle$, which have appeared in the momentum space, represent the amplitudes for the paired states in the momentum space and will be used subsequently in the definition of the superconducting gap Δ.

For simplicity, we consider the system in equilibrium, i.e. assume that the center-of-mass momentum of a single pair (or paired state) is equal to zero ($\mathbf{K} \equiv 0$). This assumption corresponds to the situation when e.g. no spontaneous current is present in the system. In that case the wave vectors $\mathbf{k}_1$, $\mathbf{k}_2$, $\mathbf{k}_3$ and $\mathbf{k}_4$ fullfil the relation $\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4 = 0$. Hence we can make the following substitution

$$\left\{\begin{array}{lcl} \mathbf{k}_1 & \longrightarrow & \mathbf{k} \\ \mathbf{k}_2 & \longrightarrow & -\mathbf{k} \end{array}\right. \quad \text{and} \quad \left\{\begin{array}{lcl} \mathbf{k}_3 & \longrightarrow & \mathbf{k}' \\ \mathbf{k}_4 & \longrightarrow & -\mathbf{k}' \end{array}\right. \,. \tag{2.19}$$

With its help the transformed Hamiltonian can be rewritten to the form

$$\begin{aligned}
\mathcal{H}_{HF} \;&= \sum_{\mathbf{k}l\sigma}(E_{\mathbf{k}l} - \mu - \sigma I\bar{S}^z)\, n_{\mathbf{k}l\sigma} \\
&+ \quad \sum_{\mathbf{k}} \left\{ \left(-\frac{2J}{N}\sum_{\mathbf{k}'} \left\langle a^\dagger_{\mathbf{k}'1\uparrow} a^\dagger_{-\mathbf{k}'2\uparrow}\right\rangle\right) a_{-\mathbf{k}2\uparrow} a_{\mathbf{k}1\uparrow} + \left(-\frac{2J}{N}\sum_{\mathbf{k}'} \left\langle a^\dagger_{\mathbf{k}'1\downarrow} a^\dagger_{-\mathbf{k}'2\downarrow}\right\rangle\right) a_{-\mathbf{k}2\downarrow} a_{\mathbf{k}1\downarrow} \right. \\
&+ \quad \left. \left(-\frac{2J}{\sqrt{2}N}\sum_{\mathbf{k}'} \left\langle a^\dagger_{\mathbf{k}'1\uparrow} a^\dagger_{-\mathbf{k}'2\downarrow} + a^\dagger_{\mathbf{k}'1\downarrow} a^\dagger_{-\mathbf{k}2\uparrow}\right\rangle\right) \frac{1}{\sqrt{2}} \left(a_{-\mathbf{k}2\downarrow} a_{\mathbf{k}1\uparrow} + a_{-\mathbf{k}2\uparrow} a_{\mathbf{k}1\downarrow}\right) + HC \right\} \\
&+ \quad \frac{N}{2J} \left\{ \left(-\frac{2J}{N}\sum_{\mathbf{k}} \left\langle a^\dagger_{\mathbf{k}1\uparrow} a^\dagger_{-\mathbf{k}2\uparrow}\right\rangle\right) \left(-\frac{2J}{N}\sum_{\mathbf{k}'} \left\langle a_{-\mathbf{k}'2\uparrow} a_{\mathbf{k}'1\uparrow}\right\rangle\right) \right. \\
&\qquad\qquad \left. + \left(-\frac{2J}{N}\sum_{\mathbf{k}} \left\langle a^\dagger_{\mathbf{k}1\downarrow} a^\dagger_{-\mathbf{k}2\downarrow}\right\rangle\right) \left(-\frac{2J}{N}\sum_{\mathbf{k}'} \left\langle a_{-\mathbf{k}'2\downarrow} a_{\mathbf{k}'1\downarrow}\right\rangle\right) \right. \\
&+ \quad \left. \left(-\frac{2J}{\sqrt{2}N}\sum_{\mathbf{k}'} \left\langle a^\dagger_{\mathbf{k}'1\uparrow} a^\dagger_{-\mathbf{k}'2\downarrow} + a^\dagger_{\mathbf{k}'1\downarrow} a^\dagger_{-\mathbf{k}2\uparrow}\right\rangle\right) \left(-\frac{2J}{\sqrt{2}N}\sum_{\mathbf{k}} \left\langle a_{-\mathbf{k}2\downarrow} a_{\mathbf{k}1\uparrow} + a_{-\mathbf{k}2\uparrow} a_{\mathbf{k}1\downarrow}\right\rangle\right) \right\} \\
&+ \quad 2NI\bar{S}^{z\,2} \,.
\end{aligned}$$

The spin-triplet pairing operators can be defined in the momentum space similarly as those in the real space presented in expression (2.4). Using the analogy, we can write the following relations for $A^\dagger_{\mathbf{k},m}$

$$A^\dagger_{\mathbf{k},m} = \left\{\begin{array}{ll} a^\dagger_{\mathbf{k}1\uparrow} a^\dagger_{-\mathbf{k}2\uparrow} & \text{for } m = 1 \;(S^z = 1) \\ a^\dagger_{\mathbf{k}1\downarrow} a^\dagger_{-\mathbf{k}2\downarrow} & \text{for } m = -1 \;(S^z = -1) \\ \frac{1}{\sqrt{2}}\left(a^\dagger_{\mathbf{k}1\uparrow} a^\dagger_{-\mathbf{k}2\downarrow} + a^\dagger_{\mathbf{k}1\downarrow} a^\dagger_{-\mathbf{k}2\uparrow}\right) & \text{for } m = 0 \;(S^z = 0) \end{array}\right. \,. \tag{2.20}$$

We recognize here the physical entities very similar to Cooper-pair operators [15], since for the pairs of particles defined by the above expressions wave vectors $\mathbf{k}$ are oriented in the opossite directions and thus their center of the mass momentum is equal to zero ($\mathbf{K} = 0$). However, the spin orientation is here different - the usual Cooper pair describes spin-singlet case, whereas the objects defined by (2.20) have an odd spin parity (i.e. the total spin $S = 1$).

Using the newly defined spin-triplet operators $A_{\mathbf{k}m}$, we can write the Hamiltonian transformed to momentum space in more compact form, namely

$$\begin{aligned}
\mathcal{H}_{HF} &= \sum_{\mathbf{k}l\sigma} (E_{\mathbf{k}l} - \mu - \sigma I \bar{S^z})\, n_{\mathbf{k}l\sigma} \\
&+ \sum_{\mathbf{k},m=-1,1} \left\{ \Delta_m^* A_{\mathbf{k},m} + A_{\mathbf{k},m}^\dagger \Delta_m \right\} + \sum_{\mathbf{k},m=0} \left\{ \sqrt{2}\Delta_0^* A_{\mathbf{k},0} + A_{\mathbf{k},0}^\dagger \sqrt{2}\Delta_0 \right\} \qquad (2.21) \\
&+ N \left\{ \frac{|\Delta_1|^2 + |\Delta_{-1}|^2 + 2|\Delta_0|^2}{2J} + 2I\bar{S^z}^2 \right\} ,
\end{aligned}$$

where we have introduced the gap parameters Δ_m defined by expressions

$$\Delta_{m=1} \equiv -\frac{2J}{N} \sum_{\mathbf{k}'} \langle A_{\mathbf{k}',1} \rangle = -\frac{2J}{N} \sum_{\mathbf{k}'} \langle a_{-\mathbf{k}'2\uparrow}\, a_{\mathbf{k}'1\uparrow} \rangle \qquad (2.22)$$

$$\Delta_{m=-1} \equiv -\frac{2J}{N} \sum_{\mathbf{k}'} \langle A_{\mathbf{k}',-1} \rangle = -\frac{2J}{N} \sum_{\mathbf{k}'} \langle a_{-\mathbf{k}'2\downarrow}\, a_{\mathbf{k}'1\downarrow} \rangle \qquad (2.23)$$

and

$$\begin{aligned}
\Delta_0 \equiv \Delta_{m=0} &\equiv -\frac{1}{\sqrt{2}} \frac{2J}{N} \sum_{\mathbf{k}'} \langle A_{\mathbf{k}',0} \rangle \\
&= -\frac{1}{2} \frac{2J}{N} \sum_{\mathbf{k}'} \left\{ \langle a_{-\mathbf{k}'2\downarrow}\, a_{\mathbf{k}'1\uparrow} \rangle + \langle a_{-\mathbf{k}'2\uparrow}\, a_{\mathbf{k}'1\downarrow} \rangle \right\} . \qquad (2.24)
\end{aligned}$$

For $\Delta_{m=0}$, the averages $\langle a_{-\mathbf{k}'2\downarrow}\, a_{\mathbf{k}'1\uparrow} \rangle$ and $\langle a_{-\mathbf{k}'2\uparrow}\, a_{\mathbf{k}'1\downarrow} \rangle$ are equal, since both describe amplitude of a paired state of indistinguishable particles located on different orbitals with their spins and wave vectors oriented in antiparallel. This results in a simplification of (2.24), which reduces to

$$\Delta_{m=0} = -\frac{2J}{N} \sum_{\mathbf{k}'} \langle a_{-\mathbf{k}'2\downarrow}\, a_{\mathbf{k}'1\uparrow} \rangle \ . \qquad (2.25)$$

Now we can write (2.22), (2.23) and (2.25) in a simpler form

$$\Delta_m = -\frac{2J}{N} \sum_{\mathbf{k}'} \langle a_{-\mathbf{k}'2\sigma}\, a_{\mathbf{k}'1\sigma'} \rangle \ , \qquad (2.26)$$

where $m = (\sigma + \sigma')/2$ and $\sigma,\ \sigma' = \pm 1$. All gap parameters are $\mathbf{k}$ *independent*, i.e. $\Delta_m \neq \Delta_m(\mathbf{k})$. This is a consequence of neglecting the hybridization of the band states in the described model.

The Hamiltonian (2.21) derived here will be used in the next Section as a starting point for introducing a generalized Bogoliubow-Nambu-de Gennes (4-dimensional) notation introduced by Klejnberg and Spałek (1999).

2.4 Generalized Bogoliubow-Nambu-de Gennes (four dimensional) notation

A generalized Nambu-Bogoliubow-de Gennes notation [9, 10, 16] is used in our approach in order to write down the Hamiltonian in a matrix form allowing an easy determination of its eigenvalues and, as a consequence, to determine the system of self-consistent equations for $\bar{S^z}$, Δ_m and the chemical potential μ. It was originally used in a 2-dimensional form to describe the spin-singlet pairs [13], [17]; here we adopt it to the case of spin-triplet pairing, which is quite nontrivial. The main benefit coming from using this approach is that the Hamiltonian written in matrix representation us to use standard algebraic methods for determining the energy eigenvalues and the eigenstate of the system in the paired state. One should note that in the following we regard the ground state with the filled Fermi volume as a vacuum state. In effect, the operator $a^{\dagger}_{\mathbf{k}\sigma}$ will describe the particle excitation, whereas the operatore $a_{-\mathbf{k}\sigma}$ the hole creation. This frazeology will be used in the remaining part of the Thesis.

We start from a slightly modified form of the Hamiltonian (2.21), namely

$$\begin{aligned}
\mathcal{H}_{HF} &= \sum_{\mathbf{k}\sigma} \left\{ (E_{\mathbf{k}1} - \mu - \sigma I \bar{S^z})\ a^{\dagger}_{\mathbf{k}1\sigma} a_{\mathbf{k}1\sigma} + (E_{\mathbf{k}2} - \mu - \sigma I \bar{S^z})\ a^{\dagger}_{\mathbf{k}2\sigma} a_{\mathbf{k}2\sigma} \right\} \\
&+ \sum_{\mathbf{k}} \left\{ \Delta_1^* a_{-\mathbf{k}2\uparrow} a_{\mathbf{k}1\uparrow} + \Delta_{-1}^* a_{-\mathbf{k}2\downarrow} a_{\mathbf{k}1\downarrow} + \Delta_0^* \left(a_{-\mathbf{k}2\downarrow} a_{\mathbf{k}1\uparrow} + a_{-\mathbf{k}2\uparrow} a_{\mathbf{k}1\downarrow} \right) + H.C. \right\} \\
&+ N \left\{ \frac{|\Delta_1|^2 + |\Delta_{-1}|^2 + 2|\Delta_0|^2}{2J} + 2I\bar{S^z}^2 \right\} ,
\end{aligned}$$

where we used the explicit expressions for spin-triplet pairing operators $A_{\mathbf{k}m}$ and $A^{\dagger}_{\mathbf{k}m}$, as well as have groupped the terms for convenience. If we count number of possible particle and antiparticle states represented by the operators $a^{\dagger}_{\mathbf{k}l\sigma}$ and $a_{-\mathbf{k}l\sigma}$, respectively, for wave vector $\mathbf{k}$, we will obtain 8 independent operators (i.e. $a^{\dagger}_{\mathbf{k}1\uparrow}$, $a^{\dagger}_{\mathbf{k}1\downarrow}$, $a^{\dagger}_{\mathbf{k}2\uparrow}$, $a^{\dagger}_{\mathbf{k}2\downarrow}$, $a_{-\mathbf{k}1\uparrow}$, $a_{-\mathbf{k}1\downarrow}$, $a_{-\mathbf{k}2\uparrow}$, and $a_{-\mathbf{k}2\downarrow}$) that could appear in the matrix representation. However, we can

reduce it to 4×4 form, if we make use of the mixed electron-hole picture considering particle from the band 1 and a hole from the band 2. In the other words, we simply convert the term representing particle energy in the $2nd$ band in the following manner

$$\begin{aligned}\sum_{\mathbf{k}\sigma}(E_{\mathbf{k}2} - \mu \;\; - \;\; \sigma I\bar{S}^z)\; a^\dagger_{\mathbf{k}2\sigma} a_{\mathbf{k}2\sigma} = \\ - \;\; \sum_{\mathbf{k}\sigma}(E_{\mathbf{k}2} - \mu - \sigma I\bar{S}^z)\; a_{-\mathbf{k}2\sigma} a^\dagger_{-\mathbf{k}2\sigma} + 2\sum_{\mathbf{k}} E_{\mathbf{k}2}\;, \end{aligned} \tag{2.27}$$

where we have substituted the identity $a^\dagger_{\mathbf{k}2\sigma} a_{\mathbf{k}2\sigma} = 1 - a_{\mathbf{k}2\sigma} a^\dagger_{\mathbf{k}2\sigma}$ arising from fermion anticommutation relations. We have also changed the sign of $\mathbf{k}$. Since the summation in (2.27) goes over all wave vectors $\mathbf{k}$ available in the momentum space, we have written $\sum_{-\mathbf{k}} \to \sum_{\mathbf{k}}$. The prefactor 2 in the front of the term $\sum_{\mathbf{k}} E_{\mathbf{k}2}$ results from the two possible spin orientations ($\sigma = \pm 1 \equiv \uparrow, \downarrow$).

In mixed particle-hole picture the Hamiltonian has the form

$$\begin{aligned}\mathcal{H}_{HF} \;\; &= \;\; \sum_{\mathbf{k}\sigma}\left\{(E_{\mathbf{k}1} - \mu - \sigma I\bar{S}^z)\; a^\dagger_{\mathbf{k}1\sigma} a_{\mathbf{k}1\sigma} - (E_{\mathbf{k}2} - \mu - \sigma I\bar{S}^z)\; a^\dagger_{\mathbf{k}2\sigma} a_{\mathbf{k}2\sigma}\right\} \\ &+ \;\; \sum_{\mathbf{k}}\Big\{\Delta_1^* a_{-\mathbf{k}2\uparrow} a_{\mathbf{k}1\uparrow} + \Delta_{-1}^* a_{-\mathbf{k}2\downarrow} a_{\mathbf{k}1\downarrow} + \Delta_0^*\left(a_{-\mathbf{k}2\downarrow} a_{\mathbf{k}1\uparrow} + a_{-\mathbf{k}2\uparrow} a_{\mathbf{k}1\downarrow}\right) \\ &+ \;\; \Delta_1 a^\dagger_{\mathbf{k}1\uparrow} a^\dagger_{-\mathbf{k}2\uparrow} + \Delta_{-1} a^\dagger_{\mathbf{k}1\downarrow} a^\dagger_{-\mathbf{k}2\downarrow} + \Delta_0\left(a^\dagger_{\mathbf{k}1\uparrow} a^\dagger_{-\mathbf{k}2\downarrow} + a^\dagger_{\mathbf{k}1\downarrow} a^\dagger_{-\mathbf{k}2\uparrow}\right)\Big\} \\ &+ \;\; 2\sum_{\mathbf{k}} E_{\mathbf{k}2} + N\left\{\frac{|\Delta_1|^2 + |\Delta_{-1}|^2 + 2|\Delta_0|^2}{2J} + 2I\bar{S}^{z\,2}\right\}\;. \end{aligned} \tag{2.28}$$

Now, we can introduce the four-dimensional notation by defining a composite creation operator (see Klejnberg and Spałek 1999, [9]) $\mathbf{f}^\dagger_{\mathbf{k}} = (a^\dagger_{\mathbf{k}1\uparrow}, a^\dagger_{\mathbf{k}1\downarrow}, a_{-\mathbf{k}2\uparrow}, a_{-\mathbf{k}2\downarrow})$, and the annihilation operator as a column $\mathbf{f}_{\mathbf{k}} = (\mathbf{f}^\dagger_{\mathbf{k}})^\dagger$. With their help we can construct 4x4 matrix representation of the Hamiltonian. Namely, it is straightforward to show that

$$\mathcal{H}_{HF} = \sum_{\mathbf{k}} \mathbf{f}^\dagger_{\mathbf{k}} \mathbf{H}_{\mathbf{k}} \mathbf{f}_{\mathbf{k}} + 2\sum_{\mathbf{k}} E_{\mathbf{k}2} + N\left\{\frac{|\Delta_1|^2 + |\Delta_{-1}|^2 + 2|\Delta_0|^2}{2J} + 2I\bar{S}^{z\,2}\right\} \tag{2.29}$$

with the Hamiltonian matrix of the form (for selected $\mathbf{k}$)

$$\mathbf{H}_{\mathbf{k}} = \begin{pmatrix} E_{\mathbf{k}1} - I\bar{S}^z, & 0, & \Delta_1, & \Delta_0 \\ 0, & E_{\mathbf{k}1} + I\bar{S}^z, & \Delta_0, & \Delta_{-1} \\ \Delta_1^*, & \Delta_0^*, & -E_{\mathbf{k}2} + I\bar{S}^z, & 0 \\ \Delta_0^*, & \Delta_{-1}^*, & 0, & -E_{\mathbf{k}2} - I\bar{S}^z \end{pmatrix}. \tag{2.30}$$

The quantities $E_{\mathbf{k}1} \equiv E_{\mathbf{k}1} - \mu$ and $E_{\mathbf{k}2} \equiv E_{\mathbf{k}2} - \mu$ are the band energies with the chemical potential as a reference point.

The Hamiltonian $\mathbf{H_k}$ can be written down in the compact form of 2x2 block matrix

$$\mathbf{H_k} = \begin{pmatrix} E_{\mathbf{k}1}\hat{\sigma}_0 - I\bar{S}^z\sigma_z, & \hat{\Delta} \\ \hat{\Delta}^*, & -E_{\mathbf{k}2}\hat{\sigma}_0 + I\bar{S}^z\sigma_z \end{pmatrix} , \tag{2.31}$$

where $\hat{\sigma}_0 \equiv \mathbf{1}$ stands for the unit 2x2 matrix and σ_z is one of the Pauli matrices. The matrix $\hat{\Delta}$ can be also defined in that case as

$$\hat{\Delta} = i(\mathbf{d}\cdot\tilde{\sigma})\sigma_y = \begin{pmatrix} -d_x + id_y, & d_z \\ d_z, & d_x + id_y \end{pmatrix} , \tag{2.32}$$

with the operator $\tilde{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, which consists of the three Pauli matrices

$$\sigma_x = \begin{pmatrix} 0, & 1 \\ 1, & 0 \end{pmatrix} , \quad \sigma_y = \begin{pmatrix} 0, & -i \\ i, & 0 \end{pmatrix} , \quad \text{and} \quad \sigma_z = \begin{pmatrix} 1, & 0 \\ 0, & -1 \end{pmatrix} , \tag{2.33}$$

and the vector $\mathbf{d}$ described in the spin space by the nonunitary-gap-parameter components $d_x = (\Delta_{-1} - \Delta_1)/2$, $d_y = -i(\Delta_{-1} + \Delta_1)/2$ and finally $d_z = \Delta_0$. The form of the Hamiltonian presented in Eq. (2.31) and parametrized with the help of the expressions introduced above is a generalization of the Nambu representation to the spin-triplet case with the three gap parameters Δ_m.

In the case of the degenerate energy bands ($E_{\mathbf{k}1} = E_{\mathbf{k}2} = E_{\mathbf{k}}$) and the real gap parameters ($\Delta_m = \Delta_m^*$), we can express (2.31) in terms of the 4x4 Dirac matrices (cf. Spałek (2001), [16])

$$\tilde{\beta} = \begin{pmatrix} \mathbf{1}, & 0 \\ 0, & \mathbf{-1} \end{pmatrix} \qquad \text{and} \qquad \tilde{\alpha}_i = \begin{pmatrix} 0, & \sigma_i \\ \sigma_i, & 0 \end{pmatrix} .$$

Hence, we have

$$\mathbf{H_k} = \tilde{\beta}\left[(E_{\mathbf{k}} - \mu)\,\mathbf{1} - I\bar{S}^z\,\Sigma_3\right] + i\,(\mathbf{d}\cdot\tilde{\alpha})\,\Sigma_2 , \tag{2.34}$$

where

$$\Sigma_2 = \begin{pmatrix} 0, & \sigma_y \\ \sigma_y, & 0 \end{pmatrix} \qquad \text{and} \qquad \Sigma_3 = \begin{pmatrix} \sigma_z, & 0 \\ 0, & \sigma_z \end{pmatrix}$$

are the y and z component of the relativistic spin operator, respectively.

In order to find the eigenstates of the matrix Hamiltonian $\mathbf{H_k}$ describe by the equation (2.34) we introduce the four component wave function

$$\hat{\Psi}(\mathbf{x}, t) = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} \begin{pmatrix} \psi_1\, a_{\mathbf{k}1\uparrow} \\ \psi_2\, a_{\mathbf{k}1\downarrow} \\ \psi_3\, a^{\dagger}_{-\mathbf{k}2\uparrow} \\ \psi_4\, a^{\dagger}_{-\mathbf{k}2\downarrow} \end{pmatrix} \exp\left[i\left(\mathbf{k}\cdot\mathbf{x} - \frac{E_{\mathbf{k}}}{\hbar}\,t\right)\right] \tag{2.35}$$

representing a single quasiparticle in the real space, with ψ_μ describing the quasiparticle amplitudes. The time-dependent Schrödinger equation written for that wave function yields

$$i\hbar\partial_t\hat{\Psi}(\mathbf{x},t) = \mathbf{H}_{\mathbf{k}\Rightarrow\frac{\nabla}{i}}\hat{\Psi}(\mathbf{x},t)\ , \tag{2.36}$$

where the wave vector $\mathbf{k}$ has been replaced in $\mathbf{H}_\mathbf{k}$ by the differential operator $(1/i)\nabla$. Inserting (2.34) and (2.35) into (2.36), we obtain the Bogolyubov-De Gennes equation in the form

$$i\hbar\partial_t\hat{\Psi}(\mathbf{x},t) = \tilde{\beta}\left\{(E_{\mathbf{k}\Rightarrow\frac{\nabla}{i}} - \mu)\ \mathbf{1} - I\bar{S}^z\ \Sigma_3\right\}\hat{\Psi}(\mathbf{x},t) + i\ (\mathbf{d}\cdot\tilde{\alpha})\ \Sigma_2\hat{\Psi}(\mathbf{x},t)\ . \tag{2.37}$$

Assuming the effective-mass approximation (i.e. energy of a quasiparticle can be estimated by its kinetic energy with the mass renormalized by the interactions) and the stationary case (then we limit our we considerations to the time-independent Schrödinger equation, i.e. $\mathbf{H}_{\mathbf{k}\Rightarrow\frac{\nabla}{i}}\hat{\Psi}(\mathbf{x},t) = \lambda\hat{\Psi}(\mathbf{x},t)$), we can finally write the wave equation for a single quasiparticle

$$\lambda\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{pmatrix} = -\left\{\left(\frac{\hbar^2}{2m^*}\nabla^2+\mu\right)\mathbf{1} + I\bar{S}^z\ \Sigma_3\right\}\begin{pmatrix}\psi_1\\ \psi_2\\ -\psi_3\\ -\psi_4\end{pmatrix} + \begin{pmatrix}\Delta_1\psi_3+\Delta_0\psi_4\\ \Delta_0\psi_3+\Delta_{-1}\psi_4\\ \Delta_1\psi_1+\Delta_0\psi_2\\ \Delta_0\psi_1+\Delta_{-1}\psi_2\end{pmatrix}\ , \tag{2.38}$$

where $\psi_\mu \equiv \psi_\mu(\mathbf{x})$ and λ is an eigenvalue of a quasiparticle state.

With the help of the wave equation derived above, eigenvalues and eigenvectors of Hamiltonian (2.29) can be found analytically. They will be used to derive system of nonlinear self-consistent equations for $\bar{S}^z$, Δ_m and the chemical potential μ. The knowledge of these quantities is necessary to determine the energetically stable solutions or, in the other words, the energetically preferred phases. A detailed discussion of these solutions is the subject of the following chapters. Our analysis of the model relies on the presumption that the isotropic part of the pairing leads already to qualitatively new features, which are only altered quantitatively when the realistic band structure is included. Hence, the hybridization among the bands can be neglected at this stage.

Chapter 3

Spin-triplet superconducting state

In this chapter we concentrate on discussing the basic properties of the superconducting spin-triplet state and its possible phases, which may appear in the system. Our considerations are based on the model formulated in the preceding chapter. For the sake of simplicity, we will neglect - for the time being - the ferromagnetic ordering and thus put $\bar{S}^z$ in the Hamiltonian (2.29) equal to zero, if an applied magnetic field is absent. We will include it later, when investigating the possibility of a coexistence of the spin-triplet superconducting state with the itinerant ferromagnetism and then behavior in an applied magnetic field.

For simplicity, we will also assume that the gap parameters do not have an imaginary part i.e. put $\Delta_m = \Delta_m^*$. This assumption is justified as long as the described system is spatialy homogenous - in that case the phase of the superconducting gap parameter can be neglected. Since we are focused rather on qualitative features of our results, we will limit our considerations to the case of the system with degenerate energy bands $E_{\mathbf{k}1} = E_{\mathbf{k}2} = E_{\mathbf{k}}$ (the analytic solution for $E_{\mathbf{k}1} \neq E_{\mathbf{k}2}$ was discussed in [16]; see also Appendix B).

Starting from the wave equation (2.38) with $\bar{S}^z = 0$, we will derive the results for the three principal phases: isotropic (all gap parameters Δ_m are equal), with equal spin pairs (only nonzero are the gap parameters with $m = -1$ and 1), and finally - totally polarized phase (only the gap parameter with $m = 1$ is nonzero). All these phases correspond to the phases B, A and $A1$ respectively, used for description of superfluidity of ^3He (see e.g. [18], [19]). This correspondence with ^3He should not be surprising, since in both systems the spin-triplet pairing is the main factor responsible for their extraordinary properties. Obviously, in the ^3He case the Cooper pairs are in the p-

orbital state (i.e. their angular momentum is $l = 1$). Here the pairing is *intraorbital* in nature, so the Copper pair has $l = 0$, if only orbital momentum of the electrons is either zero or quenched. For the convenience, we still use the nomenclature developed for superfluid ^3He to label the phases. The spin-orbit coupling is not important under these assumptions.

At the end of this chapter, we compare the properties of all three phases. We interprete the obtained results and discuss briefly their validity in the light of experiments performed on systems considered as candidates for the spin-triplet superconductors.

3.1 Solutions for the principal phases of the system

A brief analytical discussion of various superconducting phases, as well as the derivation of sets of self-consistent equations used to determine their basic parameters, can be found in [16]. Here we present briefly main results developed in that paper, as they will serve us as a starting point for detailed numerical calculations.

Following [16], we take the particle stationary amplitudes in the form $\psi_\mu(\mathbf{x}) = \frac{1}{V}\ \psi_\mu \exp(i\mathbf{k}\cdot\mathbf{x})$, where V is the volume of the system, and substitute them into the wave equation (2.38) with $\bar{S^z}$ put equal to zero, as assumed in the introduction to this chapter. In the effective mass approximation, we can also use the relation $-\frac{\hbar^2}{2m^*}\nabla^2\psi_\mu(\mathbf{x}) = E_\mathbf{k}\psi_\mu(\mathbf{x})$, in which $E_\mathbf{k}$ is the band energy of particles. In effect, the wave equation transforms to

$$\lambda \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = (E_\mathbf{k} - \mu) \begin{pmatrix} \psi_1 \\ \psi_2 \\ -\psi_3 \\ -\psi_4 \end{pmatrix} + \begin{pmatrix} \Delta_1\psi_3 + \Delta_0\psi_4 \\ \Delta_0\psi_3 + \Delta_{-1}\psi_4 \\ \Delta_1\psi_1 + \Delta_0\psi_2 \\ \Delta_0\psi_1 + \Delta_{-1}\psi_2 \end{pmatrix} . \tag{3.1}$$

In the general case we combine its components, handling particle (ψ_1 and ψ_2) and hole (ψ_3 and ψ_4) amplitudes separately. As a result, we obtain

$$\begin{cases} \lambda(\psi_1 - \psi_2) = (E_\mathbf{k} - \mu)(\psi_1 - \psi_2) + (\Delta_1 - \Delta_0)\psi_3 + (\Delta_0 - \Delta_{-1})\psi_4 \\ \lambda(\psi_3 - \psi_4) = -(E_\mathbf{k} - \mu)(\psi_3 - \psi_4) + (\Delta_1 - \Delta_0)\psi_1 + (\Delta_0 - \Delta_{-1})\psi_2 \end{cases} , \tag{3.2}$$

and

$$\begin{cases} \lambda(\psi_1 + \psi_2) = (E_\mathbf{k} - \mu)(\psi_1 + \psi_2) + (\Delta_1 + \Delta_0)\psi_3 + (\Delta_0 + \Delta_{-1})\psi_4 \\ \lambda(\psi_3 + \psi_4) = -(E_\mathbf{k} - \mu)(\psi_3 + \psi_4) + (\Delta_1 + \Delta_0)\psi_1 + (\Delta_0 + \Delta_{-1})\psi_2 \end{cases} . \tag{3.3}$$

The sets of equations developed above are used in the following sections for the calculation of particle (and hole) eigenstates.

3.1.1 Phase B - isotropic paired state

At the beginning, we consider the case of isotropic pairing in the system. It appears, when for all m the gap parameters are equal to each other, i.e. $\Delta_0 = \Delta_{-1} = \Delta_1 = \Delta$. Then Eqs. (3.2) and (3.3) take the from

$$\begin{cases} \lambda(\psi_1 - \psi_2) = (E_{\mathbf{k}} - \mu)(\psi_1 - \psi_2) \\ \lambda(\psi_3 - \psi_4) = -(E_{\mathbf{k}} - \mu)(\psi_3 - \psi_4) \end{cases} \tag{3.4}$$

and

$$\begin{cases} \lambda(\psi_1 + \psi_2) = (E_{\mathbf{k}} - \mu)(\psi_1 + \psi_2) + 2\Delta(\psi_3 + \psi_4) \\ \lambda(\psi_3 + \psi_4) = -(E_{\mathbf{k}} - \mu)(\psi_3 + \psi_4) + 2\Delta(\psi_1 + \psi_2) \end{cases} . \tag{3.5}$$

Eigenvalues λ constitute two classes of solutions - gapless and with a well defined energy gap in the energy spectrum.

The first two equations above lead to the gapless mode

$$\lambda_{\mathbf{k}1,2} = \pm(E_{\mathbf{k}} - \mu) . \tag{3.6}$$

Substituting the expression for $\lambda_{\mathbf{k}1,2}$ into (3.1), one can show that particle and hole amplitudes are equal to each other, i.e. $\psi_1 = \psi_2$ and $\psi_3 = \psi_4$. The equation (3.1) is also used for derivation of the form of the antisymmetric quasiparticle operators corresponding to the gapless mode (we must incorporate the normalization condition during the calculations additionally). Explicitly, we have

$$\begin{cases} \gamma_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left(a_{\mathbf{k}1\uparrow} - a_{\mathbf{k}1\downarrow} \right) \\ \delta^{\dagger}_{-\mathbf{k}} = \frac{1}{\sqrt{2}} \left(a^{\dagger}_{-\mathbf{k}2\uparrow} - a^{\dagger}_{-\mathbf{k}2\downarrow} \right) \end{cases} . \tag{3.7}$$

The last two equations (3.5) lead to the modes with the energy gap equal to 2Δ

$$\lambda_{\mathbf{k}3,4} = \pm\sqrt{(E_{\mathbf{k}} - \mu)^2 + (2\Delta)^2} \equiv \pm\lambda_{\mathbf{k}} , \tag{3.8}$$

with the new quasiparticle operators (derived in the same manner as the operators found for the gapless mode) in the form

$$\begin{cases} \alpha_{\mathbf{k}} = u_{\mathbf{k}} \frac{1}{\sqrt{2}} \left(a_{\mathbf{k}1\uparrow} + a_{\mathbf{k}1\downarrow} \right) + v_{\mathbf{k}} \frac{1}{\sqrt{2}} \left(a^{\dagger}_{-\mathbf{k}2\uparrow} + a^{\dagger}_{-\mathbf{k}2\downarrow} \right) \\ \beta^{\dagger}_{-\mathbf{k}} = -v_{\mathbf{k}} \frac{1}{\sqrt{2}} \left(a_{\mathbf{k}1\uparrow} + a_{\mathbf{k}1\downarrow} \right) + u_{\mathbf{k}} \frac{1}{\sqrt{2}} \left(a^{\dagger}_{-\mathbf{k}2\uparrow} - a^{\dagger}_{-\mathbf{k}2\downarrow} \right) \end{cases} . \tag{3.9}$$

Coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are the Bogolyubov coherence factors (well known from Bogolyubov-Valatin transformation used in the solution of classical BCS model)

$$u_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left(1 + \frac{E_{\mathbf{k}} - \mu}{\lambda_{\mathbf{k}}} \right)^{1/2} , \qquad v_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left(1 - \frac{E_{\mathbf{k}} - \mu}{\lambda_{\mathbf{k}}} \right)^{1/2} , \tag{3.10}$$

fulfilling the condition $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$. One can verify, that the operators $\alpha_{\mathbf{k}}$, $\beta_{\mathbf{k}}$, $\gamma_{\mathbf{k}}$ and $\delta_{\mathbf{k}}$ fulfil the fermion anticommutation relations.

