Origin and Effects of FFLO phases in Superconductors

Bachelor's Thesis

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Abstract

This thesis investigates type II superconductors consisting of Cooper pairs with different types of pairing. First, we examine time-reversal Cooper pairs using the Bardeen-Cooper-Schrieffer (BCS) theory in the simple case of no perturbations. We solve the self-consistent gap equation numerically and show how the superconductivity is suppressed by thermal fluctuations. Subsequently we add an external magnetic field for which we neglect orbital contributions, i.e., the Maki parameter is high. We investigate how the gap equation is modified by the Zeeman interaction and simulate how the superconductivity is suppressed by the field. Further we review the elusive Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state which has not yet been conclusively observed experimentally. We show that solving the self-consistent gap equation is equivalent to minimizing the free energy. Finally, we investigate if the FFLO state is favourable at low temperatures and at external magnetic fields near the Clogston-Chandrasekhar limit.

Contents

1 Introduction

Superconductors are some of the most intriguing and peculiar materials present in modern physics. Superconductivity, so far, only exists at very low temperatures and this is due to the fact that it is a direct consequence of quantum mechanics [1]. Magnetism and superconductivity are natural enimies. Eddy currents arise in superconductors in the presence of magnetic fields which lead to one of two outcomes. Either the magnetic field is excluded from the material, this is known as the Meissner effect, or the superconductivity is suppressed in the regions with a non-zero magnetic field. With a sufficiently large magnetic field the superconductivity will cease to exist. This happens at the critical field.

BCS theory was the first microscopic theoretical model of superconductors and we will use this to study the effects of a Zeeman interaction on a superconductor. First, we will consider the simple case with no external field. Secondly, we will investigate how an external magnetic field affects the superconductivity in materials where the orbital effects can be neglected. In both cases we will focus on two-dimensional type II superconductors with an s-wave, spin-singlet pairing. Furthermore, we will investigate if it could be favourable to form Cooper pairs without time-reversal symmetry at low temperatures and high magnetic fields. Thus we will search for the elusive FFLO state.

All figures, except Fig. 5 from [2], in this thesis are made by the author. Numerical plots and calculations have been produced using MATLAB™.

2 Second Quantization[1]

Second quantization representation will be presented briefly, as it is used in BCS theory. Since we are looking at a superconductor, we will only cover second quantization for fermions, but a similar representation can be made for bosons. In second quantization representation, or occupation number representation, an N-particle system is described in a basis given by

$$| n_{\nu 1}, n_{\nu 2}, n_{\nu 3}, \ldots\rangle, \qquad \sum_j n_{\nu j} = N, \tag{1}$$

where the occupation number $n_{\nu j}$ is the number of particles in a state $|\nu_j\rangle$. The occupation number operator $\hat{n}_{\nu j}$ is an eigenoperator to the state $|n_{\nu j}\rangle$ with the occupation number as eigenvalue.

$$\hat{n}_{\nu j} \mid n_{\nu j}\rangle = n_{\nu j} \mid n_{\nu j}\rangle. \tag{2}$$

States containing different numbers of particles are defined to be orthogonal. We can introduce the creation operator $\hat{c}^{\dagger}_{\nu j}$ and the annihilation operator, $\hat{c}_{\nu j} \equiv (\hat{c}^{\dagger}_{\nu j})^{\dagger}$. These operators either raise or lower the occupation number of state $\mid \nu_j\rangle$ by one. Due to Pauli's exclusion principle $n_{\nu j}$ can only be 0 or 1 for fermions. Thereby it must hold that

$$\hat{c}^{\dagger}_{\nu j}|1\rangle = 0 \quad \text{and} \quad \hat{c}_{\nu j}|0\rangle = 0. \tag{3}$$

[1]This section is based on chapter 1 of [3].