The relation between "old" (we have started with) and new quasiparticle operators is defined by the transformation

$$\begin{pmatrix} a_{\mathbf{k}1\uparrow} \\ a_{\mathbf{k}1\downarrow} \\ a^{\dagger}_{-\mathbf{k}2\uparrow} \\ a^{\dagger}_{-\mathbf{k}2\downarrow} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} u_{\mathbf{k}}, & -v_{\mathbf{k}}, & 1, & 0 \\ u_{\mathbf{k}}, & -v_{\mathbf{k}}, & -1, & 0 \\ v_{\mathbf{k}}, & u_{\mathbf{k}}, & 0, & 1 \\ v_{\mathbf{k}}, & u_{\mathbf{k}}, & 0, & -1 \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{k}} \\ \beta^{\dagger}_{-\mathbf{k}} \\ \gamma_{\mathbf{k}} \\ \delta^{\dagger}_{-\mathbf{k}} \end{pmatrix} . \tag{3.11}$$

With its help we can express the Hamiltonian (2.29) in the diagonal form

$$\begin{aligned} \mathcal{H} &= \sum_{\mathbf{k}} \lambda_{\mathbf{k}} \left(\alpha^{\dagger}_{\mathbf{k}} \alpha_{\mathbf{k}} - \beta_{-\mathbf{k}} \beta^{\dagger}_{-\mathbf{k}} \right) + \sum_{\mathbf{k}} (E_{\mathbf{k}} - \mu) \left(\gamma^{\dagger}_{\mathbf{k}} \gamma_{\mathbf{k}} - \delta_{-\mathbf{k}} \delta^{\dagger}_{-\mathbf{k}} \right) \\ &\quad + 2 \sum_{\mathbf{k}} (E_{\mathbf{k}} - \mu) + N \frac{(2\Delta)^2}{2J} , \end{aligned} \tag{3.12}$$

and after making use of anticommutation relations, it can be reduced to

$$\begin{aligned} \mathcal{H} &= \sum_{\mathbf{k}} \lambda_{\mathbf{k}} \left(\alpha^{\dagger}_{\mathbf{k}} \alpha_{\mathbf{k}} + \beta^{\dagger}_{-\mathbf{k}} \beta_{-\mathbf{k}} - 1 \right) + \sum_{\mathbf{k}} (E_{\mathbf{k}} - \mu) \left(\gamma^{\dagger}_{\mathbf{k}} \gamma_{\mathbf{k}} + \delta^{\dagger}_{-\mathbf{k}} \delta_{-\mathbf{k}} \right) \\ &\quad + \sum_{\mathbf{k}} (E_{\mathbf{k}} - \mu) + N \frac{(2\Delta)^2}{2J} . \end{aligned} \tag{3.13}$$

In order to determine the ground state energy of the phase, we have to find expressions on the gap parameter Δ and the chemical potential μ.

Self-consistent gap equation.

Self-consistent equation for Δ can be derived from the definition (2.26). As we are considering isotropic phase, we can simply put e.g. $\Delta \equiv \Delta_1 = -\frac{2J}{N} \sum_{k'} \langle a_{-\mathbf{k}'2\uparrow}\, a_{\mathbf{k}'1\uparrow} \rangle$ and substitute the original operators $a_{\mathbf{k}l\sigma}$ expressed via new (quasiparticle) operators defined by the relation (3.11). Hence, the gap equation takes the form

$$\begin{aligned} \Delta &= -\frac{2J}{N} \sum_{\mathbf{k}'} \left\langle \frac{1}{\sqrt{2}} \left(v_{\mathbf{k}'} \alpha^{\dagger}_{\mathbf{k}'} + u_{\mathbf{k}'} \beta_{-\mathbf{k}'} + \delta_{-\mathbf{k}'} \right) \times \right. \\ &\qquad \left. \times \frac{1}{\sqrt{2}} \left(u_{\mathbf{k}'} \alpha_{\mathbf{k}'} - v_{\mathbf{k}'} \beta^{\dagger}_{-\mathbf{k}'} + \gamma_{\mathbf{k}'} \right) \right\rangle . \end{aligned}$$

The average <> is taken over the quasiparticle states and therefore, the only nonzero averages are proportional to $\left\langle \alpha^{\dagger}_{\mathbf{k}'} \alpha_{\mathbf{k}'} \right\rangle$ and $\left\langle \beta_{-\mathbf{k}'} \beta^{\dagger}_{-\mathbf{k}'} \right\rangle$. Thus, our self-consistent equation for Δ reduces to

$$\Delta = -\frac{J}{N} \sum_{\mathbf{k}'} \left\langle \left(u_{\mathbf{k}'} v_{\mathbf{k}'} \alpha^{\dagger}_{\mathbf{k}'} \alpha_{\mathbf{k}'} - v_{\mathbf{k}'} u_{\mathbf{k}'} \beta_{-\mathbf{k}'} \beta^{\dagger}_{-\mathbf{k}'} \right) \right\rangle . \tag{3.14}$$

Using anti-commutation relation for $\alpha_{\mathbf{k}'}$ operators, we can rewrite (3.14) as follows

$$\Delta = -\frac{J}{N}\sum_{\mathbf{k}'} u_{\mathbf{k}'}v_{\mathbf{k}'}\left(\left\langle\alpha^{\dagger}_{\mathbf{k}'}\alpha_{\mathbf{k}'}\right\rangle + \left\langle\beta^{\dagger}_{-\mathbf{k}'}\beta_{-\mathbf{k}'}\right\rangle - 1\right) . \tag{3.15}$$

Since both types of the quasiparticles defined by the operators $\alpha_{\mathbf{k}'}$ and $\beta_{-\mathbf{k}'}$ fulfil the same dispertion relation (3.8), the averages in the equation above are equal, i.e. $\left\langle\alpha^{\dagger}_{\mathbf{k}}\alpha_{\mathbf{k}}\right\rangle = \left\langle\beta^{\dagger}_{-\mathbf{k}}\beta_{-\mathbf{k}}\right\rangle$. The same type of identity can be written for the quasiparticles with gapless spectrum ($\gamma_{\mathbf{k}'}$ and $\delta_{-\mathbf{k}'}$). Therefore the gap equation simplifies to

$$\Delta = -\frac{J}{N}\sum_{\mathbf{k}'} u_{\mathbf{k}'}v_{\mathbf{k}'}\left(2\left\langle\alpha^{\dagger}_{\mathbf{k}'}\alpha_{\mathbf{k}'}\right\rangle - 1\right) . \tag{3.16}$$

The average number of the quasiparticles $\left\langle\alpha^{\dagger}_{\mathbf{k}'}\alpha_{\mathbf{k}'}\right\rangle$ is described by the Fermi-Dirac distribution function $f(\lambda_{\mathbf{k}}) = 1/(\exp(\beta\lambda_{\mathbf{k}}) + 1)$, where $\beta = (k_B T)^{-1}$. The quantity k_B is the Boltzmann constant and T stands for the absolute temperature. When we substitute this function into (3.16), we will obtain gap equation in the form

$$\Delta_1 = \frac{J}{N}\sum_{\mathbf{k}'} u_{\mathbf{k}'}v_{\mathbf{k}'}\tanh\left(\frac{\beta\lambda_{\mathbf{k}'}}{2}\right) . \tag{3.17}$$

In the last step, we shall expand the expression $u_{\mathbf{k}'}v_{\mathbf{k}'}$ substituting definitions of Bogoliubov coherence factors (3.10). As a result we will obtain gap equation very well known from BCS theory

$$\Delta = \frac{J}{N}\sum_{\mathbf{k}'}\frac{\Delta}{\lambda_{\mathbf{k}'}}\tanh\left(\frac{\beta\lambda_{\mathbf{k}'}}{2}\right) . \tag{3.18}$$

The solution of (3.18) with $\Delta = 0$ can be neglected as it represents the normal state. Therefore, the self-consistent equation for Δ takes the final form

$$1 = \frac{J}{N}\sum_{\mathbf{k}'}\frac{1}{\sqrt{(E_{\mathbf{k}'}-\mu)^2 + 4\Delta^2}}\tanh\left(\frac{\beta\sqrt{(E_{\mathbf{k}'}-\mu)^2 + 4\Delta^2}}{2}\right) . \tag{3.19}$$

Self-consistent equation for the chemical potential.

We determine now the self-constistent equation for the chemical potential μ starting from the condition that the number of particles in the system is fixed, i.e.

$$n = \frac{1}{N}\sum_{\mathbf{k}\sigma}\left\langle a^{\dagger}_{\mathbf{k}1\sigma}a_{\mathbf{k}1\sigma} + a^{\dagger}_{\mathbf{k}2\sigma}a_{\mathbf{k}2\sigma}\right\rangle , \tag{3.20}$$

where n represents the number of particles per atom. Inserting quasipaticle operators to the above equation, in the same manner as in the case of derivation of the self-consistent equation for the gap parameter Δ, and making use of the identities for the

corresponding expectation values of the operators (namely: $\left\langle \alpha^{\dagger}_{\mathbf{k}}\alpha_{\mathbf{k}}\right\rangle = \left\langle \beta^{\dagger}_{-\mathbf{k}}\beta_{-\mathbf{k}}\right\rangle$ and $\left\langle \gamma^{\dagger}_{\mathbf{k}}\gamma_{\mathbf{k}}\right\rangle = \left\langle \delta^{\dagger}_{-\mathbf{k}}\delta_{-\mathbf{k}}\right\rangle$) we obtain

$$n = \frac{2}{N}\sum_{\mathbf{k}}\left\{\left(u^2_{\mathbf{k}} - v^2_{\mathbf{k}}\right)\left\langle \alpha^{\dagger}_{\mathbf{k}}\alpha_{\mathbf{k}}\right\rangle + v^2_{\mathbf{k}} + \left\langle \gamma^{\dagger}_{\mathbf{k}}\gamma_{\mathbf{k}}\right\rangle\right\} . \tag{3.21}$$

After substitution of the expressions for the Bogolyubov coherence factors ($u_{\mathbf{k}}$, $v_{\mathbf{k}}$), the above equation transforms to the form

$$\begin{aligned} n-1 &= \frac{1}{N}\sum_{\mathbf{k}}\left\{\frac{E_{\mathbf{k}}-\mu}{\sqrt{(E_{\mathbf{k}}-\mu)^2+4\Delta^2}}\left(2\left\langle \alpha^{\dagger}_{\mathbf{k}}\alpha_{\mathbf{k}}\right\rangle - 1\right) + 2\left\langle \gamma^{\dagger}_{\mathbf{k}}\gamma_{\mathbf{k}}\right\rangle\right\} \\ &= \frac{1}{N}\sum_{\mathbf{k}}\left\{\frac{E_{\mathbf{k}}-\mu}{\sqrt{(E_{\mathbf{k}}-\mu)^2+4\Delta^2}}\left(2f(\lambda_{\mathbf{k}})-1\right) + 2f(E_{\mathbf{k}}-\mu)\right\} . \end{aligned} \tag{3.22}$$

Equations (3.19) and (3.22) constitute a set of self-consistent equations, which will be used to determine the values of the gap parameter Δ and the chemical potential μ

$$\left\{\begin{array}{c} 1 = \frac{J}{N}\sum_{\mathbf{k}'}\frac{1}{\sqrt{(E_{\mathbf{k}'}-\mu)^2+4\Delta^2}}\tanh\left(\frac{\beta\sqrt{(E_{\mathbf{k}'}-\mu)^2+4\Delta^2}}{2}\right) \\ n-1 = \frac{1}{N}\sum_{\mathbf{k}}\left\{\frac{E_{\mathbf{k}}-\mu}{\sqrt{(E_{\mathbf{k}}-\mu)^2+4\Delta^2}}\left(2f(\lambda_{\mathbf{k}})-1\right)+2f(E_{\mathbf{k}}-\mu)\right\} \end{array}\right. . \tag{3.23}$$

In the case of nonzero magnetic moment, the set should be supplemented with the self-consistent equation for $\bar{S^z}$ (c.f. the Section on coexistence of spin-triplet superconductivity with ferromagnetism).

Finally, we write expression for the ground state energy of the system, which is

$$\begin{aligned} \frac{E_G}{N} &\equiv \frac{\langle\mathcal{H}\rangle}{N} = \frac{1}{N}\sum_{\mathbf{k}}\left\{\lambda_{\mathbf{k}}\left(2\left\langle \alpha^{\dagger}_{\mathbf{k}}\alpha_{\mathbf{k}}\right\rangle - 1\right) + E_{\mathbf{k}}\left(2\left\langle \gamma^{\dagger}_{\mathbf{k}}\gamma_{\mathbf{k}}\right\rangle + 1\right)\right\} + \frac{(2\Delta)^2}{2J} \\ &= \frac{1}{N}\sum_{\mathbf{k}}\left\{\lambda_{\mathbf{k}}\left(2f(\lambda_{\mathbf{k}})-1\right) + (E_{\mathbf{k}}-\mu)\left(2f(E_{\mathbf{k}}-\mu)+1\right)\right\} + \frac{(2\Delta)^2}{2J} . \end{aligned} \tag{3.24}$$

Its minimal value selects the stable phase of the all the three possible discussed in this and the following chapters. This in turn, will allow for determining other properties of the system, such as e.g. specific heat.

3.1.2 Phase A - equal-spin paired state

Phase A is characterized by the condition that the gap parameter $\Delta_{m=0}$ is equal to zero and those with $m \pm 1$ are nonzero, namely $\Delta_{m=-1} \neq 0$ and $\Delta_{m=1} \neq 0$. In the

absence of magnetic field these two gaps are equal. However, when the applied magnetic field is switched on, they differ.

As previously, we start from the equation (3.1), but this time we combine first with third and second with fourth component. After adding and subtracking the corresponding terms, we obtain

$$\begin{cases} (\Delta_1 - \lambda)(\psi_1 + \psi_3) + (E_{\mathbf{k}} - \mu)(\psi_1 - \psi_3) = 0 \\ (E_{\mathbf{k}} - \mu)(\psi_1 + \psi_3) - (\Delta_1 + \lambda)(\psi_1 - \psi_3) = 0 \end{cases} \tag{3.25}$$

and

$$\begin{cases} (\Delta_{-1} - \lambda)(\psi_2 + \psi_4) + (E_{\mathbf{k}} - \mu)(\psi_2 - \psi_4) = 0 \\ (E_{\mathbf{k}} - \mu)(\psi_2 + \psi_4) - (\Delta_{-1} + \lambda)(\psi_2 - \psi_4) = 0 \end{cases} . \tag{3.26}$$

The solutions of the above equations separate into two - one for spin up and one for spin down. The eigenvalues are

$$\lambda_{\mathbf{k}1,2} = \pm\sqrt{(E_{\mathbf{k}} - \mu)^2 + \Delta_1^2} \equiv \pm\lambda_{\mathbf{k}}^{(+)}, \quad \lambda_{\mathbf{k}3,4} = \pm\sqrt{(E_{\mathbf{k}} - \mu)^2 + \Delta_{-1}^2} \equiv \pm\lambda_{\mathbf{k}}^{(-)} , \tag{3.27}$$

with corresponding quasiparticle operators characterizing, respectively, the eigenstates

$$\begin{cases} \alpha_{\mathbf{k}\uparrow} = u_{\mathbf{k}}^{(+)} a_{\mathbf{k}1\uparrow} + v_{\mathbf{k}}^{(+)} a_{-\mathbf{k}2\uparrow}^{\dagger} \\ \beta_{-\mathbf{k}\uparrow}^{\dagger} = -v_{\mathbf{k}}^{(+)} a_{\mathbf{k}1\uparrow} + u_{\mathbf{k}}^{(+)} a_{-\mathbf{k}2\uparrow}^{\dagger} \end{cases} \quad \text{and} \quad \begin{cases} \alpha_{\mathbf{k}\downarrow} = u_{\mathbf{k}}^{(-)} a_{\mathbf{k}1\downarrow} + v_{\mathbf{k}}^{(-)} a_{-\mathbf{k}2\downarrow}^{\dagger} \\ \beta_{-\mathbf{k}\downarrow}^{\dagger} = -v_{\mathbf{k}}^{(-)} a_{\mathbf{k}1\downarrow} + u_{\mathbf{k}}^{(-)} a_{-\mathbf{k}2\downarrow}^{\dagger} \end{cases} , \tag{3.28}$$

where $(+)$ stands for the spin up and $(-)$ for the spin down state. As we can see, the Bogolyubov coherence factors are dependent on the pair-spin orientation. Explicitly, we have

$$\begin{cases} u_{\mathbf{k}}^{(+)} = \frac{1}{\sqrt{2}} \left(1 + \frac{E_{\mathbf{k}} - \mu}{\lambda_{\mathbf{k}}^{(+)}}\right)^{1/2} \\ v_{\mathbf{k}}^{(+)} = \frac{1}{\sqrt{2}} \left(1 - \frac{E_{\mathbf{k}} - \mu}{\lambda_{\mathbf{k}}^{(+)}}\right)^{1/2} \end{cases} \quad \text{and} \quad \begin{cases} u_{\mathbf{k}}^{(-)} = \frac{1}{\sqrt{2}} \left(1 + \frac{E_{\mathbf{k}} - \mu}{\lambda_{\mathbf{k}}^{(-)}}\right)^{1/2} \\ v_{\mathbf{k}}^{(-)} = \frac{1}{\sqrt{2}} \left(1 - \frac{E_{\mathbf{k}} - \mu}{\lambda_{\mathbf{k}}^{(-)}}\right)^{1/2} \end{cases} . \tag{3.29}$$

Similarly, as in case of phase B, they obey normalization condition but this time written separately for spin "up" and for spin "down" case, i.e.

$$\left(u_{\mathbf{k}}^{(+)}\right)^2 + \left(v_{\mathbf{k}}^{(+)}\right)^2 = 1 \qquad \text{and} \qquad \left(u_{\mathbf{k}}^{(-)}\right)^2 + \left(v_{\mathbf{k}}^{(-)}\right)^2 = 1 . \tag{3.30}$$

Thus the coherence factors, as before, set the degree of mixing of particle and hole components in the pair bound state, expressed in the quasiparticle language. Using the conditions above, one can prove that the quasiparticle operators $\alpha_{\mathbf{k}\uparrow}$, $\alpha_{\mathbf{k}\downarrow}$, $\beta_{-\mathbf{k}\uparrow}^{\dagger}$ and $\beta_{-\mathbf{k}\downarrow}^{\dagger}$ fulfil fermion anticommutation relations.

All quasiparticle states have their spectrum gapped and this constitutes the main difference with the phase B considered in the preceding Subsection. The transformation between the bare particle and the quasiparticle representations is defined by the relation

$$\begin{pmatrix} a_{\mathbf{k}1\uparrow} \\ a_{\mathbf{k}1\downarrow} \\ a^{\dagger}_{-\mathbf{k}2\uparrow} \\ a^{\dagger}_{-\mathbf{k}2\downarrow} \end{pmatrix} = \begin{pmatrix} u^{(+)}_{\mathbf{k}}, & -v^{(+)}_{\mathbf{k}}, & 0, & 0 \\ 0, & 0, & u^{(-)}_{\mathbf{k}}, & -v^{(-)}_{\mathbf{k}} \\ v^{(+)}_{\mathbf{k}}, & u^{(+)}_{\mathbf{k}}, & 0, & 0 \\ 0, & 0, & v^{(-)}_{\mathbf{k}}, & u^{(-)}_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{k}\uparrow} \\ \beta^{\dagger}_{-\mathbf{k}\uparrow} \\ \alpha_{\mathbf{k}\downarrow} \\ \beta^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix} . \tag{3.31}$$

With its help we can derive the set of self-consistent equations for the gap parameters and the chemical potential μ in the same way as previously. This time, however, we have to consider two gap parameters - for spin up (Δ_1) and spin down (Δ_{-1}) orientations. Following the procedure presented in the preceding Subsection, we obtain the following set of equations:

- for the gap parameter Δ_1:

$$1 = \frac{J}{N} \sum_{\mathbf{k}'} \frac{1}{\sqrt{(E_{\mathbf{k}'} - \mu)^2 + \Delta_1^2}} \tanh \left(\frac{\beta \sqrt{(E_{\mathbf{k}'} - \mu)^2 + \Delta_1^2}}{2} \right) \tag{3.32}$$

- for the gap parameter Δ_{-1}:

$$1 = \frac{J}{N} \sum_{\mathbf{k}'} \frac{1}{\sqrt{(E_{\mathbf{k}'} - \mu)^2 + \Delta_{-1}^2}} \tanh \left(\frac{\beta \sqrt{(E_{\mathbf{k}'} - \mu)^2 + \Delta_{-1}^2}}{2} \right) \tag{3.33}$$

- for the chemical potential μ:

$$\begin{aligned} n - 2 \;\; = \;\; & \frac{1}{N} \sum_{\mathbf{k}} \left\{ \frac{E_{\mathbf{k}} - \mu}{\sqrt{(E_{\mathbf{k}} - \mu)^2 + \Delta_1^2}} \left(2f \left(\lambda^{(+)}_{\mathbf{k}} \right) - 1 \right) \right. \\ & \left. + \frac{E_{\mathbf{k}} - \mu}{\sqrt{(E_{\mathbf{k}} - \mu)^2 + \Delta_{-1}^2}} \left(2f \left(\lambda^{(-)}_{\mathbf{k}} \right) - 1 \right) \right\} \end{aligned} \tag{3.34}$$

The equations, as noted before, above are written for the cases of magnetic field absence and lack of ferromagnetic ordering. From analysis of (3.32) and (3.33), we come to the conclusion, that there is actually no difference between both the gaps, i.e. $\Delta_1 = \Delta_{-1} = \Delta$. Therefore, the set of equations reduces to two

$$\begin{cases} 1 = \frac{J}{N} \sum_{\mathbf{k}'} \frac{1}{\sqrt{(E_{\mathbf{k}'} - \mu)^2 + \Delta^2}} \tanh \left(\frac{\beta \sqrt{(E_{\mathbf{k}'} - \mu)^2 + \Delta^2}}{2} \right) \\ n - 2 = \frac{2}{N} \sum_{\mathbf{k}} \left\{ \frac{E_{\mathbf{k}} - \mu}{\sqrt{(E_{\mathbf{k}} - \mu)^2 + \Delta^2}} \left(2f \left(\lambda_{\mathbf{k}} \right) - 1 \right) \right\} \end{cases} , \tag{3.35}$$

where $\lambda_{\mathbf{k}} = \sqrt{(E_{\mathbf{k}} - \mu)^2 + \Delta^2}$. Obviously, this is not true when the magnetic field is present.

We derive next the expression for the total energy of the system (per site) starting from the effective Hamiltonian for the phase A in the diagonal form, i.e.

$$\begin{aligned} \mathcal{H} &= \sum_{\mathbf{k}} \left\{ \lambda_{\mathbf{k}}^{(+)} \left(\alpha_{\mathbf{k}\uparrow}^{\dagger} \alpha_{\mathbf{k}\uparrow} - \beta_{-\mathbf{k}\uparrow} \beta_{-\mathbf{k}\uparrow}^{\dagger} \right) + \lambda_{\mathbf{k}}^{(-)} \left(\alpha_{\mathbf{k}\downarrow}^{\dagger} \alpha_{\mathbf{k}\downarrow} - \beta_{-\mathbf{k}\downarrow} \beta_{-\mathbf{k}\downarrow}^{\dagger} \right) \right\} \\ &+ 2 \sum_{\mathbf{k}} (E_{\mathbf{k}} - \mu) + N \frac{\Delta_1^2 + \Delta_{-1}^2}{2J} \, . \end{aligned} \tag{3.36}$$

With help of anticommutation relations for the operators it can be recast as the expression

$$\begin{aligned} \mathcal{H} &= \sum_{\mathbf{k}} \left\{ \lambda_{\mathbf{k}}^{(+)} \left(\alpha_{\mathbf{k}\uparrow}^{\dagger} \alpha_{\mathbf{k}\uparrow} + \beta_{-\mathbf{k}\uparrow}^{\dagger} \beta_{-\mathbf{k}\uparrow} - 1 \right) + \lambda_{\mathbf{k}}^{(-)} \left(\alpha_{\mathbf{k}\downarrow}^{\dagger} \alpha_{\mathbf{k}\downarrow} + \beta_{-\mathbf{k}\downarrow}^{\dagger} \beta_{-\mathbf{k}\downarrow} - 1 \right) \right\} \\ &+ 2 \sum_{\mathbf{k}} (E_{\mathbf{k}} - \mu) + N \frac{\Delta_1^2 + \Delta_{-1}^2}{2J} \, . \end{aligned} \tag{3.37}$$

Hence, the equation for the ground energy of the system in phase A has the following form

$$\begin{aligned} \frac{E_G}{N} = \frac{\langle \mathcal{H} \rangle}{N} &= \frac{1}{N} \sum_{\mathbf{k}} \left\{ \lambda_{\mathbf{k}}^{(+)} \left(\left\langle \alpha_{\mathbf{k}\uparrow}^{\dagger} \alpha_{\mathbf{k}\uparrow} \right\rangle + \left\langle \beta_{-\mathbf{k}\uparrow}^{\dagger} \beta_{-\mathbf{k}\uparrow} \right\rangle - 1 \right) \right. \\ &\left. + \lambda_{\mathbf{k}}^{(-)} \left(\left\langle \alpha_{\mathbf{k}\downarrow}^{\dagger} \alpha_{\mathbf{k}\downarrow} \right\rangle + \left\langle \beta_{-\mathbf{k}\downarrow}^{\dagger} \beta_{-\mathbf{k}\downarrow} \right\rangle - 1 \right) \right\} \\ &+ \frac{2}{N} \sum_{\mathbf{k}} (E_{\mathbf{k}} - \mu) + \frac{\Delta_1^2 + \Delta_{-1}^2}{2J} \, . \end{aligned} \tag{3.38}$$

Since the operators $\alpha_{\mathbf{k}\sigma}$ and $\beta_{-\mathbf{k}\sigma}^{\dagger}$ represent the same dispersion relation, we can (again) make use of the identities $\left\langle \alpha_{\mathbf{k}\uparrow}^{\dagger} \alpha_{\mathbf{k}\uparrow} \right\rangle = \left\langle \beta_{-\mathbf{k}\uparrow}^{\dagger} \beta_{-\mathbf{k}\uparrow} \right\rangle \equiv f(\lambda_{\mathbf{k}}^{(+)})$ and $\left\langle \alpha_{\mathbf{k}\downarrow}^{\dagger} \alpha_{\mathbf{k}\downarrow} \right\rangle = \left\langle \beta_{-\mathbf{k}\downarrow}^{\dagger} \beta_{-\mathbf{k}\downarrow} \right\rangle \equiv f(\lambda_{\mathbf{k}}^{(-)})$. As a result, we obtain

$$\begin{aligned} \frac{E_G}{N} &= \frac{1}{N} \sum_{\mathbf{k}} \left\{ \lambda_{\mathbf{k}}^{(+)} \left(2 f(\lambda_{\mathbf{k}}^{(+)}) - 1 \right) + \lambda_{\mathbf{k}}^{(-)} \left(2 f(\lambda_{\mathbf{k}}^{(-)}) - 1 \right) \right\} \\ &+ \frac{2}{N} \sum_{\mathbf{k}} (E_{\mathbf{k}} - \mu) + \frac{\Delta_1^2 + \Delta_{-1}^2}{2J} \, . \end{aligned} \tag{3.39}$$

As the parameters specific for spin up and spin down states are the same (e.g. $\Delta_1 = \Delta_{-1} \equiv \Delta \Rightarrow \lambda_{\mathbf{k}}^{(+)} = \lambda_{\mathbf{k}}^{(-)} \equiv \lambda_{\mathbf{k}}$). This results in further simplification of expression for ground state energy. Namely, we have

$$\frac{E_G}{N} = \frac{2}{N} \sum_{\mathbf{k}} \left\{ \lambda_{\mathbf{k}} \left(2 f(\lambda_{\mathbf{k}}) - 1 \right) + (E_{\mathbf{k}} - \mu) \right\} + \frac{(\Delta)^2}{J} \, . \tag{3.40}$$

Next we use this equation for comparing the energies of phase A with those for the other two phases.

The main difference between the phases A and B is that the former does not posses gapless modes - both its quasiparticle branches does have a gapped spectrum.

3.1.3 Phase A1 - spin polarized state

As the last case we consider the spin-polarized or $A1$ (according to the superfluid ^3He nomenclature) phase. It is introduced by the assumption that only the gap parameter for the spin orientation corresponding to the magnetic field direction is non-zero, i.e. $\Delta_1 \neq 0$, whereas the remaining two gap parameters are equal to zero, $\Delta_{-1} = \Delta_0 \equiv 0$. This case is the most promising, since it is most likely the phase, where the coexistence of superconductivity and ferromagnetism can be realized.

We use the same set of equations as for phase A, namely (3.25)-(3.26), and put $\Delta_{-1} = 0$. As a result, the first two equations remain unchanged

$$\begin{cases} (\Delta_1 - \lambda)(\psi_1 + \psi_3) + (E_{\mathbf{k}} - \mu)(\psi_1 - \psi_3) = 0 \\ (E_{\mathbf{k}} - \mu)(\psi_1 + \psi_3) - (\Delta_1 + \lambda)(\psi_1 - \psi_3) = 0 \end{cases} \tag{3.41}$$

and the last two take the simplier form

$$\begin{cases} -\lambda(\psi_2 + \psi_4) + (E_{\mathbf{k}} - \mu)(\psi_2 - \psi_4) = 0 \\ (E_{\mathbf{k}} - \mu)(\psi_2 + \psi_4) - \lambda(\psi_2 - \psi_4) = 0 \end{cases} . \tag{3.42}$$

In contrast to the situation in phase A, we now obtain "gapped" and gapless quasiparticle branches for spin up and spin down subspaces, respectively

$$\lambda_{\mathbf{k}1,2} = \pm\sqrt{(E_{\mathbf{k}} - \mu)^2 + \Delta_1^2} \equiv \pm\lambda_{\mathbf{k}}^{(+)} \qquad \text{and} \qquad \lambda_{\mathbf{k}3,4} = \pm(E_{\mathbf{k}} - \mu) \, . \tag{3.43}$$

The corresponding eigenstates are

$$\begin{cases} \alpha_{\mathbf{k}\uparrow} = u_{\mathbf{k}}^{(+)} a_{\mathbf{k}1\uparrow} + v_{\mathbf{k}}^{(+)} a_{-\mathbf{k}2\uparrow}^{\dagger} \\ \beta_{-\mathbf{k}\uparrow}^{\dagger} = -v_{\mathbf{k}}^{(+)} a_{\mathbf{k}1\uparrow} + u_{\mathbf{k}}^{(+)} a_{-\mathbf{k}2\uparrow}^{\dagger} \end{cases} \qquad \text{and} \qquad \begin{cases} \alpha_{\mathbf{k}\downarrow} = a_{\mathbf{k}1\downarrow} \\ \beta_{-\mathbf{k}\downarrow}^{\dagger} = a_{-\mathbf{k}2\downarrow}^{\dagger} \end{cases} , \tag{3.44}$$

where $(+)$ stands for the spin up state. The definition of Bogoliubow coherence factors is exactly the same as for phase A (see Eq. (3.29)) and with the same normalization condition imposed on them, namely $\left(u_{\mathbf{k}}^{(+)}\right)^2 + \left(v_{\mathbf{k}}^{(+)}\right)^2 = 1$. The relation between the

bare particle and the new quasiparticle states is described by the transformation

$$\begin{pmatrix} a_{\mathbf{k}1\uparrow} \\ a_{\mathbf{k}1\downarrow} \\ a^{\dagger}_{-\mathbf{k}2\uparrow} \\ a^{\dagger}_{-\mathbf{k}2\downarrow} \end{pmatrix} = \begin{pmatrix} 0, & 0, & u^{(+)}_{\mathbf{k}}, & -v^{(+)}_{\mathbf{k}} \\ 1, & 0, & 0, & 0 \\ 0, & 0, & v^{(+)}_{\mathbf{k}}, & u^{(+)}_{\mathbf{k}} \\ 0, & 1, & 0, & 0 \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{k}\downarrow} \\ \beta^{\dagger}_{-\mathbf{k}\downarrow} \\ \alpha_{\mathbf{k}\uparrow} \\ \beta^{\dagger}_{-\mathbf{k}\uparrow} \end{pmatrix} . \tag{3.45}$$

Using the results presented above, we can derive the set of self-consistent equations for the gap parameter Δ_1 and the chemical potential μ. We follow exactly the same procedure as for the phases B and A. Explicitly, we have

$$\begin{cases} 1 = \frac{J}{N} \sum_{\mathbf{k}'} \frac{1}{\sqrt{(E_{\mathbf{k}'}-\mu)^2+(\Delta_1)^2}} \tanh\left(\frac{\beta\sqrt{(E_{\mathbf{k}'}-\mu)^2+(\Delta_1)^2}}{2}\right) \\ n-1 = \frac{1}{N}\sum_{\mathbf{k}} \left\{ \frac{E_{\mathbf{k}}-\mu}{\sqrt{(E_{\mathbf{k}}-\mu)^2+(\Delta_1)^2}} \left(2f\left(\lambda^{(+)}_{\mathbf{k}}\right)-1\right) + 2f(E_{\mathbf{k}}-\mu)\right\} \end{cases} . \tag{3.46}$$

Finally, we will write expression for the ground state energy of the system for the $A1$ phase. As previously, we start from the Hamiltonian in diagonal form (obtained with help of the transformation (3.45)), which yields

$$\begin{aligned} \mathcal{H} &= \sum_{\mathbf{k}} \left\{ \lambda^{(+)}_{\mathbf{k}} \left(\alpha^{\dagger}_{\mathbf{k}\uparrow}\alpha_{\mathbf{k}\uparrow} - \beta_{-\mathbf{k}\uparrow}\beta^{\dagger}_{-\mathbf{k}\uparrow}\right) + (E_{\mathbf{k}}-\mu)\left(\alpha^{\dagger}_{\mathbf{k}\downarrow}\alpha_{\mathbf{k}\downarrow} - \beta_{-\mathbf{k}\downarrow}\beta^{\dagger}_{-\mathbf{k}\downarrow}\right)\right\} \\ &\quad +2\sum_{\mathbf{k}}(E_{\mathbf{k}}-\mu) + N\frac{\Delta_1^2}{2J} , \end{aligned} \tag{3.47}$$

and after application of the anticommutation relations (obeyed by quasiparticle operators) transforms to the form

$$\begin{aligned} \mathcal{H} &= \sum_{\mathbf{k}} \left\{ \lambda^{(+)}_{\mathbf{k}} \left(\alpha^{\dagger}_{\mathbf{k}\uparrow}\alpha_{\mathbf{k}\uparrow} + \beta^{\dagger}_{-\mathbf{k}\uparrow}\beta_{-\mathbf{k}\uparrow} - 1\right)\right. \\ &\quad \left. +(E_{\mathbf{k}}-\mu)\left(\alpha^{\dagger}_{\mathbf{k}\downarrow}\alpha_{\mathbf{k}\downarrow} + \beta^{\dagger}_{-\mathbf{k}\downarrow}\beta_{-\mathbf{k}\downarrow} + 1\right)\right\} + N\frac{\Delta_1^2}{2J} . \end{aligned} \tag{3.48}$$

Hence, the equation on the ground state energy yields

$$\frac{E_G}{N} = \frac{1}{N}\sum_{\mathbf{k}} \left\{ \lambda^{(+)}_{\mathbf{k}} \left(2f(\lambda^{(+)}_{\mathbf{k}})-1\right) + (E_{\mathbf{k}}-\mu)\left(2f(E_{\mathbf{k}}-\mu)+1\right)\right\} + \frac{\Delta_1^2}{2J} \tag{3.49}$$

Now, we have a complete set of equations we use to compare the energies of the three principal phases of the system. We have already pointed out similarities and differences of phase $A1$ to phase A. When comparing phase $A1$ to phase B, we notice that both of them have gapless quasiparticle branch, but only the phase $A1$ quasiparticles posses well defined S^z value.