The operator algebra for the fermionic creation and annihilation operators can be defined by the following anti-commutation [2] relations

$$\{\hat{c}^{\dagger}_{\nu j}, \hat{c}^{\dagger}_{\nu k}\} = 0, \quad \{\hat{c}_{\nu j}, \hat{c}_{\nu k}\} = 0, \quad \{\hat{c}_{\nu j}, \hat{c}^{\dagger}_{\nu k}\} = \delta_{\nu j \nu k}. \tag{4}$$

Introducing the Hermitian operator $\hat{c}^{\dagger}_{\nu}\hat{c}_{\nu}$ and using these anti-commutation relations, it is trivial to show that it is, in fact, the occupation number operator $\hat{n}_{\nu}$, i.e.,

$$\hat{c}^{\dagger}_{\nu}\hat{c}_{\nu} = \hat{n}_{\nu} \quad \hat{c}^{\dagger}_{\nu}\hat{c}_{\nu}|n_{\nu}\rangle = n_{\nu}|n_{\nu}\rangle \quad \text{where} \quad n_{\nu} = 0, 1. \tag{5}$$

Operators such as the Hamiltonian of a system can be expressed in terms of the relevant annihilation and creation operators.

3 Superconductivity with no perturbations

3.1 Bardeen-Cooper-Schrieffer Theory

The Bardeen-Cooper-Schrieffer (BCS) theory was published in 1957 by the physicists whom the theory is named after. BCS theory describes superconductivity as a microscopic effect due to condensation of Cooper pairs with a bosonic distribution [3]. Most superconductors known to date are spin-singlet Cooper pairs with d-wave or s-wave symmetry [4]. We will focus on the latter. This is also referred to as time-reversal pairs, i.e., the pairing arrises between states with $(\mathbf{k}, \uparrow)$ and $(-\mathbf{k}, \downarrow)$.These spin-singlet Cooper pairs have a zero center-of-mass momentum, i.e., $\mathbf{q} = 0$. In the simple case of no external perturbations, we want to investigate how the superconducting band gap is affected by thermal fluctuations. It is advantageous to work out the calculations in reciprocal space. In BCS theory the occupation number representation, described above, is used. The operator $\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}$ $(\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow})$ is the creation (annihilation) operator of a time-reversal Cooper pair. The BCS model is described by the Hamiltonian [4]

$$H_{BCS} = \sum_{\mathbf{k}} (\xi_{\mathbf{k}}\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow} + \xi_{-\mathbf{k}}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}\downarrow}) - \frac{V}{N^2}\sum_{\mathbf{k},\mathbf{k}'} \hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow} \tag{6}$$

with

$$\xi_{\mathbf{k}} = 2t[\cos(ak_x) + \cos(ak_y)] - \mu. \tag{7}$$

The first term in H_{BCS} counts the kinetic energy, i.e., it adds $\xi_{\mathbf{k}}$ to the energy if the state $(\mathbf{k}\sigma)$ is occupied. We sum over the first Brillouin zone, i.e., $-\pi/a \leq \mathbf{k} < \pi/a$. To avoid double counting due to periodic boundary conditions, we only include one of the edges. Further we assume inversion symmetry such that $\xi_{\mathbf{k}} = \xi_{-\mathbf{k}}$. The first term in the dispersion is expressed in terms of the lattice spacing a and the tunnelling strength for the nearest neighbour hopping t in accordance to the tight binding model [5]. μ denotes the chemical potential. When $\xi_{\mathbf{k}} = 0$, we are at the Fermi level. The second term describes the scattering of a Cooper pair with momentum $(\mathbf{k}', -\mathbf{k}')$ into another pair with momentum $(\mathbf{k}, -\mathbf{k})$. The scattering happens with an amplitude of $-V$.

[2] For the operators $\hat{A}$ and $\hat{B}$ the anti-commutator is defined by $\{\hat{A}, \hat{B}\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}$.