In the next Section we will present the numerical results obtained for all three phases. As a starting point, we use the equations derived in the last three sections.

3.2 Numerical results

The numerical calculations are performed for the theoretical model developed so far. Here we consider the system in the absence of applied magnetic field and without ferromagnetic ordering, i.e. we assume that both $B_a = 0$ and $\bar{S^z} = 0$. This last assumption eliminates the contributions coming from either the Zeeman term or the ferromagnetic-exchange field, responsible for ferromagnetic ordering. We include them in the next chapter when concentrating on the coexistence of superconductivity with itinerant ferromagnetism (cf. Chapter 4).

First, we transform the sets of self-consistent equations for the gaps and for the chemical potential μ to the dimensionless form, preparing the ground for numerical calculations. As the next step, we present the results for the numerical solutions of those equations for the case of nonzero temperature ($T \neq 0$). Finally, we compare basic physical quantities, such as the ground-state and internal energies and the specific heat for all three principal phases of the system.

3.2.1 Dimensionless form of the self-consistent equations

We recall once again the sets of self-consistent equations for the three considered phases:

- phase B

$$\begin{cases} 1 = \frac{J}{N}\sum_{\mathbf{k}'} \frac{1}{\sqrt{(E_{\mathbf{k}'}-\mu)^2+4\Delta^2}} \tanh\left(\frac{\beta\sqrt{(E_{\mathbf{k}'}-\mu)^2+4\Delta^2}}{2}\right) \\ n-1 = \frac{1}{N}\sum_{\mathbf{k}} \left\{ \frac{E_{\mathbf{k}}-\mu}{\sqrt{(E_{\mathbf{k}}-\mu)^2+4\Delta^2}} \left(2f(\lambda_{\mathbf{k}})-1\right) + 2f(E_{\mathbf{k}}-\mu) \right\} \end{cases},$$

- phase A

$$\begin{cases} 1 = \frac{J}{N}\sum_{\mathbf{k}'} \frac{1}{\sqrt{(E_{\mathbf{k}'}-\mu)^2+(\Delta^{(\pm)})^2}} \tanh\left(\frac{\beta\sqrt{(E_{\mathbf{k}'}-\mu)^2+(\Delta^{(\pm)})^2}}{2}\right) \\ n-2 = \frac{2}{N}\sum_{\mathbf{k}} \left\{ \frac{E_{\mathbf{k}}-\mu}{\sqrt{(E_{\mathbf{k}}-\mu)^2+(\Delta^{(\pm)})^2}} \left(2f\left(\lambda_{\mathbf{k}}^{(\pm)}\right)-1\right) \right\} \end{cases},$$

- phase $A1$

$$\begin{cases} 1 = \frac{J}{N}\sum_{\mathbf{k}'} \frac{1}{\sqrt{(E_{\mathbf{k}'}-\mu)^2+(\Delta_1)^2}} \tanh\left(\frac{\beta\sqrt{(E_{\mathbf{k}'}-\mu)^2+(\Delta_1)^2}}{2}\right) \\ n-1 = \frac{1}{N}\sum_{\mathbf{k}} \left\{ \frac{E_{\mathbf{k}}-\mu}{\sqrt{(E_{\mathbf{k}}-\mu)^2+(\Delta_1)^2}} \left(2f\left(\lambda_{\mathbf{k}}^{(+)}\right)-1\right) + 2f(E_{\mathbf{k}}-\mu) \right\} \end{cases}.$$

The summation over the wave vector $\mathbf{k}$ in the above equations can be replaced by an integration performed over the band energy E, according to the rule

$$\frac{1}{N}\sum_{\mathbf{k}} \longrightarrow \int dE\rho(E) \ ,$$

where $\rho(E)$ represents density of states (per atom per spin). For simplicity, we consider the case of "flat" density of energy states with $\rho(E) = 1/W$, where W is the bare bandwidth. If we set the integration range within the interval $[-W/2, W/2]$, we are be able to write the transformation rule in the form

$$\frac{1}{N}\sum_{\mathbf{k}} \longrightarrow \frac{1}{W}\int_{-W/2}^{W/2} dE \ . \tag{3.50}$$

Therefore, the most natural choice, when introducing dimensionless form of the equations, is to normalize all quantities to the bare bandwith W. In that case, the integral (3.50) can be rewritten as follows

$$\frac{1}{W}\int_{-W/2}^{W/2} dE \longrightarrow \int_{-1/2}^{1/2} d\epsilon \ , \tag{3.51}$$

where we have introduced dimensionless parameter ϵ representing the energy of quasiparticle relative to the energy bandwidth, i.e. $\epsilon = E/W$. We redefine all other quantities in the similar way, e.g. redefine $\Delta \longrightarrow \tilde{\Delta} \equiv \Delta/W$. As a result, we obtain the dimensionless form of the equations recalled at the beginning of this Section (note that all tilde-marked quantities are normalized according to the scheme presented above for the gap Δ). Namely,

- phase B

$$\begin{aligned} 1 &= \tilde{J}\int_{-1/2}^{1/2} d\epsilon \, \frac{1}{\tilde{\lambda}} \, \tanh\left(\frac{\tilde{\lambda}}{2\theta}\right) \\ n-1 &= \int_{-1/2}^{1/2} d\epsilon \left\{ \frac{\epsilon-\tilde{\mu}}{\tilde{\lambda}} \left(2f(\tilde{\lambda})-1\right) + 2f(\epsilon-\tilde{\mu}) \right\} \ , \end{aligned} \tag{3.52}$$

  where $\tilde{\lambda} = \sqrt{(\epsilon-\tilde{\mu})^2 + (2\tilde{\Delta}_B)^2}$;

- phase A

$$\begin{aligned} 1 &= \tilde{J}\int_{-1/2}^{1/2} d\epsilon \, \frac{1}{\tilde{\lambda}} \, \tanh\left(\frac{\tilde{\lambda}}{2\theta}\right) \\ n-2 &= 2\int_{-1/2}^{1/2} d\epsilon \, \frac{\epsilon-\tilde{\mu}}{\tilde{\lambda}} \left\{2f\left(\tilde{\lambda}\right)-1\right\} \ , \end{aligned} \tag{3.53}$$

  where $\tilde{\lambda} = \sqrt{(\epsilon-\tilde{\mu})^2 + (\tilde{\Delta}_A)^2}$;

- phase $A1$

$$\begin{aligned} 1 &= \tilde{J} \int_{-1/2}^{1/2} d\epsilon \, \frac{1}{\tilde{\lambda}} \tanh\left(\frac{\tilde{\lambda}}{2\theta}\right) \\ n-1 &= \int_{-1/2}^{1/2} d\epsilon \, \left\{ \frac{\epsilon - \tilde{\mu}}{\tilde{\lambda}} \left(2f\left(\tilde{\lambda}\right) - 1\right) + 2f(\epsilon - \tilde{\mu}) \right\} , \end{aligned} \tag{3.54}$$

where $\tilde{\lambda} = \sqrt{(\epsilon - \tilde{\mu})^2 + (\tilde{\Delta}_{A1})^2}$.

The parameter θ, which appears in the equations above, plays the role of dimensionless temperature defined by the relation $\theta = k_B T/W$.

We use the equations (3.52) - (3.54) to determine the solutions for the gap parameter(s) Δ and the chemical potential μ for each phase. Altering the parameter θ, we will be able to investigate their temperature dependence as well. From the technical point of view, this problem consists of solving a set of two non-linear integral equations.

3.2.2 Solutions for the gap parameters and the chemical potential

Solutions of Eqs. (3.52) - (3.54) are found with help of the self-consistent, or rather - the *iterative* method. The procedure is very straightforward. We describe it, taking as an example, the set of equations for the B phase, namely

$$\begin{aligned} 1 &= \tilde{J} \int_{-1/2}^{1/2} d\epsilon \, \frac{1}{\tilde{\lambda}} \, \tanh\left(\frac{\tilde{\lambda}}{2\theta}\right) \\ n-1 &= \int_{-1/2}^{1/2} d\epsilon \left\{ \frac{\epsilon - \tilde{\mu}}{\tilde{\lambda}} \left(2f(\tilde{\lambda}) - 1\right) + 2f(\epsilon - \tilde{\mu}) \right\} . \end{aligned}$$

In the first step, we determine the gap parameter $\Delta_{i=1}$ for the dimensionless temperature $\theta \simeq 0$ (note, that putting exactly $\theta = 0$ will cause the "division by zero" error). For this purpose, we solve the first equation from the set presented above using one of the standard numerical methods for root finding (e.g. *false position* or *secant* method). As the initial values of $\tilde{\mu}_{i=0}$ and $\tilde{\Delta}_{i=0}$, we take the chemical potential calculated for the normal state and the gap parameter obtained for that value of the chemical potential; in the case of $\theta = 0$, both expressions can be evaluated analytically. Once we have $\Delta_{i=1}$, we substitute it - together with $\tilde{\mu}_{i=0}$ - into the second equation, and determine the next value $\tilde{\mu}_{i=1}$. We repeat this procedure until a satisfactory accuracy is achieved, taking as an input for the next iteration ($i = j + 1$) the values of the gap parameter and the chemical potential obtained in the previous step ($i = j$). In order to obtain the

temperature dependence of both parameters, we simply repeat all steps presented above for the increased value of θ. We continue, until the critical temperature is reached, i.e. the obtained value of the gap parameter is equal (in terms of chosen accuracy) to zero.

In this section, we present the results obtained for $J/W = 0.1$ and for the band filling $n = 1$ (we should be away from the half filling, since the antiferromagnetic Slater state is stable then). The Hund's coupling constant J/W equal to 0.1 is chosen to satisfy the weak coupling limit. The case of $n = 1$ corresponds to the situation, when both bands are quarter-filled. One can easily show, that then the chemical potential value for the normal state in the limit of $\theta = 0$ is equal to $-1/4$ for the flat (rectangular) form of the bare density of states.

The chemical potential for the normal state

The expression for the chemical potential for the normal state can be derived from the equation (3.20), excplicitly

$$n = \frac{1}{N} \sum_{\mathbf{k}\sigma} \left\langle a^{\dagger}_{\mathbf{k}1\sigma} a_{\mathbf{k}1\sigma} + a^{\dagger}_{\mathbf{k}2\sigma} a_{\mathbf{k}2\sigma} \right\rangle \ .$$

The averages $\left\langle a^{\dagger}_{\mathbf{k}1\sigma} a_{\mathbf{k}1\sigma} \right\rangle$ and $\left\langle a^{\dagger}_{\mathbf{k}2\sigma} a_{\mathbf{k}2\sigma} \right\rangle$ are described by the Fermi-Dirac distribution function $f(E_{\mathbf{k}1} - \mu)$ and $f(E_{\mathbf{k}2} - \mu)$, respectively. For the case of degenerate energy bands, we can write $f(E_{\mathbf{k}1} - \mu) = f(E_{\mathbf{k}2} - \mu) \equiv f(E_{\mathbf{k}} - \mu)$, and then the equation above transforms to

$$n = \frac{4}{N} \sum_{\mathbf{k}} f(E_{\mathbf{k}} - \mu) \ , \tag{3.55}$$

where the prefactor 4 results from the summation over the spin and from the degeneracy. The dimensionless form of (3.55), obtained following the procedure presented in the previous Section, yields

$$n = 4 \int_{-1/2}^{1/2} d\epsilon \, f(\epsilon - \tilde{\mu}) \ . \tag{3.56}$$

In the limit of $\theta \to 0$, Fermi-Dirac function reduces to Heaviside step function $H(\tilde{\mu} - \epsilon)$. Hence, we have

$$n = 4 \int_{-1/2}^{1/2} d\epsilon \, H(\tilde{\mu} - \epsilon) = 4 \int_{-1/2}^{\tilde{\mu}} d\epsilon \cdot 1 = 4 \left(\tilde{\mu} + \frac{1}{2} \right) \ . \tag{3.57}$$

Substituting $n = 1$, we obtain $\tilde{\mu}_N = -1/4$.

Before we proceed with presentation of the results, we compare the sets of equations for the phases $A1$ and B. We notice, that they differ in definitions of the gap parameter

only. Hence, we can find the relation

$$\Delta_{A1} = 2\,\Delta_B\ . \tag{3.58}$$

With its help, we can evaluate the numerical results for both phases using only one common set of equations. As a consequence, we obtain the same chemical potential behavior for both $A1$ and B phase.

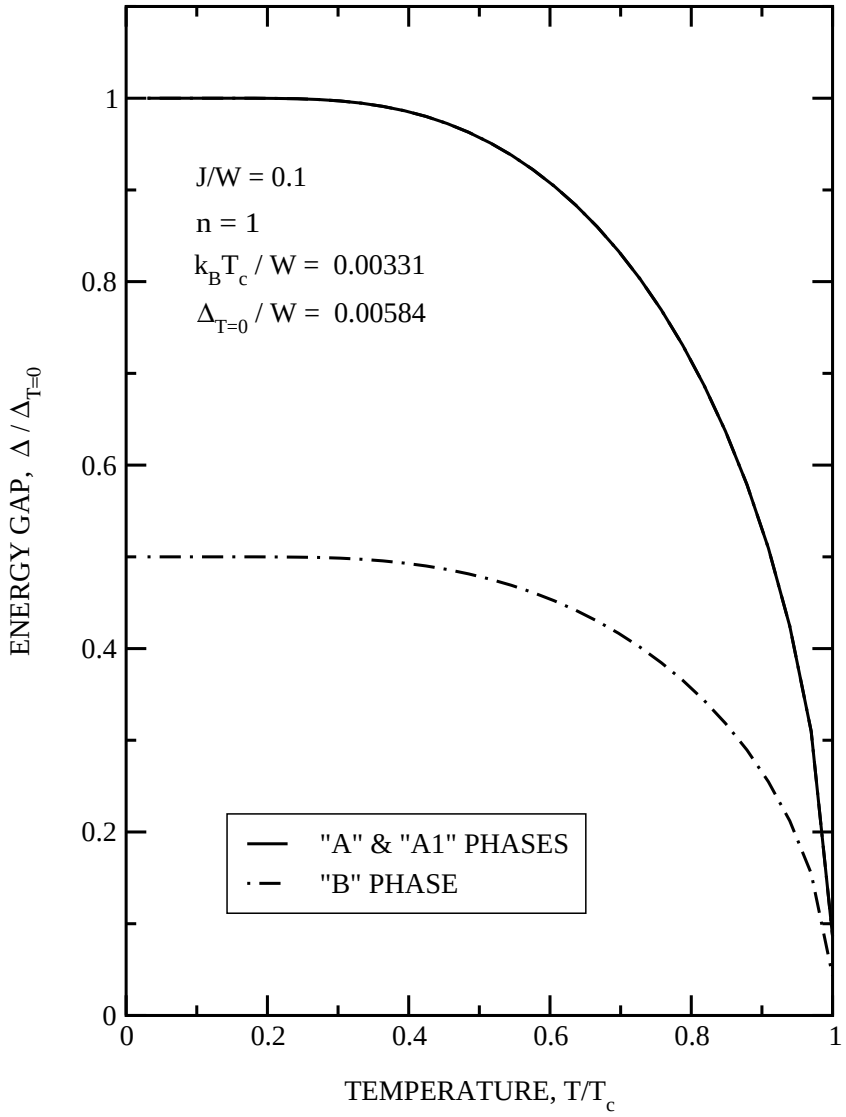

Figure 3.1: Temperature dependence of the gap parameter for all three superconducting phases.

The results evaluated from the numerical calculations are shown on Fig. 3.1 and 3.2. The gap parameters presented on both figures have been normalized to their values obtained for the $\theta \simeq 0$ case. The temperature has been presented in terms of the critical temperature θ_c - then, using the definition of $\theta = k_B T/W$, we can write directly $\theta/\theta_c = T/T_c$. The chemical potential shown in the inset of Fig. 3.2 has been expressed in the units of the energy bandwidth W.

The approximate values of the parameters characterizing each of the phases at the limit of $T = 0$ are as follows:

Parameter	Phase A	Phase A1	Phase B
$\tilde{\Delta}_{T=0}$	0.005835499	0.00583588	0.002917794
$\tilde{\mu}_{T=0}$	- 0.2500227	- 0.2500113	- 0.2500113

Table 3.1: The gap parameter and the chemical potential values for $T = 0$.

The gap parameter has nearly the same value (in terms of accuracy of numerical calculations) for phases A and $A1$, but is two times lower for the phase B. The chemical potential is the same for the phases $A1$ and B, whereas it is lower for the phase A. This means that the A phase is most stable energetically out of the three. If we consider this difference in relation to the chemical potential value for the normal state ($\tilde{\mu}_N = -0.25$), we notice that the chemical potential shift, defined as $\Delta\tilde{\mu} \equiv \tilde{\mu} - \tilde{\mu}_N$, is two times greater for the phase A.

The critical temperature T_c, determined by the condition $\tilde{\Delta} = 0$, has the same value for all three phases, and is equal to $\theta_c = k_B T_c/W = 3.31 * 10^{-3}$. In this case, Fermi-Dirac distribution function for the bare particles can be still well approximated by Heaviside function and therefore, the chemical potential value for the normal state for $\theta = \theta_c$ is practicaly the same as calculated for $\theta = 0$, namely $\tilde{\mu}_N = -0.25$.

Having calculated the values of the energy gaps at $T = 0$ and the critical temperature, we can check that the universal ratio

$$\frac{2\Delta_{T=0}}{k_B T_c} = 3.52 \tag{3.59}$$

characteristic for the BCS theory is fulfilled for all phases in our model. Namely, for the values of $\Delta_{T=0}$ and T_c presented above, we obtain the ratio value 3.53. Note, that for the phase B, its energy gap is equal to $2\Delta_B$ (see Eq. (3.8)), and thus the relation (3.59) is conserved for this phase as well.

Analysing Figs. 3.1 and 3.2, we notice that the temperature dependence of gap parameters obtained in our model exhibits a typical behavior characteristic for the BCS theory, which represents the mean-field theory, the same in all cases. All three gap parameters acquire the highest value at $T = 0$, and decrease gradually with the increasing temperature. All of them vanish, when the critical temperature T_c is reached - at this temperature the system undergoes the second-order phase transition from the superconducting to the normal state.

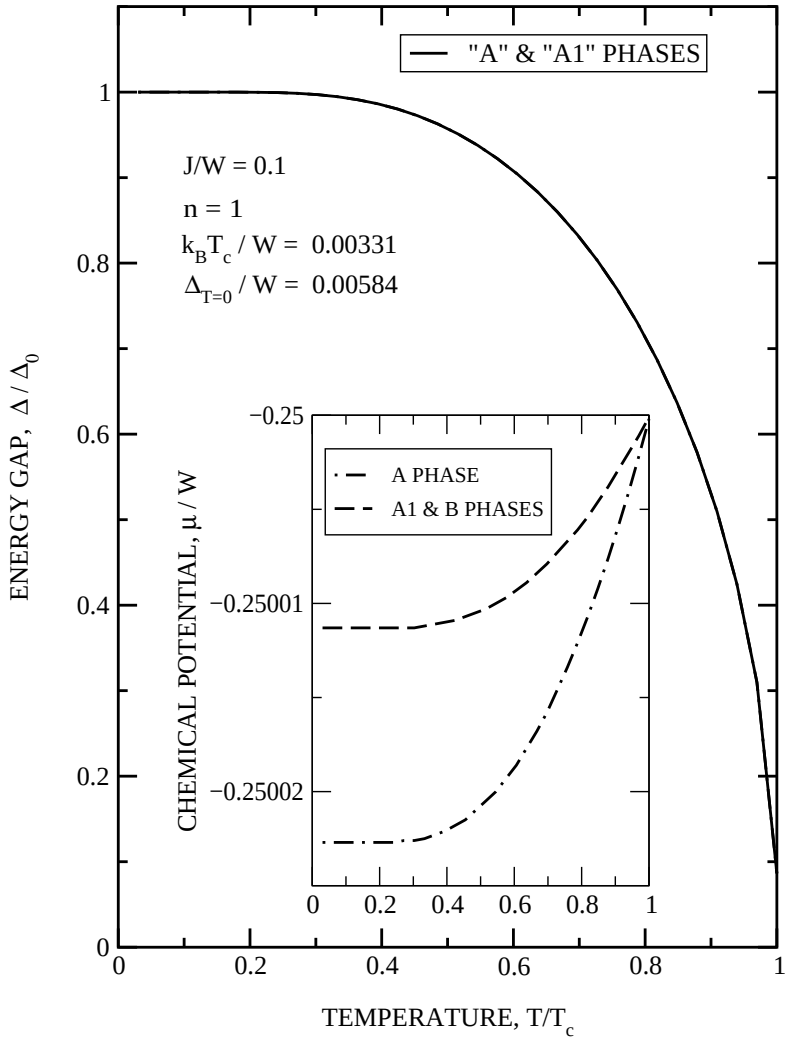

Figure 3.2: Temperature dependence of the gap parameters for the A and $A1$ phases. The inset shows the behavior of the chemical potential for all three superconducting phases.

The chemical potential behavior is complementary to the picture presented above. For $T \to 0$, it is lower for all three superconducting phases comparing to the normal state. This is a direct consequence of the existence of energy gaps in the system, what results in shifting of the chemical potential below its value characteristic for the normal state. The difference in the chemical potential shift between the phase A and the remaining phases arises from the fact, that only A phase has all quasiparticle modes gapped, whereas in the case of the phases $A1$ and B half of them is gapless. Hence, we can expect that the shift may be approximatelly two times greater for the phase A (cf. Fig. 3.2).

With the increasing temperature, the chemical potential for all three superconducting phases increases gradually and finally, for the critical temperature T_c, reaches the value characteristic for the normal state ($\tilde{\mu}_N \simeq -0.25$).

The results presented agree well with the standard behavior of a superconducting phase known from the BCS theory. They will be used in the next section as an input for the numerical calculations of the ground state energy for each phase.

3.2.3 Ground-state and internal energies and the specific heat

The internal energy for the phases B, A and $A1$ is determined from the Eqs. (3.24), (3.40), and (3.49), respectively. We transform them to the dimensionless form using the same procedure as presented previously in the Section 3.2.1. In effect, we obtain the following expressions

- phase B

$$\frac{E^B}{W} = \int_{-1/2}^{1/2} d\epsilon \, \left\{ \tilde{\lambda} \left(2f(\tilde{\lambda}) - 1 \right) + 2(\epsilon - \tilde{\mu}) f(\epsilon - \tilde{\mu}) + (\epsilon - \tilde{\mu}) \right\} + \frac{(2\tilde{\Delta}_B)^2}{2\tilde{J}} \,, \quad (3.60)$$

  where $\tilde{\lambda} = \sqrt{(\epsilon - \tilde{\mu})^2 + (2\tilde{\Delta}_B)^2}$;

- phase A

$$\frac{E^A}{W} = 2 \int_{-1/2}^{1/2} d\epsilon \, \left\{ \tilde{\lambda} \left(2f(\tilde{\lambda}) - 1 \right) + (\epsilon - \tilde{\mu}) \right\} + \frac{\tilde{\Delta}_A^2}{\tilde{J}} \,, \quad (3.61)$$

  where $\tilde{\lambda} = \sqrt{(\epsilon - \tilde{\mu})^2 + \tilde{\Delta}_A^2}$;

- phase $A1$

$$\frac{E^{A1}}{W} = \int_{-1/2}^{1/2} d\epsilon \, \left\{ \tilde{\lambda} \left(2f(\tilde{\lambda} - 1 \right) + 2(\epsilon - \tilde{\mu}) f(\epsilon - \tilde{\mu}) + (\epsilon - \tilde{\mu}) \right\} + \frac{\tilde{\Delta}_{A1}^2}{2\tilde{J}} \,, \quad (3.62)$$

where $\tilde{\lambda} = \sqrt{(\epsilon - \tilde{\mu})^2 + \tilde{\Delta}_{A1}^2}$.

Taking into account the relation between the gap parameters for the phases $A1$ and B, namely $2\tilde{\Delta}_B = \tilde{\Delta}_{A1}$, we notice that the ground state energy for these phases is described by the same equation, and thus is the same for both of them. Therefore, the phases $A1$ and B are energetically equivalent. As a result, we consider only two of the above three expressions, explicitly

- phase A

$$\frac{E^A}{W} = 2\int_{-1/2}^{1/2} d\epsilon\ \tilde{\lambda}\left(2f(\tilde{\lambda}) - 1\right) - 2\tilde{\mu} + \frac{\tilde{\Delta}_A^2}{\tilde{J}}\ , \tag{3.63}$$

- phases $A1$ and B

$$\frac{E^{A1}}{W} = \int_{-1/2}^{1/2} d\epsilon\ \left\{\tilde{\lambda}\left(2f(\tilde{\lambda} - 1\right) + 2(\epsilon - \tilde{\mu})f(\epsilon - \tilde{\mu}) + \right\} - \tilde{\mu} + \frac{\tilde{\Delta}_{A1}^2}{2\tilde{J}}\ , \tag{3.64}$$

where we have additionally evaluated the integral $\int_{-1/2}^{1/2} d\epsilon\ (\epsilon - \tilde{\mu}) = -\tilde{\mu}$. In order to obtain the temperature dependency of the internal energy, we simply calculate the expressions above for the temperatures from the interval $(0, \theta_c)$. For each considered temperature, the gap parameter $\tilde{\Delta}$ and the chemical potential $\tilde{\mu}$ must be evaluated according to the procedure presented in the previous section.

For the sake of comparison, we need to derive the equation for the internal energy of the normal state. It is defined as

$$\begin{aligned} E^N = \frac{\langle H_N \rangle}{N} &= \frac{1}{N}\sum_{\mathbf{k}l\sigma}(E_{\mathbf{k}l} - \mu_N)\left\langle a_{\mathbf{k}l\sigma}^\dagger a_{\mathbf{k}l\sigma}\right\rangle \\ &= \frac{1}{N}\sum_{\mathbf{k}l\sigma}(E_{\mathbf{k}l} - \mu_N)f(E_{\mathbf{k}l} - \mu_N)\ , \end{aligned} \tag{3.65}$$

where $f(E_{\mathbf{k}l} - \mu_N)$ is Fermi distribution function and μ_N is the chemical potential for the normal state. For the case of the degenerate energy bands and after carrying out the summation over the spin σ, we obtain

$$E^N = \frac{4}{N}\sum_{\mathbf{k}}(E_{\mathbf{k}} - \mu_N)f(E_{\mathbf{k}} - \mu_N)\ . \tag{3.66}$$

The dimensionless form of the above equation yields

$$\frac{E^N}{W} = 4\int_{-1/2}^{1/2} d\epsilon\ (\epsilon - \tilde{\mu}_N)f(\epsilon - \tilde{\mu}_N)\ . \tag{3.67}$$

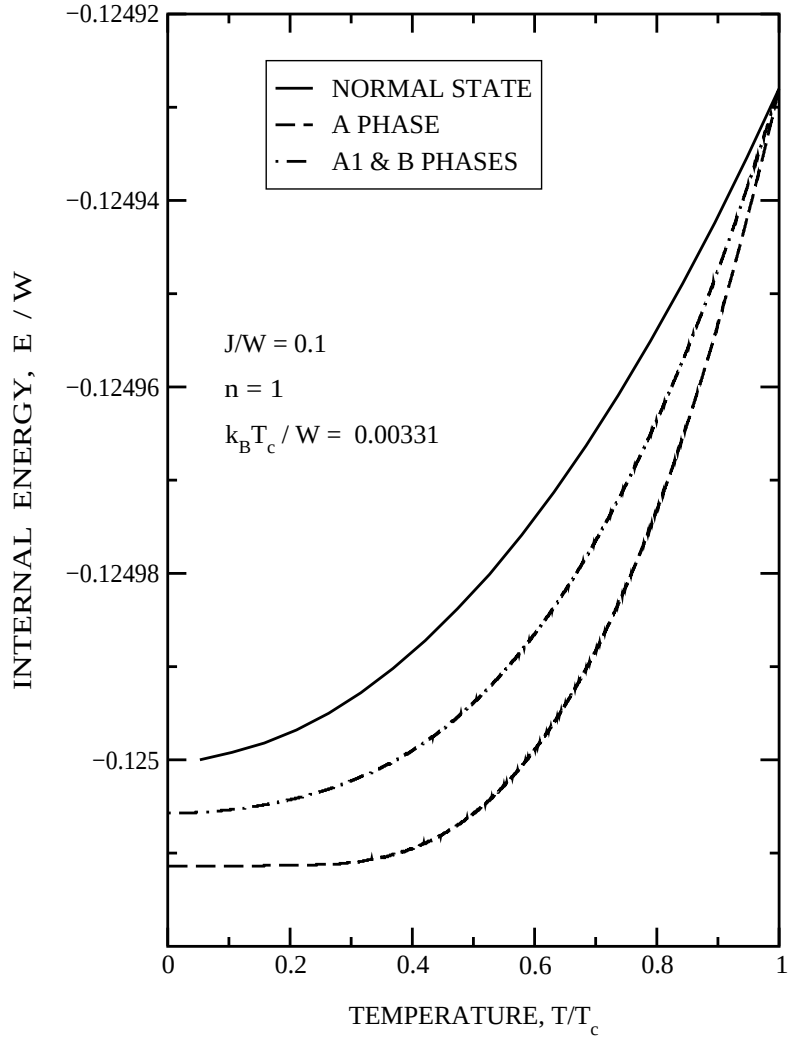

Figure 3.3: Temperature dependence of the ground state energy for all three superconducting phases. The normal state case is shown for comparison.

The temperature dependency of the internal energy for the superconducting phases and for the normal state is presented on Fig. 3.3. We notice, that (as expected) all the superconducting states are energetically lower than the normal state. Among them, the *A phase is the most stable* as it has the lowest ground state energy, since it is the only one, for which all quasiparticle modes are gapped (cf. interpretation of the results obtained for the chemical potential in the Section 3.2.2). The energy of the remaining two phases is higher due to the existence of gapless quasiparticle modes. The internal energies of all three phases increase gradually with the increasing temperature, since $\partial E/\partial T$ expresses the system heat capacity. In the limit of $\theta \to \theta_c$ ($T \to T_c$), they converge to the normal state values. At the critical temperature $\theta = \theta_c$, a second-order

phase transition from the superconducting to the normal state takes place.

Another important physical quantity, which will be presented in this section, is the specific heat (per site). It is evaluated directly from the internal energy by taking its derivative over the temperature, namely

$$c = \frac{\partial E}{\partial T} \,. \tag{3.68}$$

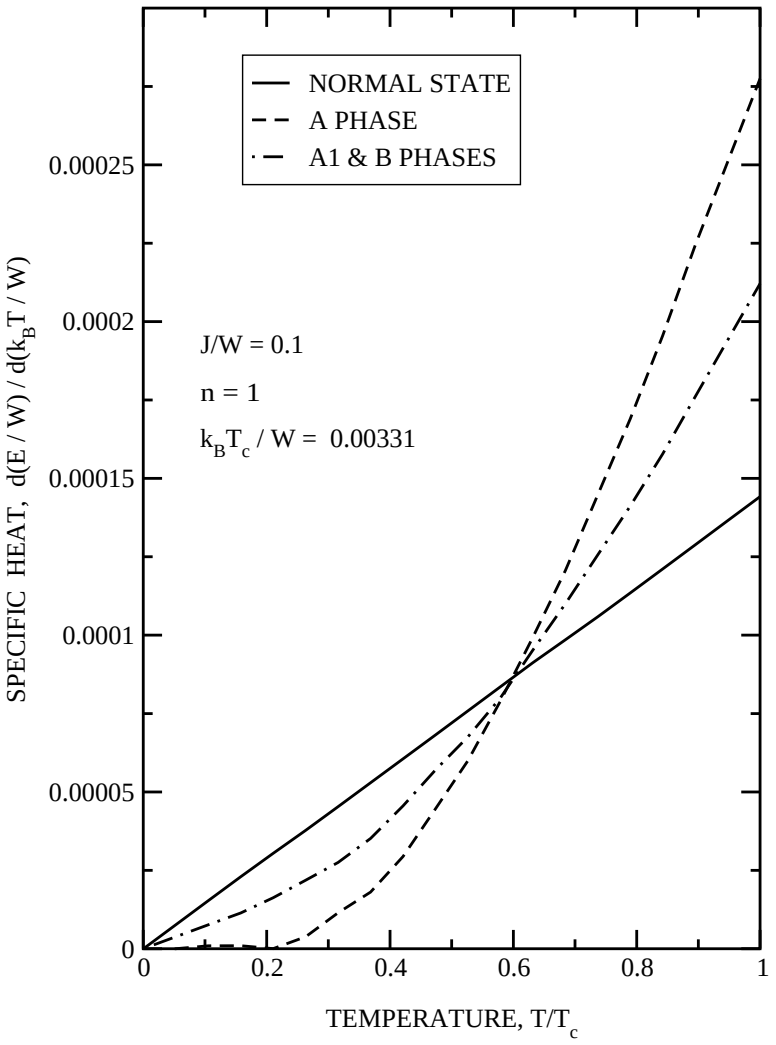

Figure 3.4: Temperature dependence of the specific heat (per site per eV) for the phases A, $A1$, and B. The normal state values are provided for comparison.

The results from the specific heat evaluation are shown on Fig. 3.4. The shape of the temperature dependence obtained for the phases A, $A1$, and B is typical for the

superconducting phase in the mean-field (BCS) approximation (c.f. e.g. M. Cyrot and D. Pavuna, [20] - Section 2.5), while the specific heat shown for the normal state exhibits the linear behavior, characteristic for the metallic state. As previously, the difference between the phase A and the remaining phases arises from the existence of the gapless modes in the phases $A1$ and B. In the first case, the contribution to the specific heat comes entirely from the exciting the paired electrons, whereas in the latter, it is the sum of contributions from the ungapped electron (normal) and the gapped states.

Analysing Fig. 3.4 we notice, that the specific heat jump at T_c, characteristic for the classical BCS superconductors ($\Delta C/C_{el} = 1.43$), is not recovered here. This is firstly the result of the temperature dependence of the chemical potential, which is not taken into account in the classic version of the BSC theory. More importantly, for $A1$ and B phase we have *gapless excitations* as well, which provide a contribution to the linear specific heat also in the superconducting state.

3.3 Summary of the basic properties of the system

In this Chapter we have analysed the basic properties of the two-band model of spin-triplet superconductivity in the absence of external magnetic field and without ferromagnetic ordering effects. We have considered three principal phases of the system: A - equal-spin paired state, $A1$ - spin polarized state, and B - isotropic paired state. We have shown, that the *phase A is the most stable phase*, as it has all quasiparticle states gapped. For the other two phases gapless modes appear even though the superconducting gap is $\mathbf{k}$-independent, thus making them less favorable energetically for the system. We have also shown the energetical equivalence (degeneracy) of the phases $A1$ and B.

In general, all three phases exhibit a typical BCS behavior such as the shape of the temperature dependences of the gap parameter and of the specific heat However, one must remember about the differencies between our model and the standard BCS theory; the most important among them is the different pairing mechanism originating from the Hund's rule introduced in real-space. As a result, we evaluate the physical quantities carrying out the integrations over the whole energy band, whereas in the BCS, the integration interval is limited by the Debye frequency regarded as a *cut-off* energy.

In the next chapter we focus on the influence of the applied magnetic field on the properties of the spin-triplet superconductivity. The main interest will be on the possibility of the coexistence of superconducting and ferromagnetic states.

Chapter 4

Magnetic properties of the spin-triplet superconducting state

In this chapter we investigate the *magnetic properties* of the two-band model of spin-triplet superconductivity. We assume that the system is spatially homogenouos and does not contain any impurities or defects. Under these circumstances and in the limit of weak magnetic field, vortices will not appear in the system. Additionally, we have shown in the Supplement that the ground state of an isolated spin-triplet pair is rather of the Landau-type than the p-type state. This means, that only the center-of-mass of the pair is rotating in the magnetic field, whereas the mutual orientation of the electrons constituting the pair remains largely unchanged in the space. Therefore, we can - as was done earlier - neglect the phases of the gap parameters Δ_m. In effect, all gap parameters are real, i.e. $\Delta^* \equiv \Delta$. This assumption is obviously valid only below the first critical field H_{c1}.

In the first Section, we consider the weak-field limit and derive the paramagnetic (spin) susceptibility for all three superconducting phases described in the previous chapter. We compare obtained results with those calculated for the BCS theory. In the last two sections, we focus on the influence of the ferromagnetic term, introduced to the Hamiltonian of the system, on its characteristic parameters and basic properties. Finally, we investigate the possible coexistence of the spin-triplet superconductivity with itinerant ferromagnetism [21, 22, 23]. For simplicity, we consider the absolute zero temperature case, $T = 0$.

4.1 Spin susceptibility in weak magnetic field

In order to derive the expression for the spin susceptibility, we have to add to Hamiltonian (2.29) the so-called Zeeman energy term $(-\mu_B B \int d^3r\ \psi^* \sigma \psi)$, which describes the interaction of spin moment of a particle with the external magnetic field. In the four dimensional representation (see Section 2.4) it takes the form

$$H_Z = -\mu_B B \sum_{\mathbf{k}} \mathbf{f}^\dagger_{\mathbf{k}} \begin{pmatrix} \sigma_z, & 0 \\ 0, & -\sigma_z \end{pmatrix} \mathbf{f}_{\mathbf{k}} \,, \tag{4.1}$$

where $\mathbf{f}^\dagger_{\mathbf{k}} = (a^\dagger_{\mathbf{k}1\uparrow}, a^\dagger_{\mathbf{k}1\downarrow}, a_{-\mathbf{k}2\uparrow}, a_{-\mathbf{k}2\downarrow})$ is the composite creation operator and σ_z is the z component of the Pauli spin operator. Addition of that term into the Hamiltonian (2.29) results in modification of diagonal elements of matrix $\mathbf{H_k}$, which for the case of degenerate energy bands and real gap parameters Δ, yields

$$\mathbf{H_k} = \begin{pmatrix} E_{\mathbf{k}} - \mathcal{E}_{B,\bar{S}^z}, & 0, & \Delta_1, & \Delta_0 \\ 0, & E_{\mathbf{k}} + \mathcal{E}_{B,\bar{S}^z}, & \Delta_0, & \Delta_{-1} \\ \Delta_1, & \Delta_0, & -E_{\mathbf{k}} + \mathcal{E}_{B,\bar{S}^z}, & 0 \\ \Delta_0, & \Delta_{-1}, & 0, & -E_{\mathbf{k}} - \mathcal{E}_{B,\bar{S}^z} \end{pmatrix} , \tag{4.2}$$

with $\mathcal{E}_{B,\bar{S}^z}$ defined as $I\bar{S}^z + \mu_B B$ and $E_{\mathbf{k}} \equiv E_{\mathbf{k}} - \mu$. This form of Hamiltonian will be used in the next sections, as it contains both ferromagnetic and Zeeman energy contributions. Here, we neglect the ferromagnetic $I\bar{S}^z$ term, as our aim is to calculate the paramagnetic spin susceptibility.

The eigenvalues of $\mathbf{H_k}$ are found in the straightforward manner, by solving the following eigen-equation

$$det \begin{pmatrix} E_{\mathbf{k}} - \mu_B B - \lambda, & 0, & \Delta_1, & \Delta_0 \\ 0, & E_{\mathbf{k}} + \mu_B B - \lambda, & \Delta_0, & \Delta_{-1} \\ \Delta_1, & \Delta_0, & -E_{\mathbf{k}} + \mu_B B - \lambda, & 0 \\ \Delta_0, & \Delta_{-1}, & 0, & -E_{\mathbf{k}} - \mu_B B - \lambda \end{pmatrix} = 0$$

for each phase. Hence, we have

- for phase B

$$\lambda^{1\ldots4}_{\mathbf{k}} = \pm\sqrt{E^2_{\mathbf{k}} + (\mu_B B)^2 + 2\Delta^2 \pm 2\sqrt{E^2_{\mathbf{k}}(\mu_B B)^2 + \Delta^2(\mu_B B)^2 + \Delta^4}} \,, \tag{4.3}$$

- for phase A

$$\lambda^{1,2}_{\mathbf{k}} = \pm\sqrt{(E_{\mathbf{k}} - \mu_B B)^2 + \Delta^2_\uparrow} \quad \text{and} \quad \lambda^{3,4}_{\mathbf{k}} = \pm\sqrt{(E_{\mathbf{k}} + \mu_B B)^2 + \Delta^2_\downarrow} \,, \tag{4.4}$$

- and finally, for phase $A1$

$$\lambda_{\mathbf{k}}^{1,2} = \pm\sqrt{(E_{\mathbf{k}} - \mu_B B)^2 + \Delta_{\uparrow}^2} \quad \text{and} \quad \lambda_{\mathbf{k}}^{3,4} = \pm(E_{\mathbf{k}} + \mu_B B) \; . \tag{4.5}$$

Note, that phase B (isotropic paired state) can be taken into account only in the weak field limit. In higher fields, it is impossible to fulfil the condition $\Delta_0 = \Delta_{-1} = \Delta_1 = \Delta_0 \equiv \Delta$, since each of the gap parameters will respond differently to the applied magnetic field.

Now, we can write the expression for the free energy of the system (per site)

$$\mathcal{F}(\lambda_{\mathbf{k}}^{(1)}, \; \ldots \; , \lambda_{\mathbf{k}}^{(4)}) = -\frac{k_B T}{N} \sum_{\mathbf{k}} \sum_{i=1\ldots4} \ln\left(1 - f(\lambda_{\mathbf{k}}^{(i)})\right) , \tag{4.6}$$

where $f(\lambda_{\mathbf{k}}^{(i)})$ is the Fermi-Dirac distribution function and $\lambda_{\mathbf{k}}^{(i)}$ represents one of the (four) eigenvalues calculated for a given phase. The index i is has been introduced to enumerate the solutions. In weak magnetic field, the free energy $\mathcal{F}$ can be expanded to the second order in B only, namely

$$\begin{aligned} \mathcal{F} \;\; (\lambda_{\mathbf{k}}^{(1)}(B), \; \ldots \; , \lambda_{\mathbf{k}}^{(4)}(B)) \;\; &\overset{B\to0}{\simeq} \;\; \mathcal{F}(\lambda_{\mathbf{k}}^{(1)}(0), \; \ldots \; , \lambda_{\mathbf{k}}^{(4)}(0)) \;\; + \\ &+ \left(\sum_{i=1\ldots4} \frac{\partial \mathcal{F}}{\partial \lambda_{\mathbf{k}}^{(i)}} \frac{\partial \lambda_{\mathbf{k}}^{(i)}}{\partial B} \bigg|_{B=0} \right) B \;\; + \;\; \frac{1}{2} \Bigg\{ \sum_{i=1\ldots4} \frac{\partial^2 \mathcal{F}}{\partial \left(\lambda_{\mathbf{k}}^{(i)}\right)^2} \left(\frac{\partial \lambda_{\mathbf{k}}^{(i)}}{\partial B} \right)^2 \Bigg|_{B=0} \; + \\ &+ \sum_{i=1\ldots4} \frac{\partial \mathcal{F}}{\partial \lambda_{\mathbf{k}}^{(i)}} \frac{\partial^2 \lambda_{\mathbf{k}}^{(i)}}{\partial B^2} \bigg|_{B=0} + \sum_{i,j=1\ldots4,\, i<j} \frac{\partial^2 \mathcal{F}}{\partial \lambda_{\mathbf{k}}^{(i)} \partial \lambda_{\mathbf{k}}^{(j)}} \frac{\partial \lambda_{\mathbf{k}}^{(i)}}{\partial B} \frac{\partial \lambda_{\mathbf{k}}^{(j)}}{\partial B} \bigg|_{B=0} \Bigg\} B^2 \; . \end{aligned} \tag{4.7}$$

The minimization condition requires the first derivative of $\mathcal{F}$ to be equal to zero, hence the second term in the expression above is dropped. The last term vanishes, since from the definition of the free energy (4.6) we have

$$\mathcal{F}(\lambda_{\mathbf{k}}^{(1)}, \; \ldots \; , \lambda_{\mathbf{k}}^{(4)}) = \sum_{i=1\ldots4} \mathcal{F}(\lambda_{\mathbf{k}}^{(i)})$$

and therefore,

$$\frac{\partial^2 \mathcal{F}}{\partial \lambda_{\mathbf{k}}^{(i)} \partial \lambda_{\mathbf{k}}^{(j)}} = 0 \; .$$

If we assume additionally, that the energy eigenvalues are considered only to the first order in B, then we can neglect the last but one term as well. In effect, the equation (4.7) reduces to the form

$$\begin{aligned} \mathcal{F}(\lambda_{\mathbf{k}}^{(1)}(B), \; \ldots \; , \lambda_{\mathbf{k}}^{(4)}(B)) \;\; &\simeq \;\; \mathcal{F}(\lambda_{\mathbf{k}}^{(1)}(0), \; \ldots \; , \lambda_{\mathbf{k}}^{(4)}(0)) \;\; + \\ &+ \;\; \frac{1}{2} \sum_{i=1\ldots4} \frac{\partial^2 \mathcal{F}}{\partial \left(\lambda_{\mathbf{k}}^{(i)}\right)^2} \left(\frac{\partial \lambda_{\mathbf{k}}^{(i)}}{\partial B} \right)^2 \Bigg|_{B=0} B^2 \; . \end{aligned} \tag{4.8}$$

By simple reasoning, one can show that $\partial\mathcal{F}/\partial\lambda_{\mathbf{k}}^{(i)} = -1/N \sum_{\mathbf{k}} f(\lambda_{\mathbf{k}}^{(i)})$, what results in the following final form of the expression for the free energy of the system

$$\begin{aligned} \mathcal{F}(\lambda_{\mathbf{k}}^{(1)}(B),\ \ldots\ ,\lambda_{\mathbf{k}}^{(4)}(B)) &\simeq \mathcal{F}(\lambda_{\mathbf{k}}^{(1)}(0),\ \ldots\ ,\lambda_{\mathbf{k}}^{(4)}(0)) + \\ &+ \frac{1}{2}\left\{-\frac{1}{N}\sum_{i=1\ldots4}\sum_{\mathbf{k}}\frac{\partial f(\lambda_{\mathbf{k}}^{(i)})}{\partial\lambda_{\mathbf{k}}^{(i)}}\left(\frac{\partial\lambda_{\mathbf{k}}^{(i)}}{\partial B}\right)^2\Bigg|_{B=0}\right\}B^2 . \end{aligned} \tag{4.9}$$

The quantity enclosed in the curly brackets is the spin susceptibility χ, explicitly

$$\chi = -\frac{1}{N}\sum_{i=1\ldots4}\sum_{\mathbf{k}}\frac{\partial f(\lambda_{\mathbf{k}}^{(i)})}{\partial\lambda_{\mathbf{k}}^{(i)}}\left(\frac{\partial\lambda_{\mathbf{k}}^{(i)}}{\partial B}\right)^2\Bigg|_{B=0} . \tag{4.10}$$

Substituting energy eigenvalues calculated earlier for the phases B, A and $A1$ (Eqs. (4.3)-(4.5)) to the above definition and evaluating the derivatives, we obtain expressions for the spin susceptibility for each phase. The obtained results are as follows

- phase B:

$$\chi_B \equiv 0 \tag{4.11}$$

- phase A:

$$\begin{aligned} \chi_A &= \frac{2\mu_B^2}{k_BT}\frac{1}{N}\sum_{\mathbf{k}}\left[\frac{\exp\left(\lambda_{\mathbf{k}}^{(1)}(0)/k_BT\right)}{\left[\exp\left(\lambda_{\mathbf{k}}^{(1)}(0)/k_BT\right)+1\right]^2}\frac{E_{\mathbf{k}}^2}{E_{\mathbf{k}}^2+\Delta_\uparrow^2(0)} + \right. \\ &\left. + \frac{\exp\left(\lambda_{\mathbf{k}}^{(3)}(0)/k_BT\right)}{\left[\exp\left(\lambda_{\mathbf{k}}^{(3)}(0)/k_BT\right)+1\right]^2}\frac{E_{\mathbf{k}}^2}{E_{\mathbf{k}}^2+\Delta_\downarrow^2(0)}\right] \end{aligned} \tag{4.12}$$

- phase $A1$:

$$\begin{aligned} \chi_{A1} &= \frac{2\mu_B^2}{k_BT}\frac{1}{N}\sum_{\mathbf{k}}\left[\frac{\exp\left(\lambda_{\mathbf{k}}^{(1)}(0)/k_BT\right)}{\left[\exp\left(\lambda_{\mathbf{k}}^{(1)}(0)/k_BT\right)+1\right]^2}\frac{E_{\mathbf{k}}^2}{E_{\mathbf{k}}^2+\Delta_\uparrow^2(0)} + \right. \\ &\left. + \frac{\exp\left(\lambda_{\mathbf{k}}^{(3)}(0)/k_BT\right)}{\left[\exp\left(\lambda_{\mathbf{k}}^{(3)}(0)/k_BT\right)+1\right]^2}\right] , \end{aligned} \tag{4.13}$$

where we have made use of the relations $f\left(\lambda_{\mathbf{k}}^{(1)}\right) = f\left(\lambda_{\mathbf{k}}^{(2)}\right)$ and $f\left(\lambda_{\mathbf{k}}^{(3)}\right) = f\left(\lambda_{\mathbf{k}}^{(4)}\right)$, valid for all phases (note the pre-factor 2 in expressions for A and $A1$ phases). As we have shown in the previous Chapter, in the case of absence of external field ($B = 0$) the gap parameters Δ_{-1} and Δ_1 calculated for the phase A are equivalent. Hence, we

can put $\Delta_\uparrow(0) = \Delta_\downarrow(0) \equiv \Delta_A$ and, as a consequence, $\lambda^{(1)}_{\mathbf{k}}(0) = \lambda^{(3)}_{\mathbf{k}}(0) \equiv \lambda^A_{\mathbf{k}}$, where $\lambda^A_{\mathbf{k}} = \sqrt{E^2_{\mathbf{k}} + \Delta^2_A}$. In effect, Eq. (4.12) simplifies to

$$\chi_A = \frac{4\mu_B^2}{k_B T}\frac{1}{N}\sum_{\mathbf{k}}\left[\frac{\exp\left(\lambda^A_{\mathbf{k}}/k_BT\right)}{\left[\exp\left(\lambda^A_{\mathbf{k}}/k_BT\right)+1\right]^2}\,\frac{E^2_{\mathbf{k}}}{E^2_{\mathbf{k}}+\Delta^2_A}\right] . \tag{4.14}$$

Similarly, we notice that the "zero" field case implies the following identities for the phase $A1$: $\Delta_\uparrow(0) \equiv \Delta_{A1}$, what results in $\lambda^{(1)}_{\mathbf{k}}(0) = \sqrt{E^2_{\mathbf{k}} + \Delta^2_{A1}} \equiv \lambda^{A1}_{\mathbf{k}}$, and finally, $\lambda^{(3)}_{\mathbf{k}}(0) \equiv E_{\mathbf{k}}$. Therefore, Eq. (4.13) reads

$$\begin{aligned}\chi_{A1} \;=\; \frac{2\mu_B^2}{k_B T}\frac{1}{N}\sum_{\mathbf{k}}\Bigg[&\frac{\exp\left(\lambda^{A1}_{\mathbf{k}}/k_BT\right)}{\left[\exp\left(\lambda^{A1}_{\mathbf{k}}/k_BT\right)+1\right]^2}\,\frac{E^2_{\mathbf{k}}}{E^2_{\mathbf{k}}+\Delta^2_{A1}} + \\ &+\frac{\exp\left(E_{\mathbf{k}}/k_BT\right)}{\left[\exp\left(E_{\mathbf{k}}/k_BT\right)+1\right]^2}\Bigg] .\end{aligned} \tag{4.15}$$

For the flat density of states considered earlier, namely $\rho(E) = 1/W$, we rewrite the above expressions to the form

$$\chi_A = \frac{4\mu_B^2}{W\,\theta}\int_{-1/2}^{1/2} d\epsilon\,\left\{\frac{\exp\left(\tilde\lambda^A/\theta\right)}{\left[\exp\left(\tilde\lambda^A/\theta\right)+1\right]^2}\,\frac{(\epsilon-\tilde\mu)^2}{(\epsilon-\tilde\mu)^2+\tilde\Delta^2_A}\right\} \tag{4.16}$$

and

$$\chi_{A1} = \frac{2\mu_B^2}{W\,\theta}\int_{-1/2}^{1/2} d\epsilon\,\left\{\frac{\exp\left(\frac{\tilde\lambda^{A1}}{\theta}\right)}{\left[\exp\left(\frac{\tilde\lambda^{A1}}{\theta}\right)+1\right]^2}\,\frac{(\epsilon-\tilde\mu)^2}{(\epsilon-\tilde\mu)^2+\tilde\Delta^2_{A1}} + \frac{\exp\left(\frac{\epsilon-\tilde\mu}{\theta}\right)}{\left[\exp\left(\frac{\epsilon-\tilde\mu}{\theta}\right)+1\right]^2}\right\} , \tag{4.17}$$

where, as previously, $\epsilon \equiv E/W$, $\theta \equiv k_BT/W$. All tilde-marked quantities are expressed in units of energy bandwidth W.

Spin susceptibility in the normal state

For comparison, we calculate the spin susceptibility for the normal state. In the external magnetic field, its energy is modified by the term $\pm\mu_B B$, dependently on the spin orientation of a single particle. Explicitly, we have

$$\lambda^{1,2}_{\mathbf{k}\uparrow} = \pm(E_{\mathbf{k}} - \mu_B B) \quad \text{and} \quad \lambda^{3,4}_{\mathbf{k}\downarrow} = \pm(E_{\mathbf{k}} + \mu_B B) , \tag{4.18}$$

with the derivatives

$$\frac{\partial\lambda^{1,2}_{\mathbf{k}\uparrow}}{\partial B} = \mp\mu_B B \quad \text{and} \quad \frac{\partial\lambda^{3,4}_{\mathbf{k}\downarrow}}{\partial B} = \pm\mu_B B . \tag{4.19}$$

Substituting (4.19) into (4.10), we obtain

$$\chi_N = -\frac{1}{N}\,\mu_B^2 \sum_{i=1\ldots4}\sum_{\mathbf{k}} \frac{\partial f(\lambda_{\mathbf{k}}^{(i)})}{\partial \lambda_{\mathbf{k}}^{(i)}}\bigg|_{B=0} \tag{4.20}$$

$$= \frac{2}{N}\,\frac{\mu_B^2}{k_BT} \sum_{\mathbf{k}} \left\{ \frac{\exp\left(\lambda_{\mathbf{k}}^{(1)}(0)/k_BT\right)}{\left[\exp\left(\lambda_{\mathbf{k}}^{(1)}(0)/k_BT\right)+1\right]^2} + \frac{\exp\left(\lambda_{\mathbf{k}}^{(3)}(0)/k_BT\right)}{\left[\exp\left(\lambda_{\mathbf{k}}^{(3)}(0)/k_BT\right)+1\right]^2} \right\},$$

where we used, again, the relations $f\left(\lambda_{\mathbf{k}}^{(1)}\right) = f\left(\lambda_{\mathbf{k}}^{(2)}\right)$ and $f\left(\lambda_{\mathbf{k}}^{(3)}\right) = f\left(\lambda_{\mathbf{k}}^{(4)}\right)$. Furthermore, we notice that $\lambda_{\mathbf{k}}^{(1)}(0) = \lambda_{\mathbf{k}}^{(3)}(0) = E_{\mathbf{k}}$. In effect, the Equation (4.20) reduces to the form

$$\chi_N = \frac{4}{N}\,\frac{\mu_B^2}{k_BT} \sum_{\mathbf{k}} \frac{\exp\left(E_{\mathbf{k}}/k_BT\right)}{\left[\exp\left(E_{\mathbf{k}}/k_BT\right)+1\right]^2}, \tag{4.21}$$

which, for the flat density of states $1/W$, can be rewritten as follows

$$\chi_N = \frac{4\mu_B^2}{W\,\theta}\int_{-1/2}^{1/2} d\epsilon\, \frac{\exp\left(\frac{\epsilon-\tilde{\mu}}{\theta}\right)}{\left[\exp\left(\frac{\epsilon-\tilde{\mu}}{\theta}\right)+1\right]^2}. \tag{4.22}$$

With help of the relation

$$-\frac{1}{\theta}\,\frac{\exp\left(\frac{\epsilon-\tilde{\mu}}{\theta}\right)}{\left[\exp\left(\frac{\epsilon-\tilde{\mu}}{\theta}\right)+1\right]^2} = \frac{d}{d\epsilon}\left(\frac{1}{\exp\left(\frac{\epsilon-\tilde{\mu}}{\theta}\right)+1}\right) = \frac{d}{d\epsilon}f(\epsilon-\tilde{\mu})$$

we evaluate the above integral in the straightforward manner, namely

$$\chi_N = -\frac{4\mu_B^2}{W}\int_{-1/2}^{1/2} d\epsilon\,\frac{d}{d\epsilon}f(\epsilon-\tilde{\mu}) = -\frac{4\mu_B^2}{W}\left[f(1/2-\tilde{\mu}) - f(-1/2-\tilde{\mu})\right]. \tag{4.23}$$

One can easily check, that for the temperature $T \simeq 0$ ($\theta \simeq 0$), $f(1/2-\tilde{\mu}) = 0$ and $f(-1/2-\tilde{\mu}) = 1$, what results in the following expression for the spin susceptibility for the normal state

$$\chi_N = 4\mu_B^2/W \equiv \frac{1}{2}\left(g\mu_B\right)^2 \rho\left(\epsilon_F\right). \tag{4.24}$$

Note, that χ_N is temperature independent as it describes the Pauli paramagnetism with a constant density of states near the Fermi energy.

Now, we express the spin susceptibility for the phases A and $A1$ in terms of χ_N. Firstly, we notice that the second term in (4.17) is exactly one half of the expression (4.22) and thus, it can be replaced by $1/2\chi_N$. Considering additionally the limit of $\theta \simeq 0$, we scale χ_A and χ_{A1} to the value of χ_N equal to $4\mu_B^2/W$

$$\chi_A/\chi_N = \frac{1}{\theta}\int_{-1/2}^{1/2} d\epsilon\, \left\{ \frac{\exp\left(\tilde{\lambda}^A/\theta\right)}{\left[\exp\left(\tilde{\lambda}^A/\theta\right)+1\right]^2}\,\frac{(\epsilon-\tilde{\mu})^2}{(\epsilon-\tilde{\mu})^2+\tilde{\Delta}_A^2} \right\} \tag{4.25}$$

and

$$\chi_{A1}/\chi_N = \frac{1}{2} + \frac{1}{2\theta}\int_{-1/2}^{1/2} d\epsilon \, \frac{\exp\left(\frac{\tilde{\lambda}^{A1}}{\theta}\right)}{\left[\exp\left(\frac{\tilde{\lambda}^{A1}}{\theta}\right)+1\right]^2} \, \frac{(\epsilon-\tilde{\mu})^2}{(\epsilon-\tilde{\mu})^2+\tilde{\Delta}_{A1}^2} \, . \tag{4.26}$$

Taking the values of the gap parameters Δ_A, Δ_{A1} and the chemical potential $\tilde{\mu}_A$, $\tilde{\mu}_{A1}$ calculated in the previous Chapter for the case of $B = 0$, and inserting them into the above equations, we obtain the temperature dependence of the spin susceptibility for both phases (as we remember $\chi_B \equiv 0$). Since the critical temperature $\theta = 0.00331$ fulfils well the condition $\theta \simeq 0$, the simplified formula for χ_N can be used, when normalizing χ_A and χ_{A1}.

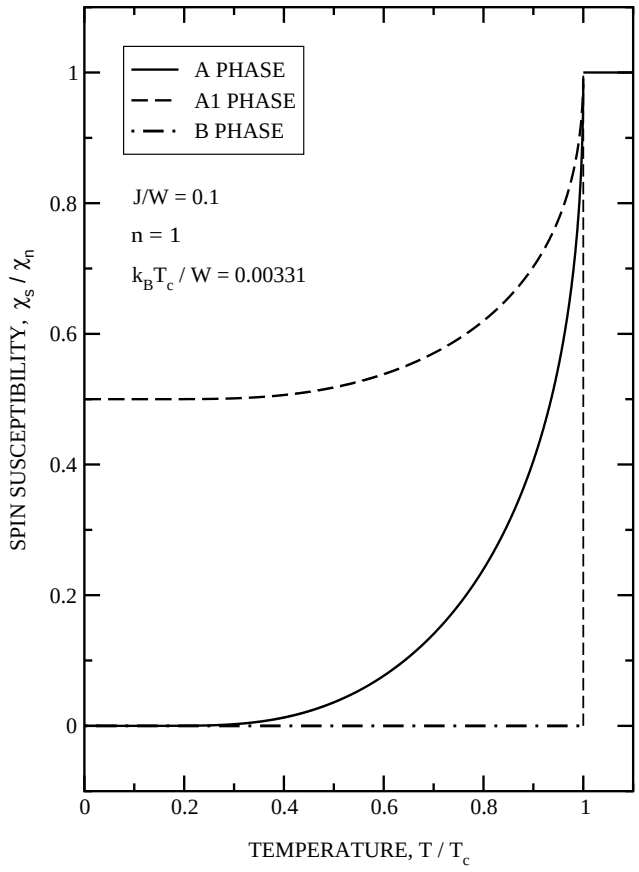

Figure 4.1: Temperature dependence of the spin susceptibility for the superconducting phases: A, $A1$ and B

The evaluated temperature dependence of the spin susceptibilities for the three superconducting phases are shown on Fig. 4.1. The behavior of χ_A (the spin susceptibility for phase A) is very similar to the results obtained for the classical BCS superconductor

[24], [25]. It is equal to zero at the temperature $T = 0$ and grows gradually to the value characteristic for the normal state, which is reached at $T = T_c$.

The phase $A1$ has non-zero value of χ_{A1} at $T = 0$, which is approximately equal to $1/2$ of the spin susceptibility calculated for the normal state. This effect is caused by the fact, that nearly half of the $A1$ quasiparticles modes are gapless, and therefore, they add the normal-state-type contribution to the calculated dependency.

The spin susceptibility for the phase B is identically equal to zero. This is the direct consequence of the fact, that the phase B quasiparticles are spinless (see the Section 3.1.1) and in effect, do not contribute to χ_B.

Strictly speaking, the just calculated susceptibility should be modified when the system approaches the ferromagnetic state (i.e. is close to the *Stoner threshold*). Namely, in the weak-field regime we have then

$$\mathcal{E}_{B,\bar{S}^z} = I\bar{S}^z + \mu_B B \simeq \left(\frac{I\tilde{\chi}}{g\mu_B} + \mu_B \right) B \, , \tag{4.27}$$

where we have assumed that $g\mu_B \bar{S}^z = \tilde{\chi} B$, with the zero field susceptibility $\tilde{\chi}$ (per site) to be calculated self-consistently. The self-consistent expression for $\tilde{\chi}$ reads then

$$\tilde{\chi} = \chi \left(1 + \frac{2I\tilde{\chi}}{(g\mu_B)^2} \right) \, , \tag{4.28}$$

where χ is given by Eq. (4.10).

In effect,

$$\tilde{\chi} = \frac{\chi}{1 - 2I\chi/(g\mu_B)^2} \, . \tag{4.29}$$

Thus, the spin susceptibility diverges at the Stoner point (see next section for the detailed numerical discussion).

In summary, in this Section, we have considered the weak field limit and thus we could use again the results obtained in the previous chapter. In the next step, we will investigate the properties of the system with the ferromagnetic term introduced to the Hamiltonian. As we will see, this will result in the qualitatively new features of the presented model.

4.2 Influence of ferromagnetism on the system at $T = 0$

So far, we have presented the results obtained for the two-band model of spin-triplet superconductivity without ferromagnetic interaction taken into account. Now, we consider the complete Hamiltonian (2.29), written for the case of degenerate energy bands, real energy gaps and with the Zeeman energy term included (4.1). The isotropic phase B will not appear in such defined system, since the condition $\Delta_0 = \Delta_{-1} = \Delta_1 \equiv \Delta$ cannot be fulfilled in the presence of magnetic ordering and applied external magnetic field. Therefore, only phases A and $A1$ are considered. For simplicity, we discuss $T = 0$ case, which is sufficient for description of the coexistence of spin-triplet superconductivity with ferromagnetism in the ground state.

4.2.1 The ferromagnetic state - the two-band model

Before we include the presence of the ferromagnetic magnetic moment in the spin-triplet superconducting state we present briefly basic results obtained for the pure ferromagnetic state.