This term is negative due to the fact that there is an attractive interaction between the electrons. The N^2 in the denominator is the number of sites in the lattice. The scattering term cannot be calculated analytically; so, we perform a mean-field approximation, $\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow} \simeq \langle\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow}\rangle\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow} + \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow}\langle\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow}\rangle - \langle\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow}\rangle\langle\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow}\rangle$ [6]. The last term is constant, and will therefore be neglected here. If we were interested in, e.g., the total energy of the system, this term could not be neglected. Since we are only interested in the gap equation, a constant shift in the energy has no conceptual implication. Defining the superconducting gap

$$\Delta \equiv \frac{V}{N^2}\sum_{\mathbf{k}}\langle\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow}\rangle, \tag{8}$$

and using the mean-field approximation, the BCS Hamiltonian can be reduced to

$$H^{mf}_{BCS} = \sum_{\mathbf{k}}(\xi_{\mathbf{k}}\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow} + \xi_{-\mathbf{k}}\hat{c}^\dagger_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}\downarrow}) - \sum_{\mathbf{k}}(\Delta\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow} + \Delta^*\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow}). \tag{9}$$

The Hamiltonian can be written in matrix form and thereby diagonalized by the following rotation of the $\hat{c}$-operators

$$\begin{pmatrix}\hat{\gamma}_{\mathbf{k}\uparrow}\\ \hat{\gamma}^\dagger_{-\mathbf{k}\downarrow}\end{pmatrix} = U^\dagger\begin{pmatrix}\hat{c}_{\mathbf{k}\uparrow}\\ \hat{c}^\dagger_{-\mathbf{k}\downarrow}\end{pmatrix} = \begin{pmatrix}u^*_{\mathbf{k}} & -v_{\mathbf{k}}\\ v^*_{\mathbf{k}} & u_{\mathbf{k}}\end{pmatrix}\begin{pmatrix}\hat{c}_{\mathbf{k}\uparrow}\\ \hat{c}^\dagger_{-\mathbf{k}\downarrow}\end{pmatrix}. \tag{10}$$

$u_{\mathbf{k}}$, $v_{\mathbf{k}}$ and Δ are assumed to be real. This is the Bogoliubov transformation. The transformation is chosen to be unitary such that the new $\hat{\gamma}$-operators represent fermions too, thus obeying the same anti-commutator relations, see Eq. (4). This is shown in Appendix A. In fact, they represent fermionic quasi excitation particles. Demanding that the transformation matrix, U, has to be unitary, i.e., $U^\dagger U = \mathbb{I}$, $UU^\dagger = \mathbb{I}$ and $|\det(U)| = 1$ we get that $u^2_{\mathbf{k}} + v^2_{\mathbf{k}} = 1$. The indices on the new operators $\hat{\gamma}_{\mathbf{k}\sigma}$ can be misleading. Since these operators are quasiparticles, the spin index on $\hat{\gamma}_{\mathbf{k}\sigma}$ should not be interpreted as spin. It should just be interpreted as a label. The Hamiltonian can now be diagonalized in the basis of these new operators.

$$U^\dagger H^{mf}_{BCS}U = \begin{pmatrix}u_{\mathbf{k}} & -v_{\mathbf{k}}\\ v_{\mathbf{k}} & u_{\mathbf{k}}\end{pmatrix}\begin{pmatrix}\xi_{\mathbf{k}} & -\Delta\\ -\Delta & -\xi_{-\mathbf{k}}\end{pmatrix}\begin{pmatrix}u_{\mathbf{k}} & v_{\mathbf{k}}\\ -v_{\mathbf{k}} & u_{\mathbf{k}}\end{pmatrix} = \begin{pmatrix}E_{\mathbf{k}} & 0\\ 0 & -E_{\mathbf{k}}\end{pmatrix}. \tag{11}$$