The effective Hamiltonian for the two-band model of ferromagnetic state is derived from the same starting Hamiltonian (2.3), but this time we do not consider anomalous averages of the type $< a_{-\mathbf{k}} a_{\mathbf{k}} >$ and $< a^{\dagger}_{\mathbf{k}} a^{\dagger}_{-\mathbf{k}} >$, specific for the BCS approach, when making the Hartee-Fock approximation. Hence, in the four-dimensional representation it has the form

$$\mathcal{H}^{ferro}_{HF} = \sum_{\mathbf{k}} \mathbf{f}^{\dagger}_{\mathbf{k}} \mathbf{H}_{\mathbf{k}} \mathbf{f}_{\mathbf{k}} + 2 \sum_{\mathbf{k}} E_{\mathbf{k}2} + 2NI\bar{S^z}^2 \tag{4.30}$$

with the matrix $\mathbf{H}_{\mathbf{k}}$ defined as

$$\mathbf{H}_{\mathbf{k}} = \begin{pmatrix} E_{\mathbf{k}1} - I\bar{S^z}, & 0, & 0, & 0 \\ 0, & E_{\mathbf{k}1} + I\bar{S^z}, & 0, & 0 \\ 0, & 0, & -E_{\mathbf{k}2} + I\bar{S^z}, & 0 \\ 0, & 0, & 0, & -E_{\mathbf{k}2} - I\bar{S^z} \end{pmatrix}. \tag{4.31}$$

For the case of degenerate energy bands and applied external magnetic field, whose contribution to the energy of the system is represented only by the Zeeman term (4.1)

(i.e. when the Landau quantization is disregarded), the above matrix transforms to

$$\mathbf{H_k} = \begin{pmatrix} E_{\mathbf{k}} - \mathcal{E}_{B,\bar{S}^z}, & 0, & 0, & 0 \\ 0, & E_{\mathbf{k}} + \mathcal{E}_{B,\bar{S}^z}, & 0, & 0 \\ 0, & 0, & -E_{\mathbf{k}} + \mathcal{E}_{B,\bar{S}^z}, & 0 \\ 0, & 0, & 0, & -E_{\mathbf{k}} - \mathcal{E}_{B,\bar{S}^z} \end{pmatrix} , \tag{4.32}$$

where $\mathcal{E}_{B,\bar{S}^z} = I\bar{S}^z + \mu_B B$ and $E_{\mathbf{k}} \equiv E_{\mathbf{k}} - \mu$. Since the Hamiltonian contains only diagonal terms, its eigenstates and eigenvectors are found immediately. Namely, for the energy eignvalues we obtain

$$\begin{cases} (\lambda_{\mathbf{k}}^{1,2})_{ferro} = \pm(E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B) , & \text{for} \quad \sigma = \uparrow \\ (\lambda_{\mathbf{k}}^{3,4})_{ferro} = \pm(E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B) , & \text{for} \quad \sigma = \downarrow \end{cases} , \tag{4.33}$$

whereas the (quasi-)particle modes remain unchanged. In effect, we can rewrite the Hamiltonian (4.30) to the form

$$\begin{aligned} H_{ferro} &= \sum_{\mathbf{k}} \Big\{ (E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B) \left(a^{\dagger}_{\mathbf{k}1\uparrow} a_{\mathbf{k}1\uparrow} + a^{\dagger}_{\mathbf{k}2\uparrow} a_{\mathbf{k}2\uparrow} \right) + \\ &\quad + (E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B) \left(a^{\dagger}_{\mathbf{k}1\downarrow} a_{\mathbf{k}1\downarrow} + a^{\dagger}_{\mathbf{k}2\downarrow} a_{\mathbf{k}2\downarrow} \right) \Big\} + 2NI\bar{S}^{z\,2} . \end{aligned} \tag{4.34}$$

Hence, the equation for the ground state energy of the ferromagnetic state yields

$$\begin{aligned} \frac{E_G^{ferro}}{N} &= \frac{2}{N} \sum_{\mathbf{k}} \Big\{ (E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B) f(E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B) + \\ &\quad + (E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B) f(E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B) \Big\} + 2I\bar{S}^{z\,2} , \end{aligned} \tag{4.35}$$

where the chemical potential μ and the magnetic moment $\bar{S}^z$ have to be evaluated self-consistently. The chemical potential is derived from the equation for the number of particles in the system

$$\begin{aligned} n &= \frac{1}{N} \sum_{\mathbf{k}\sigma} \sum_{l=1,2} < n_{\mathbf{k}l\sigma} > \\ &= \frac{2}{N} \sum_{\mathbf{k}} \Big\{ f(E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B) + f(E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B) \Big\} . \end{aligned} \tag{4.36}$$

The expression for the magnetic moment for the constant density of states near the Fermi energy is derived in Section 4.2.3 and discussed in detail in *Appendix C*.

4.2.2 Spin-triplet superconducting state - modification of equations for Δ and μ

The Hamiltonian for the spin-triplet superconducting state taking into account both the ferromagnetic-interaction and the Zeeman terms, has already been introduced in

Section 4.1. Its energy eigenvalues and eigenvectors can be found by straightforward diagonalization of the matrix Hamiltonian (4.2). Below we present the results for phases A and $A1$, as they are the only stable phases in most cases.

Phase A

- Energy eigenvalues:

$$\begin{cases} \lambda_{\mathbf{k}}^{1,2} = \pm\sqrt{(E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B)^2 + \Delta_\uparrow^2} \equiv \pm\lambda_{\mathbf{k}}^{(+)} \\ \lambda_{\mathbf{k}}^{3,4} = \pm\sqrt{(E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B)^2 + \Delta_\downarrow^2} \equiv \pm\lambda_{\mathbf{k}}^{(-)} \end{cases} \tag{4.37}$$

- The transformation matrix:

$$\begin{pmatrix} a_{\mathbf{k}1\uparrow} \\ a_{\mathbf{k}1\downarrow} \\ a^\dagger_{-\mathbf{k}2\uparrow} \\ a^\dagger_{-\mathbf{k}2\downarrow} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}}^{(+)}, & -v_{\mathbf{k}}^{(+)}, & 0, & 0 \\ 0, & 0, & u_{\mathbf{k}}^{(-)}, & -v_{\mathbf{k}}^{(-)} \\ v_{\mathbf{k}}^{(+)}, & u_{\mathbf{k}}^{(+)}, & 0, & 0 \\ 0, & 0, & v_{\mathbf{k}}^{(-)}, & u_{\mathbf{k}}^{(-)} \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{k}\uparrow} \\ \beta^\dagger_{-\mathbf{k}\uparrow} \\ \alpha_{\mathbf{k}\downarrow} \\ \beta^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix} \tag{4.38}$$

- Bogolyubow coherence factors:

$$\begin{cases} u_{\mathbf{k}}^{(+)} = \frac{1}{\sqrt{2}}\left(1 + \frac{E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B}{\lambda_{\mathbf{k}}^{(+)}}\right)^{1/2} \\ v_{\mathbf{k}}^{(+)} = \frac{1}{\sqrt{2}}\left(1 - \frac{E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B}{\lambda_{\mathbf{k}}^{(+)}}\right)^{1/2} \end{cases}, \quad \begin{cases} u_{\mathbf{k}}^{(-)} = \frac{1}{\sqrt{2}}\left(1 + \frac{E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B}{\lambda_{\mathbf{k}}^{(-)}}\right)^{1/2} \\ v_{\mathbf{k}}^{(-)} = \frac{1}{\sqrt{2}}\left(1 - \frac{E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B}{\lambda_{\mathbf{k}}^{(-)}}\right)^{1/2} \end{cases} \tag{4.39}$$

Phase $A1$

- Energy eigenvalues:

$$\begin{cases} \lambda_{\mathbf{k}}^{1,2} = \pm\sqrt{(E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B)^2 + \Delta_\uparrow^2} \equiv \pm\lambda_{\mathbf{k}}^{(+)} \\ \lambda_{\mathbf{k}}^{3,4} = \pm(E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B) \end{cases}, \tag{4.40}$$

- The transformation matrix:

$$\begin{pmatrix} a_{\mathbf{k}1\uparrow} \\ a_{\mathbf{k}1\downarrow} \\ a^\dagger_{-\mathbf{k}2\uparrow} \\ a^\dagger_{-\mathbf{k}2\downarrow} \end{pmatrix} = \begin{pmatrix} 0, & 0, & u_{\mathbf{k}}^{(+)}, & -v_{\mathbf{k}}^{(+)} \\ 1, & 0, & 0, & 0 \\ 0, & 0, & v_{\mathbf{k}}^{(+)}, & u_{\mathbf{k}}^{(+)} \\ 0, & 1, & 0, & 0 \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{k}\downarrow} \\ \beta^\dagger_{-\mathbf{k}\downarrow} \\ \alpha_{\mathbf{k}\uparrow} \\ \beta^\dagger_{-\mathbf{k}\uparrow} \end{pmatrix} \tag{4.41}$$

- Bogolyubow coherence factors - $u_{\mathbf{k}}^{(+)}$ and $v_{\mathbf{k}}^{(+)}$ - are defined in exactly the same way as for the phase A.

The only difference between these solutions and those presented in Section 3.1 lies in the presence of an extra term $I\bar{S}^z+\mu_B B$ modifying the expressions for energy eigenvalues and the coherence factors. So, we can write down the self-consistent equations for the gap parameters and the chemical potential simply by copying them from Section 3.1 here and correcting them with the extra term, where needed. Hence, we have

- for the phase A:

$$1 = \frac{J}{N}\sum_{\mathbf{k}} \frac{1}{\lambda_{\mathbf{k}}^{(+)}} \tanh\left(\frac{\beta\lambda_{\mathbf{k}}^{(+)}}{2}\right) ,$$

$$1 = \frac{J}{N}\sum_{\mathbf{k}} \frac{1}{\lambda_{\mathbf{k}}^{(-)}} \tanh\left(\frac{\beta\lambda_{\mathbf{k}}^{(-)}}{2}\right) , \tag{4.42}$$

$$n-2 = \frac{1}{N}\sum_{\mathbf{k}} \left\{ \frac{E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B}{\lambda_{\mathbf{k}}^{(+)}} \left(2f\left(\lambda_{\mathbf{k}}^{(+)}\right) - 1\right) + \frac{E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B}{\lambda_{\mathbf{k}}^{(-)}} \left(2f\left(\lambda_{\mathbf{k}}^{(-)}\right) - 1\right) \right\} ,$$

- for the phase $A1$

$$1 = \frac{J}{N}\sum_{\mathbf{k}} \frac{1}{\lambda_{\mathbf{k}}^{(+)}} \tanh\left(\frac{\beta\lambda_{\mathbf{k}}^{(+)}}{2}\right) ,$$

$$n-1 = \frac{1}{N}\sum_{\mathbf{k}} \left\{ \frac{E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B}{\lambda_{\mathbf{k}}^{(+)}} \left(2f\left(\lambda_{\mathbf{k}}^{(+)}\right) - 1\right) + 2f(E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B) \right\} . \tag{4.43}$$

Note, that for the phase A we have two separate equations for the gap parameters Δ_1 and Δ_{-1}, since they will have different values in an applied magnetic field.

4.2.3 Self-consistent equation for $\bar{S}^z$

We define the average value of $z-th$ component of the spin operator calculated per single state as

$$\bar{S}^z = \frac{1}{2N}\sum_{il} \langle S_{il}^z \rangle , \quad \text{with} \quad S_{il}^z = \frac{1}{2}\left(n_{il\uparrow} - n_{il\downarrow}\right) \tag{4.44}$$

where $\bar{n}_{il\uparrow}$ and $\bar{n}_{il\downarrow}$ represent the average number of particles on $i-th$ site and in $l-th$ band with the spin orientation "up" and "down", respectively. The factor $2N$, which appears in the denominator, results from the fact, that the number of states available is doubled by the orbital degeneracy $D=2$.

The quantity $\bar{S}^z$ can also be regarded as the average magnetic moment per orbital in the system. We have to evaluate it self-consistently, since as soon as it acquires non-zero value, the ferromagnetic interaction tends to modify the solutions. Therefore, our set of self-consistent parameters is enhanced additionally with the appearance of $\bar{S}^z$.

Taking the transformation to the momentum space, the equation for $\bar{S}^z$ has the form

$$\bar{S}^z = \frac{1}{4N} \sum_{kl} \left(\langle n_{kl\uparrow} \rangle - \langle n_{kl\downarrow} \rangle \right) \tag{4.45}$$

Expressing the operators $n_{kl\uparrow}$ and $n_{kl\downarrow}$ in terms of the quasiparticle operators, defined by the transformation rules (4.38) and (4.41), we obtain the self-consistent equations for $\bar{S}^z$ for the phases A and $A1$, respectively. Namely, we have

$$\begin{aligned} \bar{S}^z_A &= \frac{1}{4N} \sum_{\mathbf{k}} \left\{ \frac{E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B}{\lambda^{(+)}_{\mathbf{k}}} \left(2f\left(\lambda^{(+)}_{\mathbf{k}} \right) - 1 \right) \right. \\ &\qquad \left. - \frac{E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B}{\lambda^{(-)}_{\mathbf{k}}} \left(2f\left(\lambda^{(-)}_{\mathbf{k}} \right) - 1 \right) \right\} \end{aligned} \tag{4.46}$$

and

$$\begin{aligned} \bar{S}^z_{A1} &= \frac{1}{4} + \frac{1}{4N} \sum_{\mathbf{k}} \left\{ \frac{E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B}{\lambda^{(+)}_{\mathbf{k}}} \left(2f\left(\lambda^{(+)}_{\mathbf{k}} \right) - 1 \right) \right. \\ &\qquad \left. - 2f(E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B) \right\} . \end{aligned} \tag{4.47}$$

At the same time, we can write the corresponding expression for the pure ferromagnetic state

$$\bar{S}^z_N = \frac{1}{2N} \sum_{\mathbf{k}} \left\{ f(E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B) - f(E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B) \right\} . \tag{4.48}$$

Its characteristic property is the existence of non-zero spontaneous magnetization in the absence of external magnetic field. The condition for appearance of such state is determined by the *Stoner criterion*, which reads

$$I\rho(E_F) \equiv \tilde{I} = 1 , \tag{4.49}$$

where ρ is the density of states. For $\rho = \frac{1}{W}$, we obtain

$$\frac{I}{W} \equiv \tilde{I} = 1 . \tag{4.50}$$

This means, that usually at $\tilde{I} = 1$ a continuous transition from the paramagnetic to the ferromagnetic state occurs. In our case of constant density of states, a discontinuous

transition occurs at that point. The magnetic moment of the ferromagnetic state for the case of $T = 0$ and flat density of states is discussed in detail in Appendix C.

The equations for $\tilde{S}^z$ together with equations for the gap parameters and the chemical potential constitute the complete set of self-consistent equations. With their help, we determine the values of the parameters describing the system, which in the next step are used for evaluation of the ground state energy of each phase.

4.2.4 Complete set of self-consistent equations at $T = 0$ - numerical solutions

In the limit of $T = 0$ the self-consistent equations take the simpler form. For $T \to 0$, its reversal $1/T \to \infty$, and hence the Fermi-Dirac distribution function transforms to the Heaviside "step" function: $f(E) \xrightarrow{T\to 0} \theta(-E)$. Additionally, the function $\tanh(\alpha/T)$, which apears under the sum in the equations for the gap parameters, reduces to 1. Now, we have

- for the phase A:

$$1 = \frac{J}{N}\sum_{\mathbf{k}} \frac{1}{\lambda_{\mathbf{k}}^{(+)}}\,; \qquad 1 = \frac{J}{N}\sum_{\mathbf{k}} \frac{1}{\lambda_{\mathbf{k}}^{(-)}}$$

$$n - 2 = -\frac{1}{N}\sum_{\mathbf{k}} \left\{ \frac{E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B}{\lambda_{\mathbf{k}}^{(+)}} + \frac{E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B}{\lambda_{\mathbf{k}}^{(-)}} \right\} \tag{4.51}$$

$$\bar{S}^z_A = -\frac{1}{4N}\sum_{\mathbf{k}} \left\{ \frac{E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B}{\lambda_{\mathbf{k}}^{(+)}} - \frac{E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B}{\lambda_{\mathbf{k}}^{(-)}} \right\}$$

- for the phase $A1$

$$1 = \frac{J}{N}\sum_{\mathbf{k}} \frac{1}{\lambda_{\mathbf{k}}^{(+)}}$$

$$n - 1 = \frac{1}{N}\sum_{\mathbf{k}} \left\{ -\frac{E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B}{\lambda_{\mathbf{k}}^{(+)}} + 2\,\theta(\mu - E_{\mathbf{k}} - I\bar{S}^z - \mu_B B) \right\} \tag{4.52}$$

$$\bar{S}^z_{A1} = \frac{1}{4} - \frac{1}{4N}\sum_{\mathbf{k}} \left\{ \frac{E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B}{\lambda_{\mathbf{k}}^{(+)}} + 2\,\theta(\mu - E_{\mathbf{k}} - I\bar{S}^z - \mu_B B) \right\}\,,$$

where $\lambda_{\mathbf{k}}^{(+)}$ and $\lambda_{\mathbf{k}}^{(-)}$ are defined as follows

$$\begin{aligned} \lambda_{\mathbf{k}}^{(+)} &= \sqrt{(E_{\mathbf{k}} - \mu - I\bar{S}^z - \mu_B B)^2 + \Delta_\uparrow^2} \\ \lambda_{\mathbf{k}}^{(-)} &= \sqrt{(E_{\mathbf{k}} - \mu + I\bar{S}^z + \mu_B B)^2 + \Delta_\downarrow^2}\,. \end{aligned}$$

For comparison, we write down the set of self-consistent equations for the ferromagnetic phase:

$$\begin{aligned} n &= \tfrac{2}{N}\textstyle\sum_{\mathbf{k}} \Big\{\theta(\mu - E_{\mathbf{k}} + I\bar{S}^z + \mu_B B) + \theta(\mu - E_{\mathbf{k}} - I\bar{S}^z - \mu_B B)\Big\} \\ \bar{S}^z_{ferro} &= \tfrac{1}{2N}\textstyle\sum_{\mathbf{k}} \Big\{\theta(\mu - E_{\mathbf{k}} + I\bar{S}^z + \mu_B B) - \theta(\mu - E_{\mathbf{k}} - I\bar{S}^z - \mu_B B)\Big\} \end{aligned} \tag{4.53}$$

As previously, we replace the sum $\frac{1}{N}\sum_{\mathbf{k}}$ with the integral $\int_{-1/2}^{1/2} dE\rho(E)$ and, for the flat density of states $\rho(E) = 1/W$, transform the equations above to the dimensionless form. Again, we express all quantities in the units of the energy bandwidth W; traditionally, we mark them with the tilde sign (e.g. $\tilde{\Delta} = \Delta/W$). In addition, we introduce the dimensionless parameter β, defined as $\mu_B B/W$, representing the contribution of external magnetic field to the band energy of a single quasiparticle. In effect, we obtain the following integral equations

- phase A:

$$1 = \tilde{J}\int_{-1/2}^{1/2} d\epsilon\, \frac{1}{\tilde{\lambda}^{(+)}}\,; \qquad 1 = \tilde{J}\int_{-1/2}^{1/2} d\epsilon\, \frac{1}{\tilde{\lambda}^{(-)}}$$

$$\begin{aligned} n - 2 &= -\int_{-1/2}^{1/2} d\epsilon\, \left\{\frac{\epsilon - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta}{\tilde{\lambda}^{(+)}} + \frac{\epsilon - \tilde{\mu} + \tilde{I}\bar{S}^z + \beta}{\tilde{\lambda}^{(-)}}\right\} \\ \bar{S}^z_A &= -\frac{1}{4}\int_{-1/2}^{1/2} d\epsilon\, \left\{\frac{\epsilon - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta}{\tilde{\lambda}^{(+)}} - \frac{\epsilon - \tilde{\mu} + \tilde{I}\bar{S}^z + \beta}{\tilde{\lambda}^{(-)}}\right\} \end{aligned} \tag{4.54}$$

- phase $A1$

$$1 = \tilde{J}\int_{-1/2}^{1/2} d\epsilon\, \frac{1}{\tilde{\lambda}^{(+)}}$$

$$\begin{aligned} n - 1 &= \int_{-1/2}^{1/2} d\epsilon\, \left\{-\frac{\epsilon - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta}{\tilde{\lambda}^{(+)}} + 2\,\theta(\tilde{\mu} - \epsilon - \tilde{I}\bar{S}^z - \beta)\right\} \\ \bar{S}^z_{A1} &= \frac{1}{4} - \frac{1}{4}\int_{-1/2}^{1/2} d\epsilon\, \left\{\frac{\epsilon - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta}{\tilde{\lambda}^{(+)}} + 2\,\theta(\tilde{\mu} - \epsilon - \tilde{I}\bar{S}^z - \beta)\right\}\,. \end{aligned} \tag{4.55}$$

- normal state

$$\begin{aligned} n &= 2\int_{-1/2}^{1/2} d\epsilon\, \Big\{\theta(\tilde{\mu} - \epsilon + \tilde{I}\bar{S}^z + \beta) + \theta(\tilde{\mu} - \epsilon - \tilde{I}\bar{S}^z - \beta)\Big\} \\ \bar{S}^z_{ferro} &= \frac{1}{2}\int_{-1/2}^{1/2} d\epsilon\, \Big\{\theta(\tilde{\mu} - \epsilon + \tilde{I}\bar{S}^z + \beta) - \theta(\tilde{\mu} - \epsilon - \tilde{I}\bar{S}^z - \beta)\Big\}\,. \end{aligned} \tag{4.56}$$

The integrals above can be expanded analytically. The final form of the above equations is presented in Appendix D.

For d-electron systems the value of J is of the order $0.1 - 0.3\ U$. Thus, we take $J = 0.125\, I$ for numerical calculations. Using the relation $I = U + 2J$, one can easily check that then $J \simeq 0.16\ U$. As in the previous chapter, we consider the quarter-filled bands case, i.e. $n = 1$. According to the discussion provided in Appendix C, this value of band-filling implies that for the normal state at the Stoner threshold the chemical potential is $\tilde{\mu} = -0.25$ and the saturated magnetic moment is $\bar{S}^z = 0.25$. The Stoner criterion takes place at $\tilde{I} = 1$ and hence, since we have chosen $J = 0.125I$, at $\tilde{J} = 0.125$. Then the paramagnetism is unstable in a *discontinuous manner*. We understand the Stoner criterion in this manner, not in the sense of a *continuous* transition taking place for this two-band system!

In this and in the following sections we investigate the properties of the system below the modified Stoner threshold (i.e. for $\tilde{J} < 0.125$). In the magnetically saturated state spins of all quasipaticles are oriented parallel to the magnetic field direction ($\sigma = \uparrow$). Therefore, the energy gap for $m = -1$ does not appear in the system and we loose possibility for making comparisons between the phases A and $A1$.

The numerical results for Δ_m, $\tilde{\mu}$, and $\bar{S}^z$, calculated for the case of $\tilde{J} = 0.12$ are shown on Fig. 4.2. As we can see, the magnetic moment for both phases (A and $A1$) exhibits the linear dependence on applied magnetic field β, which is characteristic for the normal (paramagnetic) state. So, in terms of the type of dependence, one can say that the magnetic properties of the system are not influenced much by the pairing (but as we will show later on, pairing does modify significantly the character of phase transition between the paramagnetic and the ferromagnetic states).

The gap parameters Δ_1 (or $\Delta_{\uparrow\uparrow}$) and Δ_{-1} (or $\Delta_{\downarrow\downarrow}$) behave differently in an applied magnetic field. The first parameter increases with the increasing β, whereas the latter decreases and vanishes, when the saturation limit is reached. At this limit, no particles with spin "down" orientation exist, as all of them have already been altered by magnetic field to spin "up" orientation. Therefore, no pairs (and associated with them energy gaps) of the type $\downarrow\downarrow$ can be created. Note, that at $\beta = 0$, both gaps have similar values (cf. Fig. 3.1).

The chemical potential dependence cannot be probably explained in any simple manner. The argument, which could be used in case of phase A, is that that with the increasing magnetic field the quasiparticles migrate from the spin "down" to the spin

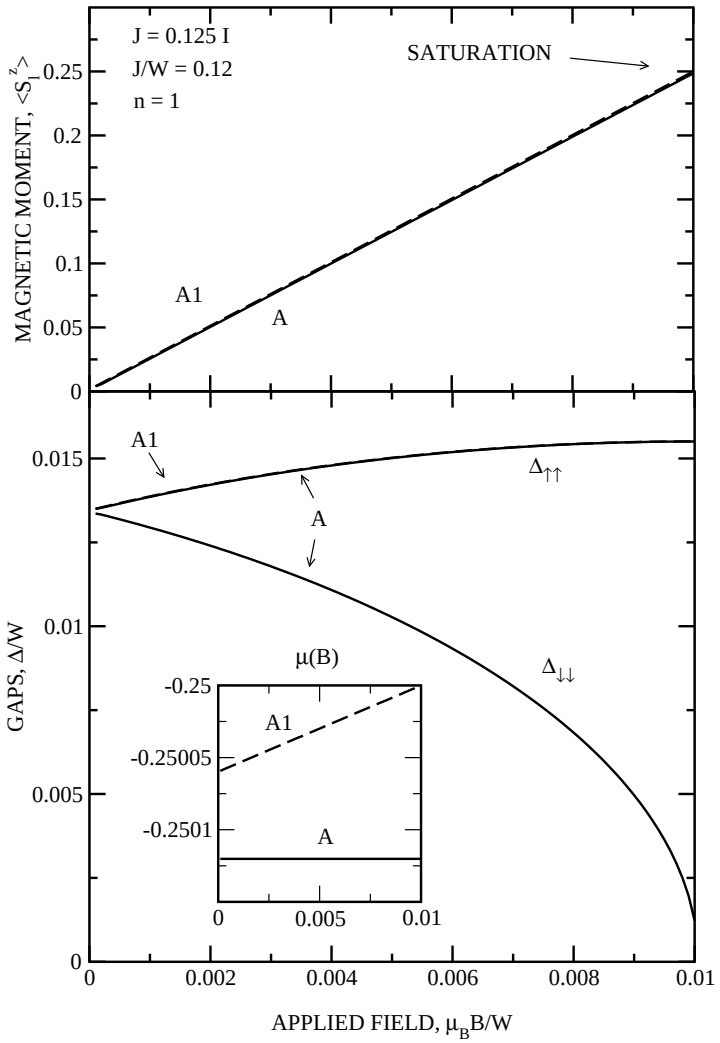

Figure 4.2: Field dependence of the basic parameters of the system. In the inset we present the field dependence of the chemical potential in the two phases.

"up" sub-bands. Since at the same time magnetic field shifts the corresponding bands upwards and downwards, respectively, the chemical potential value remains unchanged. The difference in the behavior of the phase $A1$ is probably caused by the fact, that two types of quasiparticles - *gapped and gapless* - coexist in this phase, and therefore μ reflects that circumstance. The results obtained for the case of $\beta = 0$ and $T = 0$ are qualitatively the same as those developed earlier in the absence of magnetic field (cf. Fig. 3.2).

The results presented here are used in the next section as an input in determining of ground state energy for each state. Afterwards, we will construct phase diagram and investigate the stability of the phases.

4.2.5 Ground state energy and the phase diagram

We write down the expressions for the ground state energy of the phases A and $A1$, using as a starting point Eqs. (3.40) and (3.47) derived in the previous chapter for the case of $\bar{S}^z = 0$ and $\beta = 0$. This time, we consider additionally the free term $2I\left(\bar{S}^z\right)^2$ (cf. Eq. (2.29)) and substitute previously determined energy eigenvalues with those described by (4.37) and (4.40). Hence, we obtain

- for the phase A

$$\begin{aligned}\frac{E_G^A}{N} &= \frac{1}{N}\sum_{\mathbf{k}}\left\{\lambda_{\mathbf{k}}^{(+)}\left(2f(\lambda_{\mathbf{k}}^{(+)})-1\right)+\lambda_{\mathbf{k}}^{(-)}\left(2f(\lambda_{\mathbf{k}}^{(-)})-1\right)\right\} \\ &+ \frac{2}{N}\sum_{\mathbf{k}}(E_{\mathbf{k}}-\mu)+\frac{\Delta_1^2+\Delta_{-1}^2}{2J}+2I\left(\bar{S}^z\right)^2 ,\end{aligned} \tag{4.57}$$

- for the phase $A1$

$$\begin{aligned}\frac{E_G^{A1}}{N} &= \frac{1}{N}\sum_{\mathbf{k}}\left\{\lambda_{\mathbf{k}}^{(+)}\left(2f(\lambda_{\mathbf{k}}^{(+)})-1\right)\right. \\ &\left.+\,(E_{\mathbf{k}}-\mu+I\bar{S}^z+\mu_B B)\left(2f(E_{\mathbf{k}}-\mu+I\bar{S}^z+\mu_B B)-1\right)\right\} \\ &+ \frac{2}{N}\sum_{\mathbf{k}}(E_{\mathbf{k}}-\mu)+\frac{\Delta_1^2}{2J}+2I\left(\bar{S}^z\right)^2 .\end{aligned} \tag{4.58}$$

- for the normal state

$$\begin{aligned}\frac{E_G^{A1}}{N} &= \frac{1}{N}\sum_{\mathbf{k}}\left\{(E_{\mathbf{k}}-\mu-I\bar{S}^z-\mu_B B)\left(2f(E_{\mathbf{k}}-\mu-I\bar{S}^z-\mu_B B)-1\right)\right. \\ &\left.+\,(E_{\mathbf{k}}-\mu+I\bar{S}^z+\mu_B B)\left(2f(E_{\mathbf{k}}-\mu+I\bar{S}^z+\mu_B B)-1\right)\right\} \\ &+ \frac{2}{N}\sum_{\mathbf{k}}(E_{\mathbf{k}}-\mu)+2I\left(\bar{S}^z\right)^2 .\end{aligned} \tag{4.59}$$

As previously, for the limit of $T \to 0$ we notice, that Fermi distribution function vanishes for the gapped quasiparticles (i.e. $f(\lambda^{\pm}) \to 0$), whereas for the gapless modes it simplifies to the Heaviside function: $f(E_{\mathbf{k}}-\mu+I\bar{S}^z+\mu_B B) \to \theta(\mu-I\bar{S}^z-\mu_B B-E_{\mathbf{k}})$. Simultaneously, we transform the above expressions to the dimensionless integral form, with help of the procedure carried out earlier. In effect, the equations for ground state energy yield

- for the phase A

$$\frac{E_G^A}{N} = \int_{-1/2}^{1/2} d\epsilon\ \left\{-\tilde{\lambda}^{(+)}-\tilde{\lambda}^{(-)}+2\ (\epsilon-\tilde{\mu})\right\}+\frac{\Delta_1^2+\Delta_{-1}^2}{2J}+2I\left(\bar{S}^z\right)^2 , \tag{4.60}$$

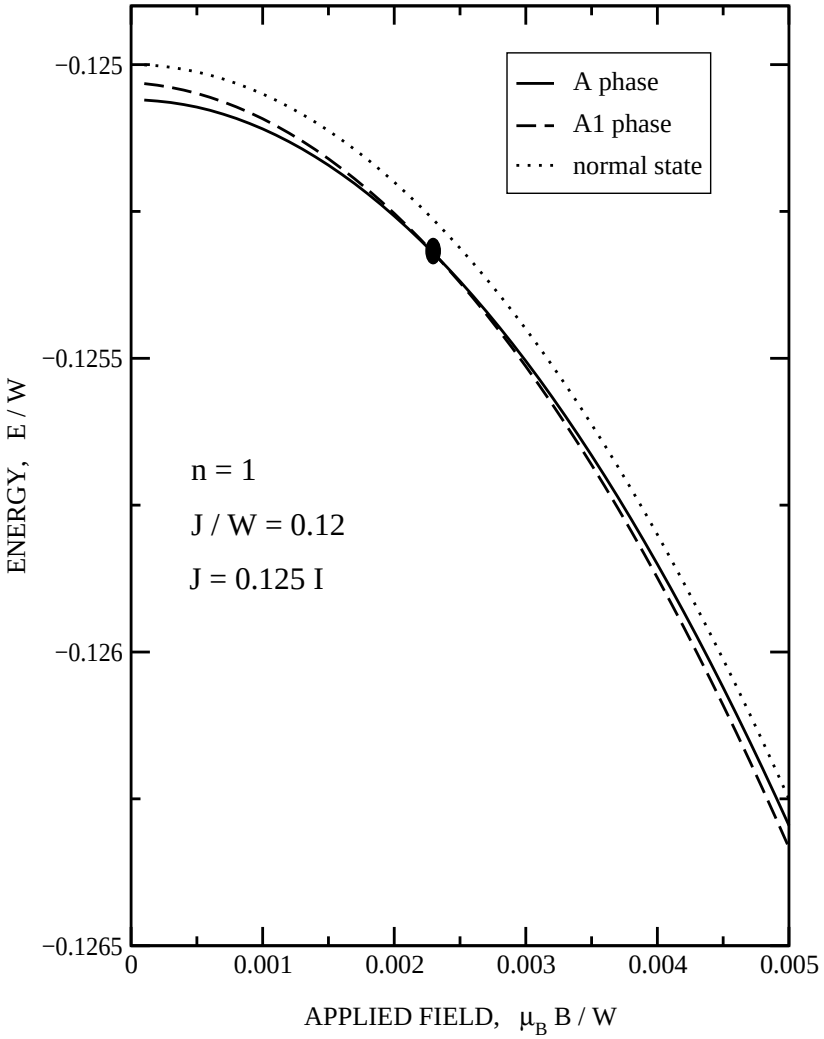

Figure 4.3: Exemplary ground state energy of A and $A1$ phases vs. applied magnetic field. Note a transition between A and $A1$ state with the increasing field.

- for the phase $A1$

$$\begin{aligned} \frac{E_G^{A1}}{N} &= \frac{\Delta_1^2}{2J} + 2I\left(\bar{S}^z\right)^2 + \int_{-1/2}^{1/2} d\epsilon \, \Big\{ -\tilde{\lambda}^{(+)} + (\epsilon - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta) \\ &\quad + 2\,(\epsilon - \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)\,\theta(\tilde{\mu} - \tilde{I}\bar{S}^z - \beta - \epsilon)\Big\}\ , \end{aligned} \tag{4.61}$$

- for the normal state

$$\begin{aligned} \frac{E_G^N}{N} &= 2\int_{-1/2}^{1/2} d\epsilon \, \Big\{ (\epsilon - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)\,\theta(\tilde{\mu} + \tilde{I}\bar{S}^z + \beta - \epsilon) \\ &+ \quad (\epsilon - \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)\,\theta(\tilde{\mu} - \tilde{I}\bar{S}^z - \beta - \epsilon)\Big\} + 2I\left(\bar{S}^z\right)^2\ . \end{aligned} \tag{4.62}$$

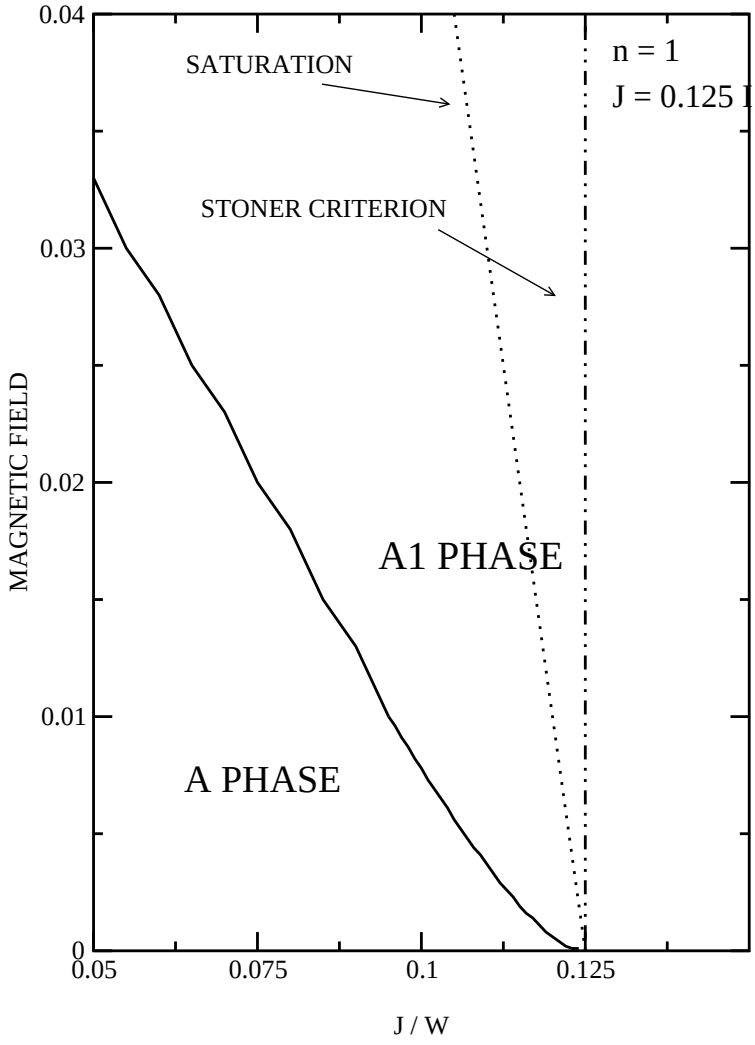

Figure 4.4: Phase diagram - transition between A and $A1$ phases *below* the Stoner threshold to the totally spin polarized state.

The exact form of calculated integrals (below the Stoner and saturation thresholds) is presented in Appendix D. Taking the results for the gap parameters, the magnetic moment, and the chemical potential obtained in the previous section and substituting them into the corresponding expressions for E_G, we evaluate the magnetic field dependence of ground state energy for superconducting and normal phases.

The numerical results are presented on Figs. 4.3 and 4.4. In the former Figure, the dependence of ground state energy as a function of magnetic field is shown. The coupling constant J and the band filling parameter have been chosen as $J = 0.12$ and $n = 1$. As we can see, at the $B = 0$ limit phase A has the lowest energy, what corresponds to the results obtained earlier in Chapter 3. However, at the value of field $\mu_B B \simeq 2 \times 10^{-3} W$

a transition from A to $A1$ phase occurs, and the new phase becomes the stable one for the system. This is probably caused by the fact, that for the phase $A1$ magnetic field re-orients the spins of gapless (unbound) quasiparticles very easily, whereas in the case of the phase A a higher energy is required to re-orient the spins of the pair by destroying of the bound state with the opposite spin directions.

The field dependence of the phase A and $A1$ stability is shown in Fig. 4.4. The border line, at which transition between both phases takes place, is marked as a solid line. It is probably the first-order line, although the confirmation of this conjecture is not to prove numerically, as the energy differences hit the accuracy ($\sim 10^{-10}$) of the solutions. For the field $B = 0$, phase A is stable up to the Stoner critical point, although the value of magnetic field, at which the phase transition appears, decreases with the increasing coupling constant J, an understandable fact. Thus, close to this point, phase A is preferred only within very narrow range of the field values. The phase A disapears exactly at the Stoner point and only the $A1$ phase survives, at least for the model density of states selected, for which only the jump to saturation occurs. Note, that the threshold for an appearance of the $A1$ phase does not coincide with the onset of saturated ferromagnetic state (marked with a dotted line).

4.3 Coexistence of spin-triplet superconductivity with itinerant ferromagnetism

One very interesting feature of our mean-field approach should be mentioned. Namely, the $\bar{S}^z(B)$ in the paired state dependence *does not* approach exactly the value $\bar{S}^z = 0$ for $B = 0$, even though the system is below the Stoner threshold. To test this very intriguing conjecture that the pairing itself may introduce a uniform ferromagnetic polarization, we have calculated the *remament* value of the spin magnetic moment in the field $B \to 0$ when approaching the Stoner critical point. The result is displayed in Fig. 4.5. We observe a beautiful critical dependence of the moment as we approach the Stoner point. So, indeed, the pairing washes out the critical Stoner point, i.e. makes it *a hidden critical point*. It should be noted that this critical behaviour is observed even though the pure magnetic transition (i.e. in the pairing absence) is discontinuous! It is interesting to ask to what extent the quantum critical fluctuations can change this mean-field result. The result also means that the superconducting coherence length

becomes infinite at the Stoner point.

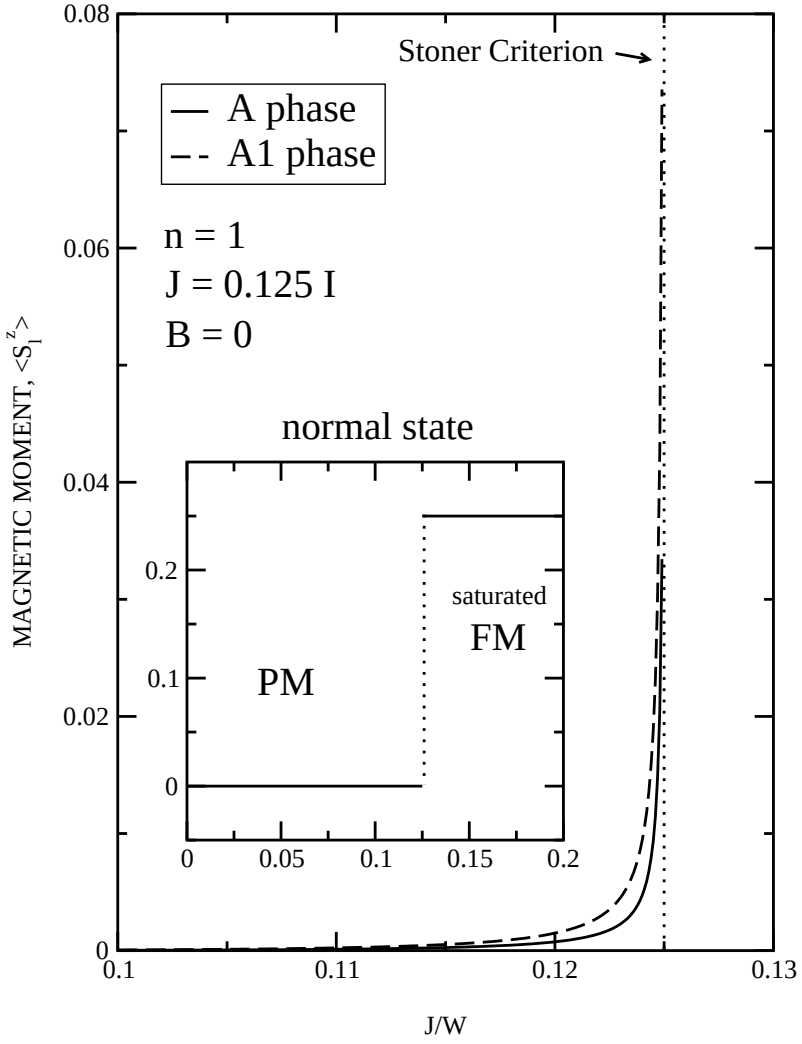

Figure 4.5: Magnetic moment per site per orbital near the Stoner threshold. The inset exhibits the nature of the magnetic transition when the pairing is absent. Note that the discontinuous magnetic transition is washed out by the effect of spin-triplet pairing making the magnetic transition point a *hidden critical point*.

The results displayed in Fig. 4.5 contain also one additional feature exhibited in the inset. Namely, the inset shows that if no pairing were present then the mean-field para-ferro-magnetic transition would be discontinuous (for the assumed constant density of states) and directly to the saturated state. The pairing smears out this discontinuity and therefore, we have an extended critical regime for $J/W \to 0.125$. Additionally, because

of the absence of the critical point for $\bar{S^z}(J)$ dependence it is difficult to say where the ferromagnetism will disappear as a function of e.g. pressure in actual systems. This is exactly what is actually observed for the newly discovered superconducting ferromagnets [26, 27].

The fact that the spin-triplet pairing can induce a weak ferromagnetic ordering must mean that the coherence length ξ of the paired states is larger than the classical distance $(V/N_e)^{1/3}$ between the electrons in this system of volume V containing N_e electrons. The overlap between the Cooper pairs effectively induces a spin-spin interaction, which can be understood in the following manner. The superconducting gap creates the effective magnetic field $H_{jm} = \chi_{ji}\Delta_{mi}$, which, in turn, induces magnetic moment $M_i \sim \chi_{ji}\Delta_{mi}$ (χ_{ji} is the superconducting susceptibility) and in turn, a negative contribution to magnetic energy $\sim (\bar{S^z})^2$.

The analytic estimates on the other side of the Stoner point, i.e. in the weakly ferromagnetic state, have been carried out elsewhere [21, 22] and will not be repeated here.

Chapter 5

A brief summary and conclusions

In this Thesis we have studied model aspects of the *spin-triplet superconductivity*, as well as its coexistence with a *weak itinerant ferromagnetism*, both induced by the Hund's rule coupling. We have concentrated on the weak coupling (the Hartree-Fock-BCS) limit to supplement the standard discussion of itinerant ferromagnetism with the detailed discussion of a local, interorbital spin-triplet pairing.

We have calculated the stability of various phases (labelled by B, A, and $A1$), as well as their basic thermodynamic properties, both expressed in terms of Bogolyubov quasiparticles, generalized to the present situation. For this purpose, a four-dimensional formalism has been used throughout the Thesis.

The most important physical result is the discovery of a *hidden character* of the Stoner quantum critical point, caused by a non-vanishing spin polarization of the Cooper pairs (i.e. by the appearance of the off-diagonal long-range ordering). Also, in the Supplement we show that even without the spin-triplet pairing, the Landau orbits of a Cooper pair with the parallel spins are possible and stable in the diluted limit, if the repulsive Coulomb interaction is taken into account.

The spin-triplet local pairing requires a simultaneous existence of occupied band $|\mathbf{k}\ 1\uparrow>$ and $|-\mathbf{k}\ 2\uparrow>$ states. This means that in realistic cases only relatively small portions of the available phase space near or on the Fermi surface is available for the pairing. Therefore, before implementing the present pairing mechanism to concrete systems (UGe_2, $URhGe$), we have to know the band structure of those systems in the ferromagnetic state. This is the reason why our considerations are to be considered as a theoretical modelling at best. The application to real materials would also require the inclusion of hybridization of the single-particle states, which will complicate essen-

tially the situation, resulting in the **k**-dependent gaps, as well as in appearance of the *intraorbital* gaps. Nevertheless, the simplicity of our present analysis, albeit in a model situation, indicates clearly that the spin-triplet real-space pairing mechanism is feasible and it would be valuable to implement it in a realistic situation.

A separate class of problems concerns the analysis of this mechanism in the *strong-correlation-limit*. In that limit, among other problems, a competition between the spin-singlet and the spin-triplet pairing channels appears. Such a competition allows for a generalization of the so-called $t - J$ *model* to the multi-orbital situation. These considerations will be detailed elsewhere [A. Klejnberg, Ph. D. Thesis in preparation].

On the basis of the present formalism one can determine a phase diagram on the plane: temperature - band filling, incorporating spin-triplet superconductivity, ferromagnetism and antiferromagnetism (or spin-density wave state, in general). This task requires a separate project, as it involves a substantial computing time and effort.

One should mention once more again that only the spatially homogeneous state has been considered, even in the presence of the applied magnetic field. This means that, strictly speaking, our results are valid only in the *Meissner state*. The most important question here, to be considered first is, whether the *vortex-lattice* formation takes place before the totally polarized state ($A1$) becomes stable. This question is particularly relevant in the paramagnetic phase close to the *Stoner point*. A derivation of the Ginzburg-Landau-type effective functional for the multiple-component order parameter would be a starting point for such a discussion. We should see progress along this line soon.

In the following *Supplement*, representing also an integral part of the Thesis, we provide a somewhat specialized discussion of a single Cooper pair, which can be in the spin-triplet state, induced by the repulsive Coulomb repulsion.

Supplement: A single Cooper pair in an applied magnetic field

In this Supplement we enclose the text of the paper submitted recently for publication [P. Wróbel and J. Spałek, submitted to Phys. Rev. B].

Two-electron bound states attracted a renewed attention recently. This interest is stimulated mainly by research in quantum dots [28, 29] and on electron states in doped two-dimensional systems [30], as well as in the high-temperature superconductors. [31] In the quantum dot systems we have reached a threshold for studying the electron states in artificial atoms and other d-dimensional quantum wells of finite size. These states are often studied in detail in the presence of an applied magnetic field, since then we can study systematically the magnetooptics, i.e. the optical or tunnel transitions as a function of well controlled external parameter. Also, the two-electron states play an important role in the scaling theory of localization as they can propagate coherently even when the single electrons cannot [32].

In this Supplement we consider pair-electron states [33] in a planar system, bound by a spin-independent pairing potential of the size $2a$. We additionally put the whole system in an applied magnetic field and determine the nature of the ground state. It turns out that the spin-triplet configuration with the center-of-mass angular momentum $L = 1$ is the stable configuration in most cases. In other words, the proper state in a magnetic field is that of the orbiting bound pair on the cyclotron orbit with $L = 1$. The effect of Coulomb repulsion is also taken explicitly into account in the second part of the paper. The long-range Coulomb repulsion enforces the $L = 1 \rightarrow l = 1$ transition in an appilied field.

The energy of first few excited states are also estimated. Finally, we also point out why the original Cooper approach [15] cannot be generalized in a strightforward manner to the nonzero-field situation.

S.1 Formulation of the problem in an applied magnetic field

The binding energy of the Cooper pair [15] is given by expression

$$\Delta_0 = \hbar\omega_D \frac{1}{\exp\left\{\frac{2}{\rho V}\right\} - 1} , \tag{S.1}$$

where $\rho \equiv \rho(\epsilon_F)$ is density of states at the Fermi energy ϵ_F, which for two-dimensional system of surface S_2 and with a parabolic dispersion relation, is equal to $mS_2/\pi\hbar^2$ (we have assumed periodic boundary conditions), ω_D is the cut-off (Debye) frequency and $(-V)$ is the coupling constant introduced originally by Cooper as a representative value of matrix element $< k'|V(r)|k >$ ($V(r)$ - the pairing potential energy, r - relative distance between the two electrons, $|k >$ - Bloch state of free electron with momentum k). In the limit of vanishing Fermi surface ($\rho(\epsilon_F) \to 0$) this bound state disappears. This is *not* the case [31] for the pairing *in real space* particularly in the presence of an applied magnetic field, as we discuss in this paper. Namely, we assume the following form of pairing energy in real space:

$$V(r) = \begin{cases} -V_0 & \text{for } r \leq a \\ 0 & \text{for } r > a \end{cases} \tag{S.2}$$

where $2a$ is the range of the attractive potential energy, which is substantially smaller than the system (or a quantum dot) size. Such a well may simulate a pair binding within a quantum dot. One can also say that we consider a single bipolaron state formed by an attractive (non-self-consistent) potential field in an external magnetic field. For the time being, we neglect the repulsive Coulomb interaction among the particles. The single-particle part is taken into account in the effective-mass approximation for the sake of simplicity (it is realistic if the bound-state size is substantially larger than the lattice parameter).

Hamiltonian of a two dimensional system of two electrons placed in a uniform magnetic field and interacting via the pairing potential (S.2) has the form

$$H = \frac{1}{2m}\left[(-i\hbar\nabla_1 - e\mathbf{A}_1)^2 + (-i\hbar\nabla_2 - e\mathbf{A}_2)^2\right] - (\vec{\mu}_1 + \vec{\mu}_2)\cdot\mathbf{B} + V(\mathbf{r}_1, \mathbf{r}_2) . \tag{S.3}$$

Indices $1, 2$ correspond to the coordinates of the electrons, respectively. The quantity $\vec{\mu} = 2\mu_B\mathbf{s}$ is the electron spin moment, where $\mathbf{s}$ - the spin operator and μ_B - the Bohr magneton (note, that we take the Zeeman energy term with minus sign). Eigenvalues

of the total spin of the system $\mathbf{S} = \mathbf{s_1} + \mathbf{s_2}$ are $S = 0, 1$. Also, $S^z = s_1^z + s_2^z = 0, \pm 1$. The quantity m is the electron effective mass.

For a magnetic field oriented perpendicularly to the system plane, (z-axis), the rotational symmetry of the problem allows for the choice of the symmetric gauge of vector potential $\mathbf{A} = (-y, x, 0)B/2$, which is also a convienient choice for the shape of the proposed pairing potential. Introducing the center of the mass and relative coordinates, defined as follows:

$$\begin{cases} \mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2} \\ \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \end{cases} \Longrightarrow \begin{cases} \mathbf{r}_1 = \mathbf{R} + \frac{\mathbf{r}}{2} \\ \mathbf{r}_2 = \mathbf{R} - \frac{\mathbf{r}}{2} \end{cases} ,$$

we separate Hamiltonian (S.3) into two parts, which describe respectively the motion of the pair center of the mass and their relative motion with the reduced mass μ. This is possible because the pairing potential depends only on the relative distance r of the two interacting particles. Next, the transformation to polar coordinates can be performed resulting in the following expression for the Hamiltonian:

$$\begin{aligned} H &= -\frac{\hbar^2}{2M}\left[\frac{1}{R}\partial_R(R\partial_R) + \frac{1}{R^2}\partial_\Phi^2\right] + \frac{M\omega_c^2}{8}R^2 - \frac{i\hbar\omega_c}{2}\partial_\Phi \\ &\quad -\frac{\hbar^2}{2\mu}\left[\frac{1}{r}\partial_r(r\partial_r) + \frac{1}{r^2}\partial_\phi^2\right] + \frac{\mu\omega_c^2}{8}r^2 - \frac{i\hbar\omega_c}{2}\partial_\phi - 2\mu_B B\hat{S}_z + V(r) \ . \end{aligned} \tag{S.4}$$

Coordinates R, Φ and r, ϕ correspond respectively to the center-of-mass (with the mass $M = 2m$) and the relative coordinates (with the mass $\mu = m/2$). The cyclotron frequency ω_c is defined as $|e|B/m$ (in SI units). Thus, we have a system of two independent harmonic oscillators: one describing the Lorentz orbit of the pair (center of mass) and the other accounting for the relative motion of the particles.

A. Noninteracting pair: a brief summary

In the absence of the pairing potential energy eigenvalues and eigenfunctions of the system of two noninteracting electrons are given by the respective formulae [34]:

$$(E_0)_{NLnl}^{S,S_z} = \hbar\omega_c\left(N + L + n + l - S_z + 1\right) \ , \tag{S.5}$$

$$\Psi_{NLnl}^{S,S_z}(\zeta, \Phi, \xi, \phi) = \frac{1}{2\pi}\, e^{iL\Phi}\, e^{il\phi}\, U_{NL}(\zeta)\, u_{nl}(\xi)\, \chi(S, S_z), \tag{S.6}$$

$$U_{NL}(\zeta) = \frac{1}{R_H\sqrt{N!(N+L)!}}\, e^{-\frac{\zeta}{2}}\zeta^{\frac{L}{2}}L_N^L(\zeta) \ ,$$

and

$$u_{nl}(\xi) = \frac{1}{r_H\sqrt{n!(n+l)!}}\, e^{-\frac{\xi}{2}} \xi^{\frac{l}{2}} L_n^l(\xi) \; .$$

where N, L and n, l are characterizing the orbital (N, n) and angular-momentum quantum number (L, l) for the center-of-mass and the reduced-mass parts, respectively. The term $\chi(S, S_z)$ represents the spin part of the wave function and for given values of (S, S_z), it is described by following expressions: $\chi(0,0) = 1/\sqrt{2}(|\uparrow\downarrow> - |\downarrow\uparrow>)$, $\chi(1,1) = |\uparrow\uparrow>$, $\chi(1,0) = 1/\sqrt{2}(|\uparrow\downarrow> + |\downarrow\uparrow>)$, $\chi(1,-1) = |\downarrow\downarrow>$. Only positive values of L and l are allowed, Φ and ϕ are the corresponding azimuthal angles. Dimensionless coordinates ζ and ξ are given by the expressions:

$$\zeta = \frac{R^2}{2R_H^2} \;\; \text{with} \;\; R_H^2 = \frac{\hbar}{M\omega_c} \; , \;\; \text{and} \;\; \xi = \frac{r^2}{2r_H^2} \;\; \text{with} \;\; r_H^2 = \frac{\hbar}{\mu\omega_c} \; . \tag{S.7}$$

Parameters R_H and r_H represent the magnetic lengths for the corresponding wave-function parts. They represent the classical cyclotron radii of the whole pair (that encircles their center of mass) and the radius of orbiting one electron relative to the other.

The parity of the wave function (S.6) is provided by the factor $(-1)^{L+l}(-1)^{S+1}$. Due to Pauli's principle the total wave function must have an odd parity. Hence, even values of $L+l$ yield $S=0$ (spin singlet state) and odd $L+l$ values require $S=1$ (spin triplet state). However, for a non-interacting system the energy levels (S.5) are degenerate with respect to the possible location of the cyclotron orbit center. Hence, the states with $S=1$, $S_z=1$ are energetically distinguishable as states with the lowest energy for all allowed sets of quantum numbers N, n, L, l corresponding to the two-electron Landau levels, with their spin moments oriented parallel to the applied magnetic field B. The energy of non-interacting two-electron system is thus equal to

$$E^0_{NnLl} = \hbar\omega_c(N+n+L+l) \; . \tag{S.8}$$

B. Real-space bound pair in magnetic field

In a direct analogy to the Cooper-pair problem [15], we can build the ground-state wave function as a linear superposition of the functions obtained for the non-iteracting system, namely

$$\Phi^{S,S_z}_{NLl}(R, \Phi, r, \phi) = \sum_n \alpha_n \; \Psi^{S,S_z}_{NLnl}(\zeta(R), \Phi, \xi(r), \phi) \; . \tag{S.9}$$

Note that only the sumation over n is performed, since operators of angular momentum $\hat{L}_z$, $\hat{l}_z$, operator $\hat{S}_z$ and part of the Hamiltonian dependend on coordinates of centre of the mass does commute with the full Hamiltonian (S.4). Hence, only the quantum number n is not conserved in the presence of interaction. Thus, the parity of the ground-state wave function is defined in the same way as before, i.e. the spin singlet pairing is performed only for even values of $L+l$ and the spin triplet - for the odd $L+l$ values.

Taking the expectation value $< \Phi^{S,S_z}_{NLl}|H|\Phi^{S,S_z}_{NLl} >$ and making use of the orthonormality relations we obtain the self-consistent equation for the coefficients α_n

$$\alpha_{n'} = -\frac{\sum_n \alpha_n V_{n'nl}}{(E_0)^{S,S_z}_{NLn'l} - E^{S,S_z}_{Ll}} \ , \tag{S.10}$$

where $V_{n'nl} = \int_0^\infty dr\ r\ u_{n'l}(\xi(r))\ V(r)\ u_{nl}(\xi(r))$, and E^{S,S_z}_{Ll} is the energy of the system, which depends on the quantum numbers S, S_z, L, l. Substituting into the above equation $V(r)$ of the form (S.2) and changing the integration variable from r to $\xi = r^2/2r_H^2$, we can rewrite the matrix element $V_{n'nl}$ in the form

$$V_{n'nl} = -\frac{V_0}{\sqrt{n!(n+l)!n'!(n'+l)!}} \int_0^{\frac{a^2}{2r_H^2}} d\xi\ e^{-\xi}\ \xi^l\ L^l_{n'}(\xi)\ L^l_n(\xi) \ . \tag{S.11}$$

Thus, the pairing potential is renormalized by extension of the pair wave function. We are interested only in the states with the lowest energy, so we can put main quantum number of the centre of the mass N as equal to zero (it represents the case with the vanishing center-of-mass kinetic energy). In result, we arrive at the Fredholm-type integral equation:

$$\alpha_{n'l} = -\frac{\sum_n \alpha_{nl} V_{n'nl}}{(E_0)^{S,S_z}_{n'Ll} - E^{S,S_z}_{Ll}} \ , \tag{S.12}$$

where $(E_0)^{S,S_z}_{nLl} = \hbar\omega_c\,(n+l+L-S_z+1)$. The essential difficulty in solving this equation is rooted in the calculation of matrix element $V_{n'nl}$. It cannot be carried out analytically for all values of magnetic field. Nevertheless, the analysis of the limits of weak ($r_H >> a$) and strong magnetic fields ($r_H << a$) can be easily performed, as we show next.

C. Weak magnetic field: $a \ll r_H$

The limit of weak magnetic field is obtained in the case, when the range a of the pairing potential well is small compared to the magnetic length r_H. In that limit the relative motion is only weakly perturbed by the magnetic field. Then upper limit of an integral

in (S.11) $\xi_a = a^2/2r_H^2$ becomes very small (for $B \to 0$ magnetic length $r_H \to \infty$). In this case integration goes over values of ξ, which are very close to zero, allows us to expand the integrand function in the power series of ξ, as well as and limit our considerations to the lowest nontrivial order. Such analysis yields the following form of the pairing amplitude in the presence of an applied field:

$$V_{n'nl}(\xi \ll 1) = -\frac{V}{\sqrt{n!(n+|l|)!n'!(n'+|l|)!}} \int_0^{\frac{a^2}{2r_H^2}} d\xi \; \xi^{|l|} \; (1 + o(\xi)) \; . \tag{S.13}$$

Integrating out this expression, we obtain the following formula for matrix element

$$V_{n'nl} = -\frac{V_0}{(l+1)\sqrt{n!(n+l)!n'!(n'+l)!}} \left(\frac{a^2}{2r_H^2}\right)^{l+1} . \tag{S.14}$$

Substituting this result into (S.12) and performing few elementary steps (following the original derivation of Cooper), we finally obtain the equation for the energy eigenvalues in the form

$$1 = \frac{V_0}{l+1} \left(\frac{a^2}{2r_H^2}\right)^{l+1} \sum_{n'} \frac{1}{n'!(n'+l)!} \frac{1}{(E_0)_{n'Ll}^{S,S_z} - E_{Ll}^{S,S_z}} \; . \tag{S.15}$$

This expression can be rewritten in the following dimensionless form:

$$1 = \frac{1}{l+1} \chi^{l+1} \beta^{l+1} \sum_{n'} \frac{1}{n'!(n'+l)!} \frac{1}{\beta(n'+l+L-S_z+1) - \tilde{E}_{Ll}^{S,S_z}} \; , \tag{S.16}$$

where $\chi = V_0 m a^2/2\hbar^2$ characterizes the relative depth of the potential well; $\beta = B/B_0$ is dimensionless magnetic field expressed in units $B_0 \equiv mV_0/\hbar e$ and $\tilde{E}_{Ll}^{S,S_z} = E_{Ll}^{S,S_z}/V_0$ is self-energy of the system relative to the pairing energy depth V_0. Binding energy $\tilde{\Delta}_{Ll}^{S,S_z} = \Delta_{Ll}^{S,S_z}/V_0$ of the pair of electrons is defined as follows

$$\tilde{\Delta}_{Ll}^{S,S_z} = \tilde{E}_{Ll}^{S,S_z} - (\tilde{E}_g)_{Ll} \; , \tag{S.17}$$

where $(\tilde{E}_g)_{Ll} = \hbar\omega_c(L+l)/V_0 = \beta(L+l)$ (cf. eq. (S.8)) corresponds to the lowest energy level occupied by the electrons with angular momenta L, l in the absence of the pairing iteraction.

Numerical solution of (S.16) is shown in Fig S.1 for $\chi = 10$. For given $\chi = 1$ and the range of the potential, $a = 100$ Å, we obtain for $m = m_0$ the potential depth equal to $V_0 = 1,5$ meV and $B_0 \approx 13$ T. The following three initial states were considered:

1) $L = 0$, $l = 0$, $S = 0$, $S_z = 0$ - spin- and orbital-singlet state

2) $L = 1$, $l = 0$, $S = 1$, $S_z = 1$ - spin-triplet state with non-zero center-of-mass angular momentum;

3) $L = 0$, $l = 1$, $S = 1$, $S_z = 1$ - spin-triplet, p orbital state of the pair.

One should note that the state $L = 1$ and $l = 0$ is the Landau state for the pair, whereas the $l = 1$, $L = 0$ state represents orbitally antisymmetric (p) state of the pair.

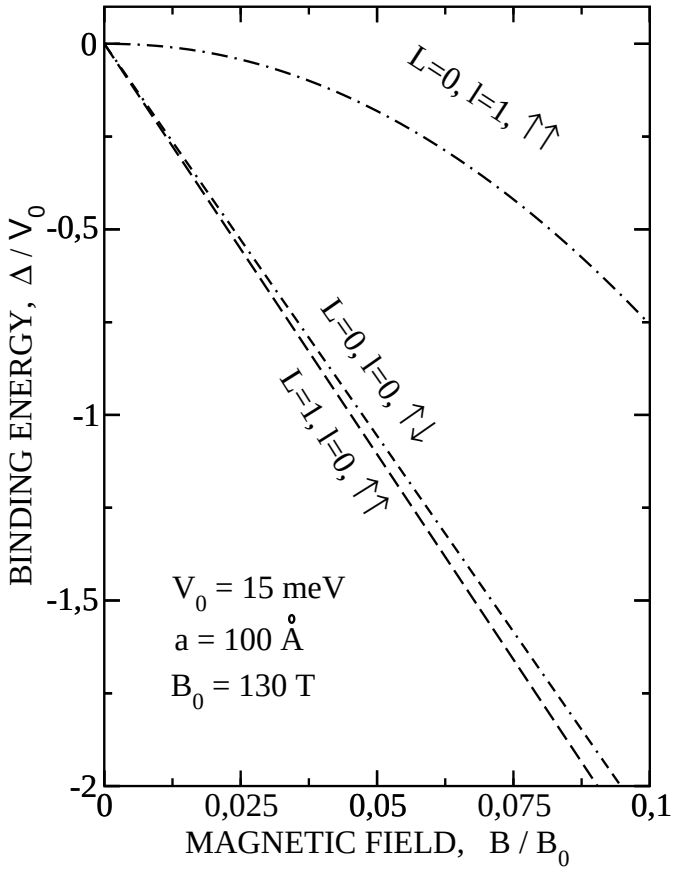

Figure S.1: Binding energy of two electron system in a weak magnetic fields. The inset specifies exemplary set of the model parameters for $\chi = 10$.

The binding energy increases with the increasing magnetic field. This Δ increase is connected with the circumstance that the electron wave function shrinks with the increasing B. However, the growth rate strongly depends on the value of the relative angular momentum l. This result is also in good correspondence with the physical intuition, since the pair with non-zero relative angular momentum can resist more efficiently the compressing action of the applied magnetic field. In the other words, it is

much harder to squeeze the wave function of a rotating system. The difference between the solutions for $L = 0$ and $L = 1$ is caused by an additional negative contribution arising from the advantageous spin orientation appearing in the latter case.

Surprisingly, the binding energy of the pair vanishes while approaching the limit of zero magnetic field. This is the result of an improper choice of the set of basis functions used to construct the ground-state wave function. In other-words, for $B \to 0$ the size of the wave function is rather provided by the Cooper-pair coherence length rather then by magnetic length. These functions and the corresponding energy eigenvalues were calculated in the case of vanishing wave function in infinity. In effect the wave function magnitude vanishes identically in the $B \to 0$ limit. This is not correct, since we expect a bound pair state at $B = 0$. This nonanalyticity will be corrected in Next section, when we proposed a wave function diffrent from (S.9), which will provide a correct Cooper-pair binding in the limit $B = 0$.

D. Strong magnetic field: $r_H \ll a$

The decomposition (S.9) of the wave function should describe properly the physics in the limit of strong magnetic fields i.e. when $r_H \ll a$. In this case the upper limit $\xi_a = a^2/2r_H^2$ of the integral in (S.11) becomes very large and therefore, can be approximated by infinity. In effect, the matrix elements take now the form

$$V_{n'nl} = -\frac{V_0}{\sqrt{n!(n+l)!n'!(n'+l)!}} \int_0^\infty d\xi \; e^{-\xi} \; \xi^l \; L^l_{n'}(\xi) \; L^l_n(\xi) \; . \tag{S.18}$$

Using the orthonormality of the Laguerre polynomials

$$\int_0^\infty d\xi \; e^{-\xi} \; \xi^l \; L^l_{n'}(\xi) \; L^l_n(\xi) = n!(n+l)! \; \delta_{n'n},$$

we obtain the following expression for matrix elements

$$V_{n'nl} = -V_0 \; \delta_{n'n}. \tag{S.19}$$

Substituting this result into (S.12) yields the following equation for the energy eigenvalues of the pair

$$E^{S,S_z}_{Ll} = (E^0)^{S,S_z}_{n'Ll} - V_0 \; . \tag{S.20}$$

Hence, the binding energy is

$$\Delta^{S,S_z}_{Ll} = E^{S,S_z}_{Ll} - (E_g)_{Ll} = (E^0)^{S,S_z}_{n'Ll} - V_0 - (E_g)_{Ll} \; .$$

For the three particular cases considered above, it provides the following limiting value

- for $L=0$, $l=0$, $S=0$, $S_z=0$: $\Delta_{L=0,l=0}^{S=0,S_z=0} = \hbar\omega_c - V_0$
- for $L=1$, $l=0$, $S=1$, $S_z=1$: $\Delta_{L=1,l=0}^{S=1,S_z=1} = -V_0$
- for $L=0$, $l=1$, $S=1$, $S_z=1$ $\Delta_{L=0,l=1}^{S=1,S_z=1} = -V_0$

In the case $S=1$, $S_z=1$ (spin triplet, parallel spin orientation) the binding energy reaches its maximal value V_0. This result can be easily explained. For strong magnetic fields whole ground state wave function of the pair is confined within the range of the potential well. Hence, a further increase of the field B does not change anything, since the expectation value of the pairing part will remain the same.

The situation is quite different in the case of the spin singlet ($S=0$). Here, the bound state is destroyed as it is the state of higher energy than the state of the two non-interacting electrons with parallel spin orientation.