Writing the Hamiltonian on matrix form in this way also shifts the energy with a constant due to the anti-commutator relations viewed previously, Eq. (4). We will neglect this with the same argumentation as above. From this we can obtain the following 2 equations

$$(u^2_{\mathbf{k}} - v^2_{\mathbf{k}})\xi_{\mathbf{k}} + 2u_{\mathbf{k}}v_{\mathbf{k}}\Delta = E_{\mathbf{k}}, \tag{12}$$
$$2u_{\mathbf{k}}v_{\mathbf{k}}\xi_{\mathbf{k}} + (v^2_{\mathbf{k}} - u^2_{\mathbf{k}})\Delta = 0. \tag{13}$$

Using that U is unitary, we can now isolate $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ from these equations. The eigenenergies can be found by solving $H^{mf}_{BCS} - E_{\mathbf{k}}\mathbb{I} = 0$. Thus we obtain

$$bu_{\mathbf{k}} = \pm\sqrt{\frac{1}{2}\left(1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right)}, \quad v_{\mathbf{k}} = \pm\sqrt{\frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right)} \quad \text{and} \quad E_{\mathbf{k}} = \sqrt{\xi^2_{\mathbf{k}} + \Delta^2}. \tag{14}$$

$E_{\mathbf{k}}$ is the quasiparticle energies. Varying $\mathbf{k}$ this energy can never become zero due to the presence of Δ. Thus, a gap opens in the dispersion around zero with a size of 2Δ. Multiplying $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ we get

$$u_{\mathbf{k}}v_{\mathbf{k}} = \sqrt{\frac{1}{4}\left(1+\frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right)\left(1-\frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right)} = \frac{1}{2}\sqrt{1-\frac{E_{\mathbf{k}}^2-\Delta^2}{E_{\mathbf{k}}^2}} = \frac{\Delta}{2E_{\mathbf{k}}}. \tag{15}$$

The rotation can further be used to rewrite Eq. (8)

$$\Delta = \frac{V}{N^2}\sum_{\mathbf{k}}\langle(u_{\mathbf{k}}\hat{\gamma}_{-\mathbf{k}\downarrow} - v_{\mathbf{k}}\hat{\gamma}^{\dagger}_{\mathbf{k}\uparrow})(u_{\mathbf{k}}\hat{\gamma}_{\mathbf{k}\uparrow} + v_{\mathbf{k}}\hat{\gamma}^{\dagger}_{-\mathbf{k}\downarrow})\rangle \tag{16}$$

$$= \frac{V}{N^2}\sum_{\mathbf{k}}(u_{\mathbf{k}}^2\langle\hat{\gamma}_{-\mathbf{k}\downarrow}\hat{\gamma}_{\mathbf{k}\uparrow}\rangle - v_{\mathbf{k}}^2\langle\hat{\gamma}^{\dagger}_{\mathbf{k}\uparrow}\hat{\gamma}^{\dagger}_{-\mathbf{k}\downarrow}\rangle + u_{\mathbf{k}}v_{\mathbf{k}}(\langle\hat{\gamma}_{-\mathbf{k}\downarrow}\hat{\gamma}^{\dagger}_{-\mathbf{k}\downarrow}\rangle - \langle\hat{\gamma}^{\dagger}_{\mathbf{k}\uparrow}\hat{\gamma}_{\mathbf{k}\uparrow}\rangle)). \tag{17}$$