S.2 Variational approach for an arbitrary applied field

In this Section we apply a variational method to the Cooper problem for $B \neq 0$. This is because the limit of weak magnetic field the Cooper-like approach does not yield a non-zero pair binding energy for $B=0$. Analysing Eq.(S.14) we notice that the matrix element $V_{n'nl}$ vanishes in that limit, and hence the equation (S.15) for eigenvalues may have solution only in the case when the eigenvalues of energy are equal to the energies of non-interacting pair of electrons, i.e. $\Delta = 0$. Vanishing of these matrix elements is caused by the improper choice of a set of basis functions used. These functions are simply spread over the whole space. Hence, it is necessary to introduce a factor, which will keep them localised, if a bound state exists. Obviously, such an approach must also reproduce correctly the $B \to \infty$ limit.

The ground state energy of the pair can be estimated by the well-known variational formula

$$E_G \leq E = \frac{<\Psi|\hat{H}|\Psi>}{<\Psi|\Psi>}\,, \tag{S.21}$$

where $|\Psi>$ is a trial function. We discuss again the three situations discussed in the previous section.

Case A: $L = 0$, $l = 0$, $S = 0$, $S_z = 0$ - spin singlet state, s orbital state

We can choose the wave function (S.6) with $N = n = 0$ (ground state) as the trial function

$$\Psi(r, R) = \frac{1}{\sqrt{2\pi}} \frac{1}{r_H} \, e^{-\frac{r^2}{4r_H^2}} \, \frac{1}{\sqrt{2\pi}} \frac{1}{R_H} \, e^{-\frac{R^2}{4R_H^2}} \tag{S.22}$$

However, due to the discussion at the beginning of this paragraph, we must introduce variational parameters into it, which are responsible for localization of the wave function. It can be realized by defining the function

$$\Psi(r, R) = \frac{1}{\sqrt{2\pi}\alpha} \, e^{-\frac{r^2}{4\alpha^2}} \, \frac{1}{\sqrt{2\pi}\eta} \, e^{-\frac{R^2}{4\eta^2}} \, , \tag{S.23}$$

where α is the parameter in the relative part of wave function and η is inserted into the center-of-mass part. Both parameters characterize the size of respective parts of the total wave function. The trial function is normalized (we have assumed here that the correlation length of the wave function is negligibly small in comparison with the crystal size in order to perform integration over r and R over the interval $(0, \infty)$).

Substituting the function (S.23) into Eq.(S.21) and taking Hamiltonian in the form (S.4), we obtain after the integration over R, r, Φ and ϕ

$$E_G \leq E(\alpha, \eta) = \frac{M\omega_c^2\eta^2}{4} + \frac{\hbar^2}{4M\eta^2} + \frac{\mu\omega_c^2\alpha^2}{4} + \frac{\hbar^2}{4\mu\alpha^2} - \hbar\omega_c S_z - V_0 \left(1 - e^{-a^2/2\alpha^2}\right) \, . \tag{S.24}$$

Minimizing this expression with respect to α and η, we obtain the upper estimate for the ground state energy. Condition $\partial E(\alpha, \eta)/\partial\eta = 0$ yields $\eta_{min} = R_H$. Hence, we can rewrite the dimensionless version of (S.24) for $S_z = 0$ as follows

$$\frac{E(\alpha, \eta_{min} = R_H)}{V_0} = \frac{\beta}{2} + \frac{\alpha^2}{4a^2} \, \chi \, \beta^2 + \frac{1}{4\alpha^2\chi} a^2 - (1 - e^{-a^2/2\alpha^2}) \, , \tag{S.25}$$

where $\beta = B/B_0$ and χ were defined previously. It is convienient to define a new dimensionless, variational parameter $\lambda = \alpha/a$. In effect, we can write

$$\frac{E(\lambda, R_H)}{V_0} = \frac{\beta}{2} + \frac{\lambda^2}{4} \, \chi \, \beta^2 + \frac{1}{4\lambda^2\chi} - (1 - e^{-1/2\lambda^2}) \, . \tag{S.26}$$

Minimizing this equation with respect to λ for different values of β, we can determine the influence of the applied field on the binding energy $\tilde{\Delta}_{L=0,l=0}^{S=0,S_z=0} = \tilde{E}_{min}(\lambda, \eta) - (\tilde{E}_g)_{L=0,l=0}$. The related numerical results are shown in Fig. S.2 for $\chi = 10$ (for $a = 100$ Å, we obtain $V_0 = 15$ meV, and $B_0 = 130$ T). The binding energy of the singlet pair decreases with the increasing magnetic field. The bound state is destroyed at the critical value $B_c \approx B_0$.

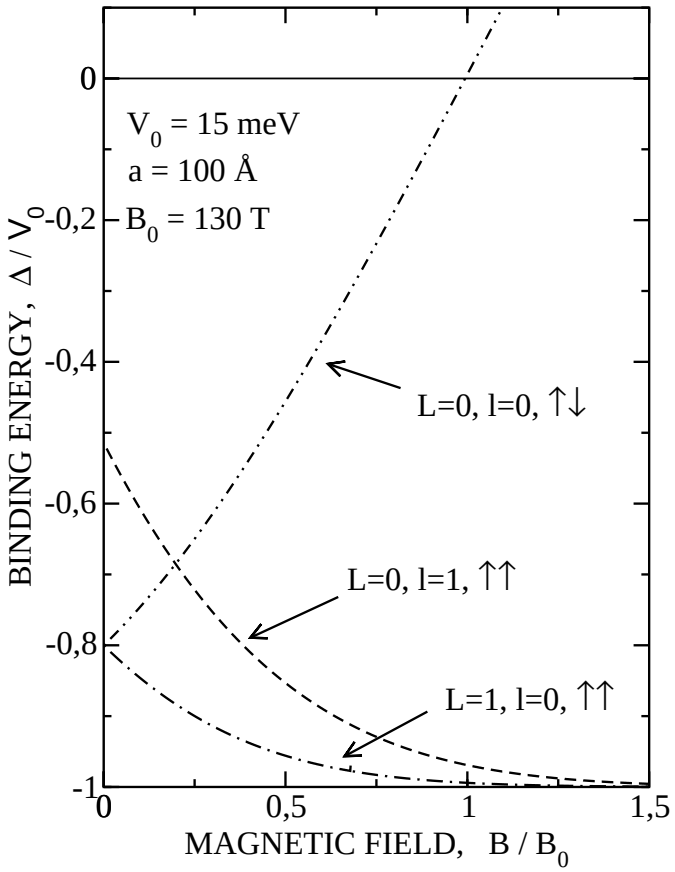

Figure S.2: Binding energy vs. magnetic field - variational solution for three different quantum states.

The pair binding energy depends strongly on the value of parameter χ describing potential well. In the absence of magnetic field ($\beta = 0$), minimum of energy is reached for $\lambda^2_{min} = 1/2ln(2\chi)$, where $\chi > 1/2$. Below this value there is no solution (bound state). Hence, the expression for the energy is

$$\tilde{E}_{min}(\beta = 0) = \frac{ln2\chi + 1}{2\chi} - 1 \, .$$

This dependence of energy on parameter χ in zero field is displayed in Fig. S.3.

To conclude, the binding energy depends on two parameters: $\chi = V_0 m a^2/2\hbar^2$ and $B_0 = V_0/2\mu_B$. The first of them is nonzero even in the limit $a \to 0$ and $V_0 \to \infty$, with $V_0 a^2$ finite, i.e. for a contact attraction $-V_0 a^2 \delta(\mathbf{r})$. The second expresses rather large applied-field value, for which the Zeeman energy is equal to the electrostatic binding potential. The additional parameter is the self-consistently adjusted pair orbit size $\lambda \equiv \alpha/a$.

Case B: $L = 1$, $l = 0$, $S = 1$, $S_z = 1$ - *spin-triplet state*

In this case the wave function for non-interacting system with quantum numbers $N = n = l = 0$ and $L = 1$ can be chosen as the trial function. Variational parameters α and η are introduced as follows:

$$\Psi(r, R, \Phi) = \frac{1}{\sqrt{2\pi}\alpha}\, e^{-\frac{r^2}{4\alpha^2}}\, \frac{R}{2\sqrt{\pi}\eta^2}\, e^{i\Phi} e^{-\frac{R^2}{4\eta^2}} \ . \tag{S.27}$$

After some algebra we obtain the following expressionfor the trial energy

$$E(\alpha, \eta) = \frac{M\omega_c^2\eta^2}{2} + \frac{\hbar^2}{2M\eta^2} + \frac{\hbar\omega_c}{2} + \frac{\mu\omega_c^2\alpha^2}{4} + \frac{\hbar^2}{4\mu\alpha^2} - \hbar\omega_c S_z - V_0\left(1 - e^{-a^2/2\alpha^2}\right) \ . \tag{S.28}$$

Condition $\partial E(\alpha, \eta)/\partial\eta = 0$ yields $\eta = R_H$. The dimensionless form (for $S_z = 1$) of the energy is

$$\frac{E(\lambda, \eta = R_H)}{V_0} = \frac{\beta}{2} + \frac{\lambda^2}{4}\, \chi\, \beta^2 + \frac{1}{4\lambda^2\chi} - \left(1 - e^{-1/2\lambda^2}\right) \ . \tag{S.29}$$

The binding energy $\Delta_{L=1,l=0}^{S=1,S_z=1} = E_{min}(\alpha, \eta) - (E_g)_{L=1,l=0}$ vs field β investigated from above expression is shown also in Fig.S.2. The binding energy increases in this case up to maximal value 1, in good correspondence with the result obtained with the Cooper approach for the case of strong field. The bound state is preserved thanks to the parallel spin orientation. The state represents the ground state of the pair in $L = 1$ state.

This solution in the field absence ($\beta = 0$) is the same as that in case A with the same restriction $\chi > 1/2$.

Case C: $L = 0$, $l = 1$, $S = 1$, $S_z = 1$ - *spin triplet-state, p-orbital state*

The trial function selection is based on the wave function (S.6) written for quantum numbers $N = n = L = 0$ and $l = 1$ with variational parameters α and η, i.e. has the form

$$\Psi(r, \phi, R) = \frac{1}{\sqrt{2\pi}\eta}\, e^{-\frac{R^2}{4\eta^2}}\, \frac{r}{2\sqrt{\pi}\alpha^2}\, e^{i\phi} e^{-\frac{r^2}{4\alpha^2}} \ . \tag{S.30}$$

The trial energy has then the form

$$\begin{aligned} E(\alpha, \eta) \ = \ & \frac{M\omega_c^2\eta^2}{4} + \frac{\hbar^2}{4M\eta^2} + \frac{\mu\omega_c^2\alpha^2}{2} + \frac{\hbar^2}{2\mu\alpha^2} + \frac{\hbar\omega_c}{2} - \hbar\omega_c S_z \\ & -V_0\left[1 - e^{-a^2/2\alpha^2}\left(1 + \frac{a^2}{2\alpha^2}\right)\right] \ . \end{aligned} \tag{S.31}$$

Substituting $\eta = R_H$ (obtained from the condition $\partial E(\alpha, \eta)/\partial\eta = 0$), and taking $S_z = 1$, we can write the dimensionless version of $E(\alpha, \eta)$ as

$$\frac{E(\lambda, \eta = R_H)}{V_0} = \frac{\lambda^2}{2}\, \chi\, \beta^2 + \frac{1}{2\lambda^2\chi} - \left[1 - e^{-1/2\lambda^2}\left(1 + \frac{1}{2\lambda^2}\right)\right] \ . \tag{S.32}$$

The binding energy $\Delta_{L=0,l=1}^{S=1,S_z=1} = E_{min}(\alpha,\eta) - (E_g)_{L=0,l=1}$ vs field β is shown in Fig. S.2. Similarly as in the case B binding energy grows up to maximal value 1. However, the growth is slower and all the time binding energy in the case of non-zero relative angular momentum is smaller than in the case of non-zero center-of-mass angular momentum. This can be explained as follows: the center-of-mass rotation does not affect pairing process, while the relative part does.

Solution for the energy in the field absence vs parameter χ is presented in Fig. S.3. In this case the bound state appears for χ greater than 3.35 (see the inset).

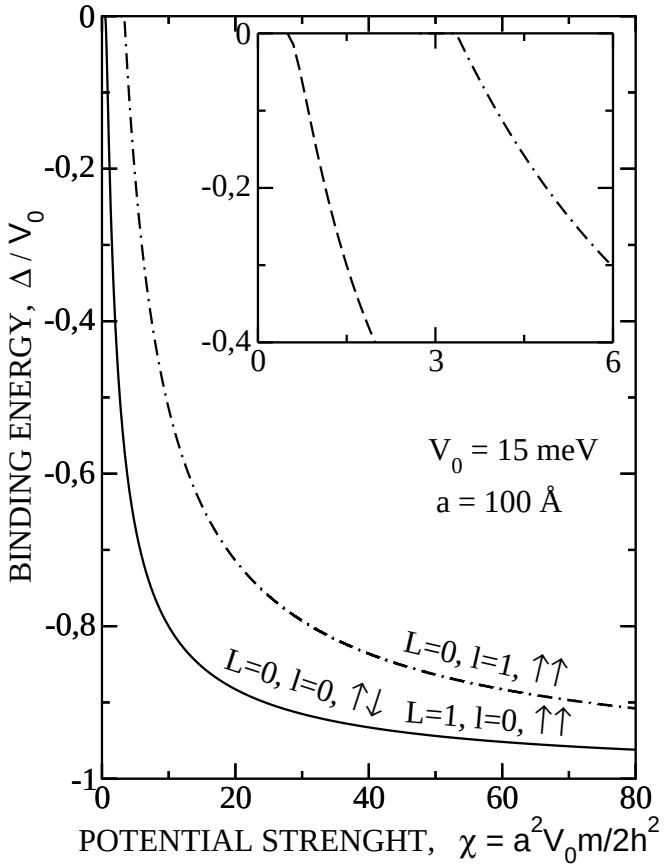

Figure S.3: Binding energy vs. potential well parameter $\chi = mV_0a^2/2\hbar^2$ for $B = 0$. The inset shows the detailed behaviour in the $\chi \to 0$ limit.

It is interesting to see how the variational parameter λ behaves with increasing field. This dependence is shown in Fig.S.4 for three considered sets of quantum numbers and

for $\chi = 10$. Parameter λ can be considered as a dimensionless correlation length of the relative part of the wave function. In the case of fixed $\lambda = r_H/a$, and for $\beta \to 0$ (dotted line) the correlation length diverges, what corresponds to the fact that wave function is not localized. This is not the case, when λ is obtained from the minimization of the system energy. The correlation length is finite in zero field and approches asymptotically the value r_H with increasing B. The relative wave function is always localized inside the potential well range, since $\lambda < 1$ for all values of magnetic field B/B_0.

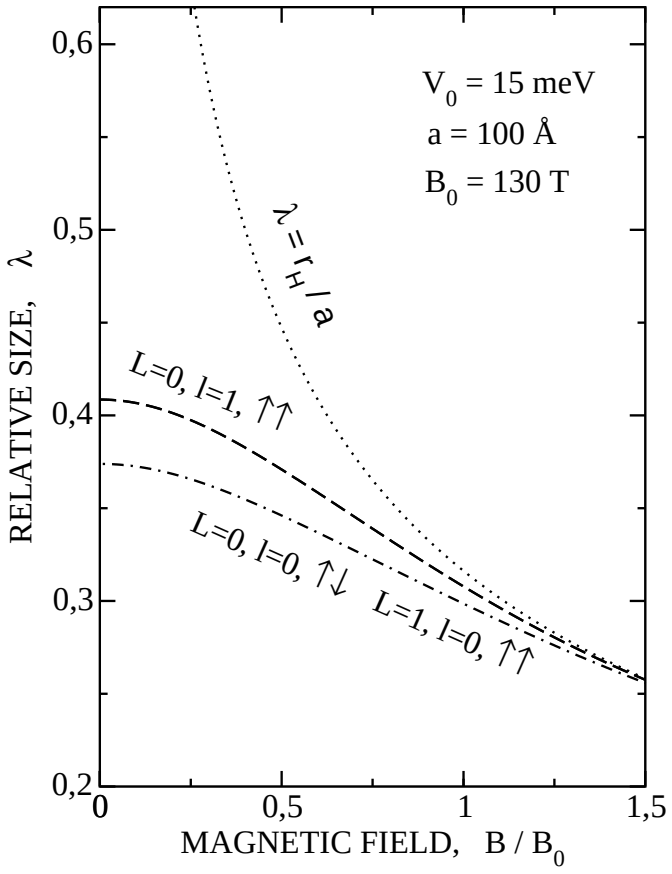

Figure S.4: Variational parameter $\lambda = \alpha/a$ (considered as size of relative wave function) vs magnetic field. Dotted line represents fixed variational parameter at the value $\lambda = r_H/a$.

Summarizing this Section, the states: spin-singlet with $L = l = 0$ and the spin-triplet with $L = 1$ and $l = 0$, are degenerate in the field absence, but the spin-triplet state with $L = 1$ is favored for $B > 0$. In other words, a stable pair state in the absence of the

Coulomb interaction is a pair rotating together ($l = 0$) on a Landau orbit with $L = 1$. The binding into a pair takes place only above the critical value of χ. The parameter ratio $\chi = V_0/\frac{\hbar^2}{(m/2)a^2}$ has a simple interpretation. Namely, the momentum uncertainty in a box of the radius $2a$ is of the order $\Delta p \sim \hbar/a$. Therefore, the kinetic energy uncertainty for the pair in its relative motion is of the order $(\Delta p)^2/(m/2) \sim \hbar^2/\left[(m/2)a^2\right]$. Thus, the parameter χ expresses the ratio of pair binding potential to the kinetic energy increase due to the formation of the bound state inside the potential well.

S.3 Effect of the Coulomb repulsion

As we have seen above, the applied field favors the rotating spin-triplet state with the canter-of-mass angular momentum $L = 1$ and the relative angular momentum $l = 0$. There is no critical magnetic field for a singlet-triplet transition if the repulsive interaction is absent. This critical field absence is caused by the circumstance that for a single pair there is no wave-function rigidity [35] induced by the interaction with other pairs. Also, the repulsive Coulomb interaction will favor an antisymmetric space part of the of the wave function, i.e. the spin-singlet configuration. In this Section we analyse the effect of the repulsive interactions among the partners. We model this interaction with the help of the two forms of the potential energy $V_{rep}(r)$, namely

1) $V(r) = U\,\frac{a}{r}$, and

2) $V(\mathbf{r}) = Ua^2\delta^{(2)}(\mathbf{r})$.

The first case with $U = \frac{e^2}{\kappa a}$, where κ is the static dielectric constant of the environment, describes the long-range nature of the potential in this planar system. The second case describes the well screened potential center placed in the center of the attractive well.

To calculate the system energy in the present situation we take again the total wave function in the form (S.23) with $\eta = R_H$. The trial energy in the case 1) for $L = 1$, $l = 0$ state has the form

$$\frac{E(\lambda, R_H)}{V_0} = \frac{\beta}{2} + \frac{\lambda^2}{4}\,\chi\,\beta^2 + \frac{1}{4\lambda^2\chi} - (1 - e^{-1/2\lambda^2}) + \sqrt{\frac{\pi}{2}}U\frac{1}{\lambda}\,. \tag{S.33}$$

The binding energy in this case is

$$\frac{\Delta^{S=1,S_z=1}_{L=1,l=0}}{V_0} = \frac{E_{min}(\alpha,\eta)}{V_0} - \beta\,. \tag{S.34}$$

The expression for the energy of other states can be obtained in a strightforward manner and will not be reproduced explicitly here.

In case 2) we represent the δ function in the polar coordinates in the form $\delta^{(2)}(\mathbf{r}) = \frac{1}{r}\delta(r)\delta(\phi)$. Within this representation (and leaving aside the problem of indeterminacy of the angle ϕ for $\mathbf{r} = 0$) we obtain the trial pair energy for the $L = 1$, $l = 0$ state in form

$$\frac{E(\lambda, R_H)}{V_0} = \frac{\beta}{2} + \frac{\lambda^2}{4}\,\chi\,\beta^2 + \frac{1}{4\lambda^2\chi} - (1 - e^{-1/2\lambda^2}) + \frac{1}{2\pi}U\frac{1}{\lambda^2}\,. \tag{S.35}$$

The binding energy is described in the same way as before (S.34). Note that in the state with $L = 0$, $l = 1$ the δ-potential does not influence the pairing, since its wave function vanishes in the potential well center.

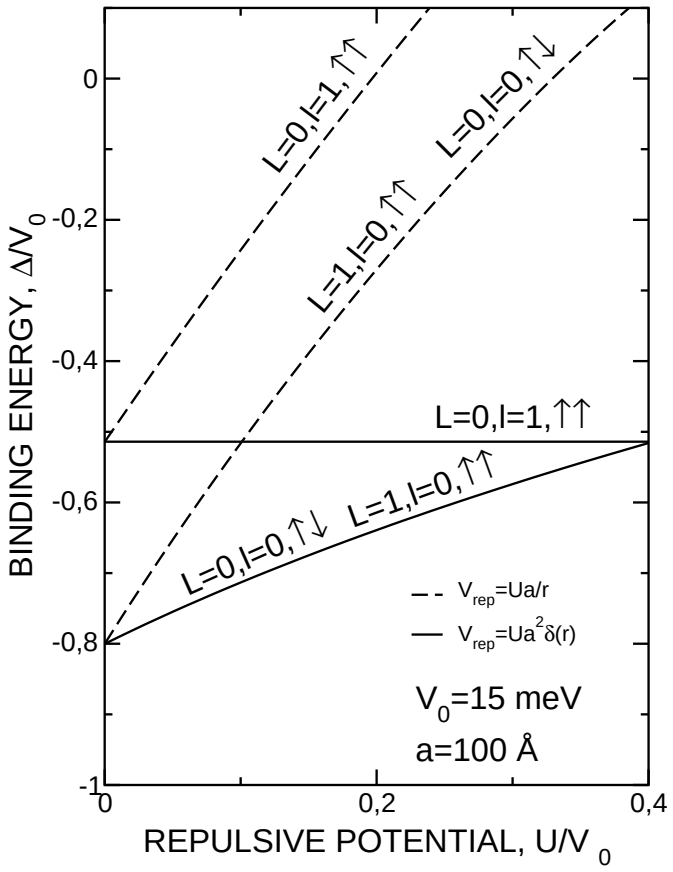

Figure S.5: The pair binding energy as a function of relative interaction magnitude U/V_0 and for the field $B = 0$. A comparison is made between the long- and the short-range interactions.

In Fig. S.5 we plot the binding energy of the pair as a function of relative interaction magnitude U/V_0 for the field $B = 0$. As expected, the repulsive contribution reduces the binding energy of the $L = 1$, $l = 0$ state, if the interaction is of long-range nature. However, for $U/V_0 > 0.4$ (cf. Fig. S.6) in the case of the short-range interaction, the $L = 0$, $l = 1$ state with parallel spins becomes stable. The relative stability of the $l = 1$, $S_z = 1$ state in the presence of the repulsive (δ-like) interaction is reminiscent of the instability with a large l invoked long time ago [36] and induced by a purely repulsive interaction when the higher-order effects (and screening) are both important.

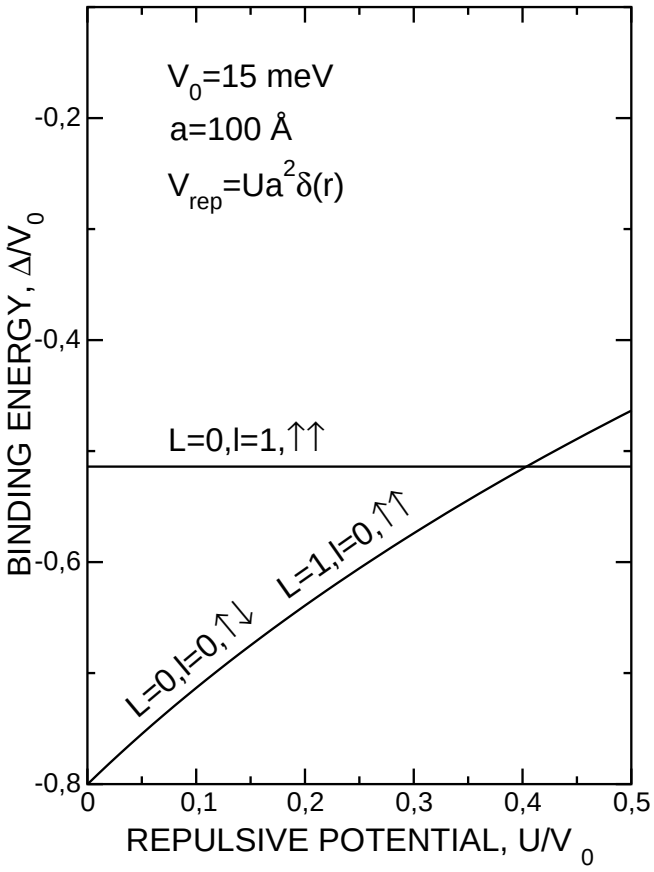

Figure S.6: The binding energy of the pair in the states indicated as a function of relative interaction magnitude U/V_0 and for the field $B = 0$ in the case of the δ-type repulsive potential.

The combined effect of the repulsive interaction and the magnetic field is illustrated in Figs. S.7 a-b. In extremely high field the pair states become unstable for the long-

range repulsive potential. Obviously all the Figures were plotted for a rather weak repulsive interactions. This means that in order to observe those states $\chi = V_0 m a^2/2\hbar^2$ must be rather large and U/V_0 rather small, i.e. the artificial atom must be rather large and placed in a highly polarizable medium.

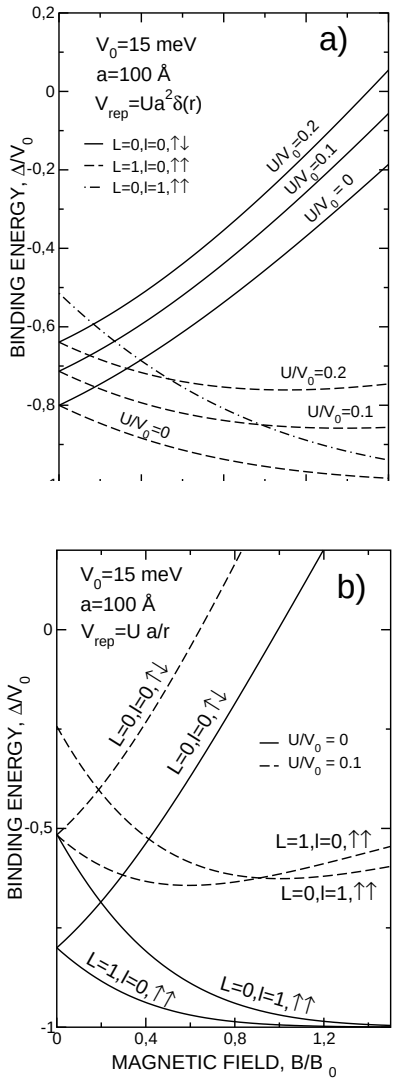

Figure S.7: Combined effect of the repulsive interaction and the magnetic field on the binding energy: a) for the δ-type of repulsive potential, and b) for the screened Coulomb potential. Note the singlet-triplet transition in the case b) for $U/V_0 > 0$.

Finally, in Fig. S.8 we display a typical dependence of the pair size as a function of the applied field for the cases specified (the $L = l = 0$ singlet and $L = 1$, $l = 0$ triplet states have the same size). The pair size α is always substantially smaller than

the pairing potential range $2a$, i.e. $\lambda = \alpha/a \sim \frac{1}{2}$. Thus, the orbiting pair in the applied field can be easily accomodated within the potential well boundaries at relatively low fields.

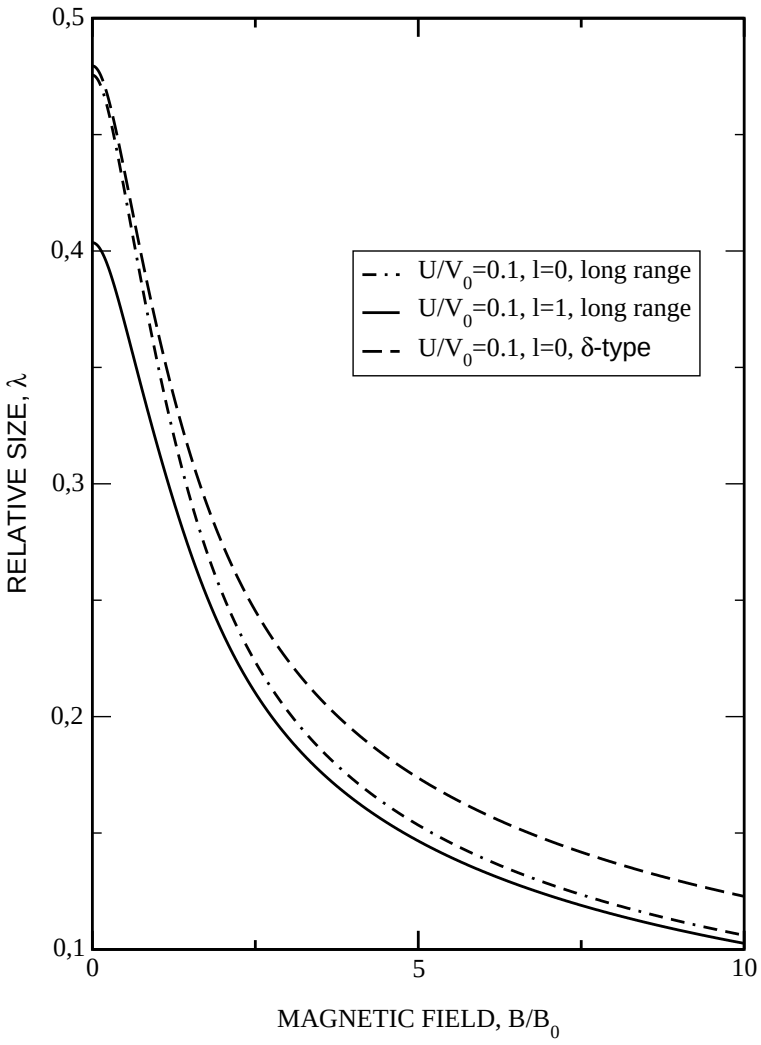

Figure S.8: Typical bound-pair size vs. applied magnetic field.

S.4 Conclusions

We have considered two-electron states induced by a pairing potential in real space in an external, uniform magnetic field. Due to the difficulties with the direct calculation of matrix element $V_{n'nl}$, our studies were limited first to the cases of weak and strong

applied field. As in the standard Cooper-pair case, we compose the pair wave function from those of noninteracting particles taken here in a nonzero magnetic field. In both cases the presence of the field increases the binding energy of the pair, approaching with $B \to \infty$ to its maximal value provided by the depth V_0 of the potential well. Within such a direct approach, the limit of zero magnetic field is not properly restored, since binding energy of the pair decreases to zero. This result is inconsistent with the calculations performed in the field absence. This inconsistency has its source in the improper choice of the basis of noninteracting functions to describe the ground state.

This problem is fixed within a variational approach. The trial function is constructed with a variational parameter, which is responsible for the localization of the pair wave function in the system. This approach leads to a non-zero binding energy in the field absence, and properly restores the solution for very strong magnetic fields in both cases of the spin singlet and the spin triplet paired states. The repulsive interaction has a strong influence on the magnitude of the binding, but still favors *the spin-triplet* configuration. We point out that this triplet ground-state configuration can be observed when a planar quantum dot is deposited on a substrate of highly polarized medium. The most interesting result is that for $B \neq 0$ the triplet state with the center-of-mass angular momentum $L = 1$ is stable, *not* the usual spin-triplet state with the relative angular momentum $l = 1$.

Appendices

A. Expression of Hund's rule term by the pairing operators A and $A^{\dagger}$

B. Two-band model: general solution ($\Delta_0 \neq \Delta_{-1} \neq \Delta_1 \neq \Delta_0$, $E_{\mathbf{k}1} \neq E_{\mathbf{k}2}$)

C. Magnetic moment of the ferromagnetic state: $T = 0$, $\rho = 1/W$ case

D. Final form of self-consistent equations for Δ, μ, $\bar{S}^z$ and E_G

Appendix A

Expression of Hund's rule term by the pairing operators A_{im} and $A^{\dagger}_{im}$

The Hund's rule coupling term can be expressed either by the spin operators $\hat{\mathbf{S}}_{il}$ expressed via fermionic operators or by the local spin-triplet pair operators A, $A^{\dagger}$. Here, we show in a straightforward manner the equivalence of both representations.

We start from the full Hund's rule term written with help of the spin operators $\hat{\mathbf{S}}_{il}$, $\hat{\mathbf{S}}_{il'}$

$$\sum_{ill'(l\neq l')} \left(\mathbf{S}_{il} \cdot \mathbf{S}_{il'} + \frac{3}{4}\, n_{il} n_{il'} \right) . \tag{A.1}$$

In the spin space, operator $\mathbf{S}_{il}$ has the Cartesian components $(S^x_{il}, S^y_{il}, S^z_{il})$, where each of them is responsible for the projection of a spin of a single particle on the selected axis. As usually, one expresses the S^x_{il} and S^y_{il} components in terms of the spin creation and annihilation operators S^+_{il} and S^-_{il} defined as $a^{\dagger}_{il\uparrow} a_{il\downarrow}$ and $a^{\dagger}_{il\downarrow} a_{il\uparrow}$, repectively, where the first of them changes the spin orientation of a particle from down to up, and the second - vice versa. For this purpose, we use the following relation

$$\begin{cases} S^x = \frac{1}{2}\,(S^+ + S^-) \\ S^y = \frac{1}{2i}\,(S^+ - S^-) \end{cases} . \tag{A.2}$$

Simultaneously, the component S^z_{il} expressed in the language of second quantization yields

$$S^z_{il} = \frac{1}{2}(n_{il\uparrow} - n_{il\downarrow}) , \tag{A.3}$$

where $n_{il\uparrow}$ is the operator of number of particles with spin up, whereas $n_{il\downarrow}$ counts particles with spin down. As a result, the spin operator $\mathbf{S}_{il}$ can be rewritten to the form

$$\mathbf{S}_{il} = \frac{1}{2} \left(S^+_{il} + S^-_{il}\,,\ \frac{1}{i}(S^+_{il} - S^-_{il}),\ n_{il\uparrow} - n_{il\downarrow} \right) . \tag{A.4}$$

Now, we can decompose the first term from (A.1) as follows

$$\begin{aligned}\mathbf{S}_{il}\cdot\mathbf{S}_{il'} &= \frac{1}{2}\left(S^+_{il}+S^-_{il},\ \frac{1}{i}(S^+_{il}-S^-_{il}),\ n_{il\uparrow}-n_{il\downarrow}\right)\times \\ &\quad\times\frac{1}{2}\left(S^+_{il'}+S^-_{il'},\ \frac{1}{i}(S^+_{il'}-S^-_{il'}),\ n_{il'\uparrow}-n_{il'\downarrow}\right) \\ &= \frac{1}{4}\left(S^+_{il}+S^-_{il}\right)\left(S^+_{il'}+S^-_{il'}\right)-\frac{1}{4}\left(S^+_{il}-S^-_{il}\right)\left(S^+_{il'}-S^-_{il'}\right) \\ &\quad+\frac{1}{4}\left(n_{il\uparrow}-n_{il\downarrow}\right)\left(n_{il'\uparrow}-n_{il'\downarrow}\right)\ .\end{aligned}$$

Since the terms $S^+_{il}S^+_{il'}$ and $S^-_{il}S^-_{il'}$ vanish in the expression above, it reduces to

$$\mathbf{S}_{il}\cdot\mathbf{S}_{il'}=\frac{1}{2}\left(S^+_{il}S^-_{il'}+S^-_{il}S^+_{il'}\right)+\frac{1}{4}\left(n_{il\uparrow}n_{il'\uparrow}+n_{il\downarrow}n_{il'\downarrow}-n_{il\uparrow}n_{il'\downarrow}-n_{il\downarrow}n_{il'\uparrow}\right)\ . \tag{A.5}$$

In the case of the second term from (A.1), we make use of the definition of the operator n_{il}, namely $n_{il}=n_{il\uparrow}+n_{il\downarrow}$, as it represents the total number of particles on site i and orbital l, and thus should consider both spin orientations. Therefore, we obtain

$$n_{il}n_{il'}=n_{il\uparrow}n_{il'\uparrow}+n_{il\downarrow}n_{il'\downarrow}+n_{il\uparrow}n_{il'\downarrow}+n_{il\downarrow}n_{il'\uparrow} \tag{A.6}$$

Substituting (A.5) and (A.6) into (A.1), we can rewrite it to the form

$$\begin{aligned}\sum_{ill'(l\neq l')}\left(\mathbf{S}_{il}\cdot\mathbf{S}_{il'}+\frac{3}{4}\,n_{il}n_{il'}\right) &= \sum_{ill'(l\neq l')}\Big(\frac{1}{2}\left(S^+_{il}S^-_{il'}+S^-_{il}S^+_{il'}+n_{il\uparrow}n_{il'\downarrow}+n_{il\downarrow}n_{il'\uparrow}\right) \\ &\qquad +n_{il\uparrow}n_{il'\uparrow}+n_{il\downarrow}n_{il'\downarrow}\Big)\end{aligned} \tag{A.7}$$

It is straightforward to show, that $n_{il\uparrow}n_{il'\uparrow}$ and $n_{il\downarrow}n_{il'\downarrow}$ can be directly expressed by the operators A and $A^\dagger$ (see Eq. (2.4) for the definition of operators). Explicitly,

$$n_{il\uparrow}n_{il'\uparrow}=a^\dagger_{il\uparrow}a_{il\uparrow}a^\dagger_{il'\uparrow}a_{il'\uparrow}=a^\dagger_{il\uparrow}a^\dagger_{il'\uparrow}a_{il'\uparrow}a_{il\uparrow}=A^\dagger_{ill',m=1}A_{il'l,m=1}\ , \tag{A.8}$$

where we have used the anticommutation relations fulfilled by the operators a and $a^\dagger$ (note that $l\neq l'$). Similarly, we can show that

$$n_{il\downarrow}n_{il'\downarrow}=A^\dagger_{ill',m=-1}A_{il'l,m=-1}\ . \tag{A.9}$$

In the last step, we take into account the remaining terms in (A.7). Expressing the operators S^+ and S^- in terms of the operators a, $a^\dagger$, we obtain

$$\begin{aligned}&\tfrac{1}{2}\quad\left(S^+_{il}S^-_{il'}+S^-_{il}S^+_{il'}+n_{il\uparrow}n_{il'\downarrow}+n_{il\downarrow}n_{il'\uparrow}\right)= \\ &=\quad\frac{1}{2}\left(a^\dagger_{il\uparrow}a_{il\downarrow}a^\dagger_{il'\downarrow}a_{il'\uparrow}+a^\dagger_{il\downarrow}a_{il\uparrow}a^\dagger_{il'\uparrow}a_{il'\downarrow}+a^\dagger_{il\uparrow}a_{il\uparrow}a^\dagger_{il'\downarrow}a_{il'\downarrow}+a^\dagger_{il\downarrow}a_{il\downarrow}a^\dagger_{il'\uparrow}a_{il'\uparrow}\right)\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{2}\left(a^{\dagger}_{il\uparrow}a^{\dagger}_{il'\downarrow}a_{il'\uparrow}a_{il\downarrow} + a^{\dagger}_{il\downarrow}a^{\dagger}_{il'\uparrow}a_{il'\downarrow}a_{il\uparrow} + a^{\dagger}_{il\uparrow}a^{\dagger}_{il'\downarrow}a_{il'\downarrow}a_{il\uparrow} + a^{\dagger}_{il\downarrow}a^{\dagger}_{il'\uparrow}a_{il'\uparrow}a_{il\downarrow}\right) \\
&= \frac{1}{2}\left[a^{\dagger}_{il\uparrow}a^{\dagger}_{il'\downarrow}\left(a_{il'\uparrow}a_{il\downarrow} + a_{il'\downarrow}a_{il\uparrow}\right) + a^{\dagger}_{il\downarrow}a^{\dagger}_{il'\uparrow}\left(a_{il'\downarrow}a_{il\uparrow} + a_{il'\uparrow}a_{il\downarrow}\right)\right] \\
&= \frac{1}{\sqrt{2}}\left(a^{\dagger}_{il\uparrow}a^{\dagger}_{il'\downarrow} + a^{\dagger}_{il\downarrow}a^{\dagger}_{il'\uparrow}\right) \times \frac{1}{\sqrt{2}}\left(a_{il'\downarrow}a_{il\uparrow} + a_{il'\uparrow}a_{il\downarrow}\right) = A^{\dagger}_{ill',m=0}A_{il'l,m=0} \quad \text{(A.10)}
\end{aligned}
$$

Combining the results from (A.8)-(A.10), we can recast (A.1) in the form

$$
\sum_{ill'(l\neq l')}\left(\mathbf{S}_{il}\cdot\mathbf{S}_{il'} + \frac{3}{4}\,n_{il}n_{il'}\right) = \sum_{ill'(l\neq l')m} A^{\dagger}_{ill',m}A_{il'l,m}\ . \qquad \text{(A.11)}
$$

One can easily show, that $A^{\dagger}_{ill',m}A_{il'l,m} = A^{\dagger}_{il'l,m}A_{ill',m} \equiv A^{\dagger}_{im}A_{im}$. In the case of a two-band system, this gives additional factor 2 on the right side of (A.11), when executing summation over l and l'. Namely,

$$
\sum_{ill'(l\neq l')}\left(\mathbf{S}_{il}\cdot\mathbf{S}_{il'} + \frac{3}{4}\,n_{il}n_{il'}\right) = 2\sum_{im} A^{\dagger}_{ill',m}A_{il'l,m}\ . \qquad \text{(A.12)}
$$

This provides us with the identity (2.5).

Appendix B

Two-band model: general solution ($\Delta_0 \neq \Delta_{-1} \neq \Delta_1 \neq \Delta_0$, $E_{\mathbf{k}1} \neq E_{\mathbf{k}2}$)

In Section 3.1 we have discussed the solutions of the Hamiltonian (2.29) for the three principal phases of the system in the absence of magnetic field and ferromagnetic ordering ($S^z = 0$). Here we present the most general case, i.e. for arbitrary band energies $E_{\mathbf{k}1} \neq E_{\mathbf{k}2}$ and for arbitrary values of the gap parameters, which all are nonzero and differ from each other, namely $\Delta_0 \neq \Delta_1 \neq \Delta_{-1} \neq \Delta_0$ (cf. also [16]).

The Hamiltonian has the $4x4$ matrix form

$$\mathcal{H}_{HF} = \sum_{\mathbf{k}} \mathbf{f}_{\mathbf{k}}^{\dagger} \mathbf{H}_{\mathbf{k}} \mathbf{f}_{\mathbf{k}} + 2 \sum_{\mathbf{k}} E_{\mathbf{k}2} + N \, \frac{|\Delta_1|^2 + |\Delta_{-1}|^2 + 2|\Delta_0|^2}{2J} \,, \tag{B.1}$$

where

$$\mathbf{H}_{\mathbf{k}} = \begin{pmatrix} E_{\mathbf{k}1}, & 0, & \Delta_1, & \Delta_0 \\ 0, & E_{\mathbf{k}1}, & \Delta_0, & \Delta_{-1} \\ \Delta_1, & \Delta_0, & -E_{\mathbf{k}2}, & 0 \\ \Delta_0, & \Delta_{-1}, & 0, & -E_{\mathbf{k}2} \end{pmatrix} , \tag{B.2}$$

with $E_{\mathbf{k}1} \equiv E_{\mathbf{k}1} - \mu$ and $E_{\mathbf{k}2} \equiv E_{\mathbf{k}2} - \mu$, for simplicity. As previously, we assume that all the gap parameters are real.

In the case of arbitrary band energies, it is not possible to write down the set of equations based on Bogolyubow-de Gennes wave equation (2.38) in the same manner as before (cf. Eqs. (3.2)-(3.3), (3.25)-(3.26), (3.41)-(3.42)). Thus, in order to find the eigenvalues of the Hamiltonian (B.1), we have to diagonalize the matrix $\mathbf{H}_{\mathbf{k}}$. The

problem relies on solving the following equation

$$det \begin{pmatrix} E_{\mathbf{k}1} - \lambda, & 0, & \Delta_1, & \Delta_0 \\ 0, & E_{\mathbf{k}1} - \lambda, & \Delta_0, & \Delta_{-1} \\ \Delta_1, & \Delta_0, & -E_{\mathbf{k}2} - \lambda, & 0 \\ \Delta_0, & \Delta_{-1}, & 0, & -E_{\mathbf{k}2-\lambda} \end{pmatrix} = 0 \, . \tag{B.3}$$

The obtained eigenvalues are described by the expression

$$\lambda_{\mathbf{k}1\ldots4} = \frac{1}{2}\left(E_{\mathbf{k}1} - E_{\mathbf{k}2}\right) \pm \frac{1}{2}\left\{ \left(E_{\mathbf{k}1} + E_{\mathbf{k}2}\right)^2 + 2\tilde{\Delta}^2 \pm 2\sqrt{\tilde{\Delta}^4 - 4\tilde{\delta}^4} \right\}^{1/2} \, , \tag{B.4}$$

where the total gap $\tilde{\Delta}$ is characterized by the relation

$$\tilde{\Delta} = \left(\Delta_1^2 + \Delta_{-1}^2 + 2\Delta_0^2\right)^{1/2} \, , \tag{B.5}$$

and the gap asymmetry parameter $\tilde{\delta}$ is expressed as follows

$$\tilde{\delta} = \sqrt{|\Delta_0^2 - \Delta_1 \Delta_{-1}|} \, . \tag{B.6}$$

Note, that for the gap anisotropy parameter equal to zero ($\tilde{\delta} = 0$) gapless modes appear in the system, explicitly $\lambda_{\mathbf{k}1} = E_{\mathbf{k}1}$ and $\lambda_{\mathbf{k}2} = -E_{\mathbf{k}2}$.

One can easily check, that after substituting the conditions defining the phases A, $A1$, and B, respectively, into the general solution (B.4), it reduces nicely to the eigenvalues for the corresponding phases.

The eigenstates for the general case $\Delta_0 \neq \Delta_{-1} \neq \Delta_1 \neq \Delta_0$ and $E_{\mathbf{k}1} \neq E_{\mathbf{k}2}$ can be found with help of standard algebraic methods, and therefore will not be presented here.

Appendix C

Magnetic moment of purely ferromagnetic state: $T = 0$, $\rho = 1/W$ case

The dimensionless equations for the magnetic moment and the chemical potential of the ferromagnetic state, written for the case of $T = 0$ and the flat density of states $\rho = 1/W$, read

$$\bar{S}^z_{ferro} = \frac{1}{2}\int_{-1/2}^{1/2} d\epsilon \, \left\{ \theta(\tilde{\mu} - \epsilon + \tilde{I}\bar{S}^z + \beta) - \theta(\tilde{\mu} - \epsilon - \tilde{I}\bar{S}^z - \beta) \right\} , \tag{C.1}$$

$$n = 2\int_{-1/2}^{1/2} d\epsilon \, \left\{ \theta(\tilde{\mu} - \epsilon + \tilde{I}\bar{S}^z + \beta) + \theta(\tilde{\mu} - \epsilon - \tilde{I}\bar{S}^z - \beta) \right\} , \tag{C.2}$$

where θ is the Heaviside step function and β is defined as $\mu_B B/W$. The first integrands in the expressions above represent the occupation for the spin "up", and the second - spin "down" states.

For the two-band system the maximum number of particles per site is $n = 4$. We consider the case with $0 < n < 2$ here, which is equivalent to the situation with $2 < n < 4$ (the result of particle-antiparticle symmetry). For $n = 2$ the Slater antiferromagnetism arises, and for $n = 4$ we have the state, when all the states are occupied and where no magnetic state is possible.

The saturated ferromagnetic state for $n < 2$ occurs when all particles have the same spin orientation and no further change of magnetic moment is possible. Then, all particles occupy the bands with the spin orientation preferred by the system, whereas the bands with the opposite spin orientation are empty. Hence, the magnetic moment

(per site per orbital) for the saturated state simply yields

$$\bar{S}^z_{sat} = \frac{n}{4} \, . \tag{C.3}$$

Below the saturation point both types of bands are filled with the particles and therefore, both integrands in Eqs. (C.1) and (C.2) are non-zero. Hence, we can rewrite the equation for the chemical potential in the form

$$n = 2 \left[\int_{-1/2}^{\tilde{\mu}+\tilde{I}\bar{S}^z+\beta} d\epsilon \, + \int_{-1/2}^{\tilde{\mu}-\tilde{I}\bar{S}^z-\beta} d\epsilon \right] \, , \tag{C.4}$$

what results in the following expression for $\tilde{\mu}$

$$\tilde{\mu} = \frac{n-2}{4} \, . \tag{C.5}$$

As we can see, it depends neither on the magnetic field nor on the magnetic moment value.

Similarly, we evaluate the expression for the magnetic moment, for which the integral equation yieds

$$\bar{S}^z = \frac{1}{2} \left[\int_{-1/2}^{\tilde{\mu}+\tilde{I}\bar{S}^z+\beta} d\epsilon \, - \int_{-1/2}^{\tilde{\mu}-\tilde{I}\bar{S}^z-\beta} d\epsilon \right] \tag{C.6}$$

and hence, we obtain

$$\bar{S}^z = \frac{1}{1-\tilde{I}} \, \beta \implies \tilde{I} = 1 \, . \tag{C.7}$$

We recovered the Stoner criterion here. Normally, for $\tilde{I} < 1$ the magnetic moment depends linearly from the applied magnetic field and is equal to zero in its absence. The situation changes dramatically at the value of $\tilde{I}$ equal to 1. Then the magnetic moment diverges, what results in the possibility of existence of non-zero magnetic moment for $\beta \to 0$, i.e. spontaneous magnetization appears in the system. Therefore, the Stoner criterion defines the value of $\tilde{I} = 1$, at which the system undergoes the continouus phase transition from paramagnetic to ferromagnetic state.

Finally, we determine the critical value of $\tilde{I}$, for which the saturation occurs in the absence of magnetic field. For the saturated state the second integral in (C.6) should vanish, as it represents the average number of particles with the opposite spin orientation. This condition is fulfilled, when all the particles are transferred from the spin-down subband to the spin-up subband, i.e. when

$$\tilde{\mu} - \tilde{I}\bar{S}^z_{sat} \leq -1/2 \, . \tag{C.8}$$

Substituting (C.5) and (C.3) into the expression above, we obtain

$$\tilde{I} \geq 1 \, . \tag{C.9}$$

This means, that at the Stoner critical point the magnetic moment acquires the value characteristic for the saturated state, i.e. the transition is discontinuous.

Taking into account the results obtained for the magnetic moment below and above the Stoner threshold, we can describe its dependence on the *Stoner parameter* $\tilde{I}$ in the case of $\beta = 0$. Namely,

$$\begin{cases} \bar{S}^z = 0 & \text{for} \quad \tilde{I} < 1 \\ \bar{S}^z = \frac{n}{4} & \text{for} \quad \tilde{I} \geq 1 \end{cases} , \tag{C.10}$$

where we can observe the jump in the magnetic moment value at the Stoner critical point (cf. Fig. 4.3).

The results obtained in this Appendix are widely used in Section 4.3 as a reference solution for the superconducting state.

Appendix D

Final form of the self-consistent equations for Δ, μ, $\bar{S}^z$ and E_G

In this Appendix, we present the final form of the equations derived in Section 4.2, where they have been reduced to the integral form written for the case of $T = 0$. Here, we show the explicit analytical solutions for the integrals, thus presenting the exact expressions used in the numerical calculations.

Self-consistent equations for Δ, μ and $\bar{S}^z$

The sets of self-consistent equations have been collected in Eqs. (4.54) - (4.56). Solutions for the normal state case have been already presented and discussed in the previous appendix (cf. (C.5) and (C.7)). Thus, we focus on integrals written for the phases A and $A1$ only.

There are three types of integrals, we need to take into account. Explicitly,

$$\text{a)} \int_{-1/2}^{1/2} d\epsilon \, \frac{1}{\sqrt{(\epsilon - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta)^2 + \Delta^2_{\uparrow/\downarrow}}} \, ,$$

$$\text{b)} \int_{-1/2}^{1/2} d\epsilon \, \frac{\epsilon - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta}{\sqrt{(\epsilon - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta)^2 + \Delta^2_{\uparrow/\downarrow}}} \, ,$$

and

$$\text{c)} \int_{-1/2}^{1/2} d\epsilon \, \theta(\tilde{\mu} - \epsilon - \tilde{I}\bar{S}^z - \beta) \, .$$

The last integral, for the system below the saturation and Stoner threshold, simply yields

$$\int_{-1/2}^{1/2} d\epsilon \, \theta(\tilde{\mu} - \epsilon - \tilde{I}\bar{S}^z - \beta) = \int_{-1/2}^{\tilde{\mu} - \tilde{I}\bar{S}^z - \beta} d\epsilon \; = \tilde{\mu} - \tilde{I}\bar{S}^z - \beta + \frac{1}{2} \, . \qquad \text{(D.1)}$$

In the case of integrals a) and b), we substitute $\epsilon - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta \equiv \epsilon'$, and then recast them into the form

$$\text{a)} \int_{-1/2-\tilde{\mu}\mp\tilde{I}\bar{S}^z\mp\beta}^{1/2-\tilde{\mu}\mp\tilde{I}\bar{S}^z\mp\beta} d\epsilon' \, \frac{1}{\sqrt{(\epsilon')^2 + \Delta^2_{\uparrow/\downarrow}}} \, ,$$

and

$$\text{b)} \int_{-1/2-\tilde{\mu}\mp\tilde{I}\bar{S}^z\mp\beta}^{1/2-\tilde{\mu}\mp\tilde{I}\bar{S}^z\mp\beta} d\epsilon' \, \frac{\epsilon'}{\sqrt{(\epsilon')^2 + \Delta^2_{\uparrow/\downarrow}}} \, .$$

We notice, that a) is the integral of the very well known type $\int dx \; 1/\sqrt{x^2+a^2}$, which has the following solution

$$\int dx \; 1/\sqrt{x^2+a^2} = \ln|x + \sqrt{x^2+a^2}| + C \, ,$$

whereas the integral b) is expanded as follows

$$\int dx \; x/\sqrt{x^2+a^2} = \sqrt{x^2+a^2} + C \, .$$

Hence, the expressions for integrals a) and b) yield

$$\text{a)} \; = \; \ln \frac{1/2 - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta + \sqrt{(1/2 - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta)^2 + \Delta^2_{\uparrow/\downarrow}}}{-1/2 - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta + \sqrt{(-1/2 - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta)^2 + \Delta^2_{\uparrow/\downarrow}}} \, , \qquad \text{(D.2)}$$

and

$$\text{b)} \; = \; \sqrt{(1/2 - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta)^2 + \Delta^2_{\uparrow/\downarrow}} - \sqrt{(-1/2 - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta)^2 + \Delta^2_{\uparrow/\downarrow}} \, . \qquad \text{(D.3)}$$

Now, collecting the results (D.1) - (D.3), we write the final form of self-consistent equations for phases A and $A1$.

- phase A

$$1 = \tilde{J} \ln \frac{1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta + \sqrt{(1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)^2 + \Delta^2_{\uparrow}}}{-1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta + \sqrt{(1/2 + \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta^2_{\uparrow}}}$$

$$1 = \tilde{J} \ln \frac{1/2 - \tilde{\mu} + \tilde{I}\bar{S}^z + \beta + \sqrt{(1/2 - \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta^2_{\downarrow}}}{-1/2 - \tilde{\mu} + \tilde{I}\bar{S}^z + \beta + \sqrt{(1/2 + \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)^2 + \Delta^2_{\downarrow}}}$$

$$\begin{aligned} n - 2 \; = \; & \sqrt{(1/2 + \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta^2_{\uparrow}} - \sqrt{(1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)^2 + \Delta^2_{\uparrow}} \\ & + \sqrt{(-1/2 - \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta^2_{\downarrow}} - \sqrt{(1/2 - \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta^2_{\downarrow}} \end{aligned}$$

$$\begin{aligned} \bar{S}^z_A \; = \; & 1/4 \sqrt{(1/2 + \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta^2_{\uparrow}} - 1/4 \sqrt{(1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)^2 + \Delta^2_{\uparrow}} \\ & + 1/4 \sqrt{(1/2 - \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta^2_{\downarrow}} - 1/4 \sqrt{(-1/2 - \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta^2_{\downarrow}} \end{aligned}$$

- phase $A1$

$$1 = \tilde{J} \ln \frac{1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta + \sqrt{(1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)^2 + \Delta_\uparrow^2}}{-1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta + \sqrt{(1/2 + \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta_\uparrow^2}}$$

$$\begin{aligned} n - 2 &= \sqrt{(1/2 + \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta_\uparrow^2} - \sqrt{(1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)^2 + \Delta_\uparrow^2} \\ &\quad + 2\,(\tilde{\mu} - \tilde{I}\bar{S}^z - \beta) \end{aligned}$$

$$\begin{aligned} \bar{S}^z_{A1} &= 1/4\,\sqrt{(1/2 + \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta_\uparrow^2} - 1/4\,\sqrt{(1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)^2 + \Delta_\uparrow^2} \\ &\quad - 1/2\,(\tilde{\mu} - \tilde{I}\bar{S}^z - \beta) \end{aligned}$$

The sets above were evaluated with the help of iterative method. The parameters were determined with the numerical accuracy of the order $\sim 10^{-10}$.

Equations for ground state energy E_G

The expressions for the ground state energy are presented in Eqs. (4.60) - (4.62). As previously, all integrals encountered in these equations can be expanded analytically. We will present here the solutions only for the two of them, namely

$$\text{a)} \int_{-1/2}^{1/2} d\epsilon\, \sqrt{(\epsilon - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta)^2 + \Delta_{\uparrow/\downarrow}^2}\,,$$

and

$$\text{b)} \int_{-1/2}^{1/2} d\epsilon\, (\epsilon - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta)\, \theta(\tilde{\mu} \pm \tilde{I}\bar{S}^z \pm \beta - \epsilon)\,.$$

The remaining integrals are of the type $\int dx\; x$ and $\int dx$, and thus their solutions are trivial.

The integral a), with the help of substitution introduced previously, can be simplified to the more general form $\int dx\sqrt{x^2 + a^2}$, whose expansion reads

$$\int dx\sqrt{x^2 + a^2} = \frac{1}{2}\, x\, \sqrt{x^2 + a^2} + \frac{1}{2}\, a\, \ln|x + \sqrt{x^2 + a^2}| + C\,.$$

Hence, the solution for a) is as follows

$$\begin{aligned} \text{a)} \quad &= 1/2\,(1/2 - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta)\sqrt{(1/2 - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta)^2 + \Delta_{\uparrow/\downarrow}^2} \\ &- 1/2\,(-1/2 - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta)\sqrt{(-1/2 - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta)^2 + \Delta_{\uparrow/\downarrow}^2} \\ &+ 1/2\,\Delta_{\uparrow/\downarrow}^2 \ln \frac{1/2 - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta + \sqrt{(1/2 - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta)^2 + \Delta_{\uparrow/\downarrow}^2}}{-1/2 - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta + \sqrt{(-1/2 - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta)^2 + \Delta_{\uparrow/\downarrow}^2}}\,. \end{aligned} \tag{D.4}$$

In order to evaluate the integral b), we execute the Heaviside function (the same assumptions are made as previously), what results in change of upper limit in the integration range, explicitly

$$\int_{-1/2}^{1/2} d\epsilon \; (\epsilon - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta) \; \theta(\tilde{\mu} \pm \tilde{I}\bar{S}^z \pm \beta - \epsilon) = \int_{-1/2}^{\tilde{\mu} \pm \tilde{I}\bar{S}^z \pm \beta} d\epsilon \; (\epsilon - \tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta) \; .$$

Hence, we obtain

$$\text{b)} \; = \; -1/4 - \tilde{\mu} \pm \tilde{I}\bar{S}^z \pm \beta - (\tilde{\mu} \mp \tilde{I}\bar{S}^z \mp \beta)^2 \; . \tag{D.5}$$

With the help of the results (D.4) and (D.5), we can derive the final form of the expressions for ground state energy for both phases (A and $A1$) and for the normal state.

- phase A

$$\begin{aligned}
\frac{E_G^A}{N} \; = \; & -1/2 \; (1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)\sqrt{(1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)^2 + \Delta_\uparrow^2} \\
& - \; 1/2 \; (1/2 + \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)\sqrt{(1/2 + \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta_\uparrow^2} \\
& - \; 1/2 \; \Delta_\uparrow^2 \ln \frac{1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta + \sqrt{(1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)^2 + \Delta_\uparrow^2}}{-1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta + \sqrt{(1/2 + \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta_\uparrow^2}} \\
& - \; 1/2 \; (1/2 - \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)\sqrt{(1/2 - \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta_\downarrow^2} \\
& - \; 1/2 \; (1/2 + \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)\sqrt{(1/2 + \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)^2 + \Delta_\downarrow^2} \\
& - \; 1/2 \; \Delta_\downarrow^2 \ln \frac{1/2 - \tilde{\mu} + \tilde{I}\bar{S}^z + \beta + \sqrt{(1/2 - \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta_\downarrow^2}}{-1/2 - \tilde{\mu} + \tilde{I}\bar{S}^z + \beta + \sqrt{(1/2 + \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)^2 + \Delta_\downarrow^2}} \\
& - \; 2 \; \tilde{\mu} + \frac{\Delta_1^2 + \Delta_{-1}^2}{2J} + 2I \left(\bar{S}^z\right)^2
\end{aligned}$$

- phase $A1$

$$\begin{aligned}
\frac{E_G^{A1}}{N} \; = \; & -1/2 \; (1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)\sqrt{(1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)^2 + \Delta_\uparrow^2} \\
& - \; 1/2 \; (1/2 + \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)\sqrt{(1/2 + \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta_\uparrow^2} \\
& - \; 1/2 \; \Delta_\uparrow^2 \ln \frac{1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta + \sqrt{(1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta)^2 + \Delta_\uparrow^2}}{-1/2 - \tilde{\mu} - \tilde{I}\bar{S}^z - \beta + \sqrt{(1/2 + \tilde{\mu} + \tilde{I}\bar{S}^z + \beta)^2 + \Delta_\uparrow^2}} \\
& - \; 2 \; \tilde{\mu} - (\tilde{\mu} - \tilde{I}\bar{S}^z - \beta)^2 + \frac{\Delta_1^2}{2J} + 2I \left(\bar{S}^z\right)^2 - \frac{1}{4}
\end{aligned}$$

- normal state

$$\frac{E_G^N}{N} = -1/2 - 2\tilde{\mu} - 2\tilde{\mu}^2 - 2(\tilde{I}\bar{S}^z + \beta)^2 + 2I\left(\bar{S}^z\right)^2$$

This completes the formal expressions for the basic physical quantities.

Bibliography

[1] A. Layzer and D. Fay, Int. J. Magn. **1**, 135 (1971); Solid State Commun. **15**, 599 (1974).

[2] P. W. Anderson and W. F. Brinkman, Phys. Rev. Lett. (1973); for review see: P. W. Anderson and W. F. Brinkman 1975, 1978 in *Liquid and Solid Helium.*

[3] D. Fay and J. Appel, Phys. Rev. B **16**, 2325 (1977); A. J. Legget (1979?).

[4] G. Baskaran, Physica B **223-224**, 498 (1996).

[5] D. van der Marel and G. Sawatzky, Solid State Commun. **55**, 937 (1985).

[6] D. Agterberg, T. M. Rice, and M. Sigirst, Phys. Rev. Lett. **78**, 3374 (1997).

[7] J. F. Annett, B. L. Györffy, G. Litak, and K. Wysokiński, Eur. Phys. J. B **36**, 301 (2003)

[8] K. I. Wysokiński, G. Litak, J. F. Annett, and B. L. Györffy, Phys. Stat. Solidi (b) **236**, 325 (2003)

[9] A. Klejnberg and J. Spałek, J. Phys.: Condensed Matter **11**, 6553 (1999).

[10] A. Klejnberg and J. Spałek, Phys. Rev. B **61**, 15542 (2000).

[11] J. Bardeen, L. N. Cooper, J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

[12] D. Aoki et al., Nature **413**, 58 (2001).

[13] P. G. De Gennes *Superconductivity of Metals and Alloys* (W. A. Benjamin, New York, 1966)

[14] J. R. Schrieffer *Theory of Superconductivity* (Addison-Wesley, Redwood City, CA, fourth printing, 1988)

[15] L.N. Cooper, Phys. Rev. **104**, 1189 (1956)

[16] J. Spałek, Phys. Rev. B **63**, 104513 (2001).

[17] Y. Nambu, Phys. Rev. **117**, 648 (1960); *Midwest Conference on Theoretical Physics* (Purdue University, 1960), in preprint only.

[18] A.J. Leggett, Rev. Mod. Phys. **47**, 331 (1975)

[19] D. Vollhardt and P. Wölfle, *The Superfluid Phases of Helium 3* (Taylor&Francis, London 1990 - chapter 3 and 5)

[20] M. Cyrot and D. Pavuna *Wstęp do nadprzewodnictwa* (Wydawnictwo Naukowe PWN, Warszawa 1996)

[21] J. Spałek, P. Wróbel, W. Wójcik, *Proc. Int. Conf. Ruthenate and Rutheno-Cuprate Materials*, Springer Series Lecture Notes in Physics, vol. 603 (Springer, Berlin, 2002), pp 60-75.

[22] J. Spałek, P. Wróbel, W. Wójcik, Physica C **387**, 1-6 (2003)

[23] P. Wróbel, J. Spałek, W. Wójcik, Acta Physica Polonica B **34**, 527 (2003)

[24] G. Rickayzen *Theory of Superconductivity* (J. Wiley & Sons, New York, 1965).

[25] K. Yosida, Phys. Rev. **110**, 769-770 (1958).

[26] S.S. Saxena et al., Nature **406**, 587 (2000); A. Huxley et al., Phys. Rev. B**63**, 144519 (2001); N. Tateiwa et al., J. Phys. C: Condensed Matter C**13**, L17(2001).

[27] C. Pfleiderer, M. Uhlarz, S.M. Hayden, R. Vollmer, H.v.Löhneysen, N.R. Bernhoeft, and G.G. Lonzarich, Nature **412**, 58 (2001).

[28] Cf. e.g. L. Jacak, P. Hawrylak, and A. Wójs, *Quantum dots*, (Springer Vg., Berlin, 1998).

[29] A. Aharony, O. Entin-Wohlman, and Y. Imry, Phys. Rev. B **61**, 5452 (2000); J. Adamowski et al., Phys. Rev. B **62** 4234 (2000).

[30] The role of the electron-electron repulsive interactions in the two-dimensional case was discussed in: D. L. Shepelyansky, Phys. Rev. Lett. **73**, 2607 (1994); Y. Imry, Europhys. Lett. **30**, 405 (1995); Phys. Stat. Solidi (b) **205**, 249 (1998). Here we discuss first the attractive interaction and include the repulsive part later.

[31] S. Schmitt-Rink, C. M. Varma, and A. E. Ruckenstein, Phys. Rev. Lett. **63**, 445 (1989); M. Randeria, J.-M. Duan, and L.-Y. Shieh, Phys. Rev. B **41**, 327 (1990); K. Byczuk, J. Spałek, and W. Wójcik, Phys. Rev. B **46**, 14134 (1992).

[32] M. Ortuño and E. Cuevas, Europhys. Lett. **46**, 224 (1999); G. Benedetti and D. L. Shepelyansky, cond-mat/0011461, and references therein.

[33] Strictly speaking the pair-bound states are neither those of Cooper pair, nor those of bipolaron. This is because for the Cooper pair we have pairing in the momentum space, whereas the bipolaron state is formed by a self-consistent potential. Instead, we consider here a pairing *in real space*.

[34] For the case of a single electron see e.g. L. D. Landau and E. M. Lifshitz *"Quantum Mechanics"* (Pergamon Press, Oxford, 1980).

[35] See e.g. P. W. Anderson, *Basic Notions of Condensed Matter Physics*, (The Benjamin/Cummings Publishing Co., London, 1984), chapter 2. The second critical field (H_{c2}) estimate for a planar lattice is provided in: M. Mierzejewski and M. Maśka, Phys. Rev. B **60**, 6300 (1999), and to be published.

[36] W. Kohn and J. M. Luttinger, Phys. Rev. Lett. **15**, 524 (1965).