In the last two steps, we have used the anti-commutation relations given in Eq. (4). Since the operators $\hat{\gamma}_{\mathbf{k}\sigma}$,$\hat{\gamma}^{\dagger}_{\mathbf{k}\sigma}$ represent fermions, they obey Fermi-Dirac statistics. This implies that $\langle\hat{\gamma}^{\dagger}_{\mathbf{k}\sigma}\hat{\gamma}_{\mathbf{k}'\sigma'}\rangle = f(E_{\mathbf{k}})\delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'}$, whereas $\langle\hat{\gamma}^{\dagger}_{\mathbf{k}\sigma}\hat{\gamma}^{\dagger}_{\mathbf{k}'\sigma'}\rangle = 0$ and $\langle\hat{\gamma}_{\mathbf{k}\sigma}\hat{\gamma}_{\mathbf{k}'\sigma'}\rangle = 0$. Here $f(E_{\mathbf{k}}) = [1+e^{E_{\mathbf{k}}/k_BT}]^{-1}$ is the Fermi-Dirac distribution function, where k_B and T are the Boltzmann constant and temperature respectively. The new number operator $\hat{\gamma}^{\dagger}_{\mathbf{k}\sigma}\hat{\gamma}_{\mathbf{k}\sigma}$ counts the number of excitations above the superconducting ground state, i.e., states with energy $E_{\mathbf{k}} > 0$. Using these characteristics of the new operators, the gap equation can be written as

$$\begin{aligned}\Delta &= \frac{V}{N^2}\sum_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}}(\langle\hat{\gamma}_{-\mathbf{k}\downarrow}\hat{\gamma}^{\dagger}_{-\mathbf{k}\downarrow}\rangle - \langle\hat{\gamma}^{\dagger}_{\mathbf{k}\uparrow}\hat{\gamma}_{\mathbf{k}\uparrow}\rangle)\\ &= \frac{V}{N^2}\sum_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}}(1-\langle\hat{\gamma}^{\dagger}_{-\mathbf{k}\downarrow}\hat{\gamma}_{-\mathbf{k}\downarrow}\rangle - \langle\hat{\gamma}^{\dagger}_{\mathbf{k}\uparrow}\hat{\gamma}_{\mathbf{k}\uparrow}\rangle)\\ &= \frac{V}{N^2}\sum_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}}(1-2f(E_{\mathbf{k}})).\end{aligned} \tag{18}$$

Inserting Eq. (15) and using that $1-2f(E_{\mathbf{k}}) = \tanh(E_{\mathbf{k}}/2k_BT)$ it reduces to

$$\Delta = \frac{V}{N^2}\sum_{\mathbf{k}}\frac{\Delta}{2E_{\mathbf{k}}}\tanh\left(\frac{E_{\mathbf{k}}}{2k_BT}\right). \tag{19}$$

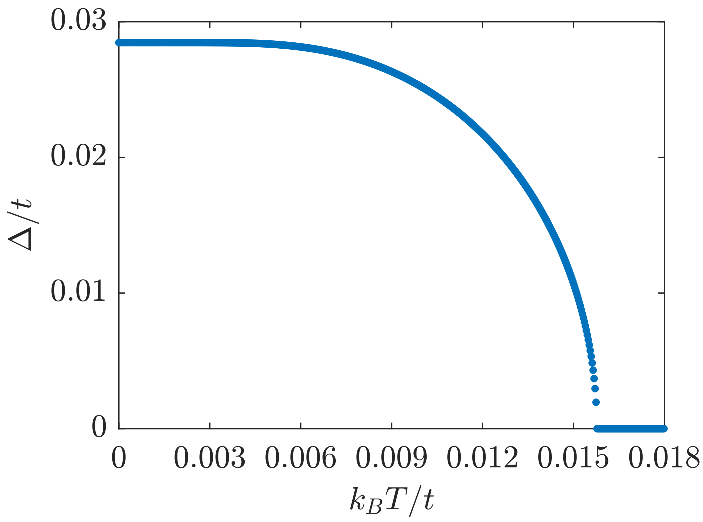


Fig. 1: Temperature dependence of the superconducting gap, Δ, given in terms of the hopping constant, t. The plot simulates how the superconductivity is suppressed by thermal fluctuations as the temperature increases.

This equation invokes self-consistency. A self-consistency equation has a trivial solution with $\Delta = 0$, and we will investigate whether there exists a nontrivial solution too. Using Eq. (14) and (19) to simulate how the bandgap changes with the temperature, we get the tendency plotted in Fig. 1. In the numerical solution, everything is given in terms of t, the hopping constant. The chemical potential, μ, is chosen such that the Fermi surface is not in touch with the edges of the Brillouin zone. The scattering potential, V, is chosen such that $\Delta \ll t$, i.e., $\Delta \sim 0.01t$. It is clear that as the temperature is increased, the superconducting gap is decreased. It can be shown that the superconducting band gap in fact is the microscopically derived order parameter of the superconducting state [4]. Thereby we observe the superconductivity being suppressed with increasing temperatures in Fig. 1. Eventually the superconductivity is completely destroyed by thermal fluctuations when Δ reaches zero at the critical temperature. An observable consequence of the order parameter is the gap that arises in the density of states. This is described in Appendix B.

4 Magnetic Perturbation of a Superconductor

In this section, we investigate how a superconductor is affected by an external magnetic field. An applied magnetic field can suppress the superconductivity in two different ways, i.e., by orbital effects due to the Lorentz force and by spin effects due to Pauli paramagnetic pair breaking. The Maki parameter describes the relative importance of these two effects.

4.1 The Maki Parameter

The orbital effect is often the dominant mechanism in breaking the superconducting state. There exist materials in which the opposite holds, e.g., materials with a heavy effective electron mass or in layered materials where the magnetic field lines are perpendicular to these layers [7]. The Maki parameter is given by [8]

$$\alpha_M = \frac{\sqrt{2}H_{c2}^{orb}}{H_{c2}^{P}}, \tag{20}$$

where H_{c2}^{orb} is the critical field for a type II superconductor only including the orbital effects, H_{c2}^{P} is the critical field in the paramagnetic limit. In this thesis we will neglect the orbital effect and focus on the Zeeman interaction, i.e., systems where $\alpha_M \geq 1$. This limit is denominated the Pauli limit.

4.2 The Clogston-Chandrasekhar limit [3]

Let us now focus on the Pauli paramagnetic pair breaking and find $H_{c2}^{P}(T)$. For small magnetic fields, the paramagnetism will be eliminated by the formation of spin-singlet Cooper-pairs in the superconducting state. When the magnetic field is sufficiently large, the Pauli paramagnetic pair-breaking will instead destroy the superconducting state. This happens when the normal state paramagnetic energy, E_P, exceeds the superconducting condensation energy, i.e., the binding energy of the Cooper pairs, E_c. The two quantities mentioned is given by

$$E_P = \frac{1}{2}\chi_n (H_{c2}^{P})^2, \quad E_c = \frac{1}{2}N_0\Delta^2(T), \tag{21}$$

N_0 being the density of states at the Fermi energy per spin polarization and χ_n being the normal spin susceptibility. The latter is given by

$$\chi_n = \frac{1}{2}g^2\mu_B^2 N_0, \tag{22}$$

where g is the gyromagnetic ratio and μ_B is the Bohr magneton. Setting $E_P = E_c$ and isolating $H_{c2}^{P}(T)$ we get

$$H_{c2}^{P}(T) = \frac{\sqrt{2}\Delta(T)}{|g|\mu_B}. \tag{23}$$

This is the Clogston-Chandrasekhar limit. It tells us how big the external field has to be to destroy the superconductivity. At this point there will be a first order transition from the BCS state to the depaired state. Since $H_{c2}^{P}(T)$ is directly proportional to Δ, the temperature dependence of these must have the same form, see Fig. 1. Thus the superconducting state can survive bigger magnetic fields at lower temperatures. Here we have assumed that the curvature of $\Delta(T)$ is the same for $B \neq 0$ as for $B = 0$. Whether this is true or not, we will investigate in the following section.

4.3 Modulation of the Gap Equation by a Zeeman Interaction in s-wave Superconductors

We want to investigate how the gap equation is modulated when a Zeeman interaction is added. In this section we are dealing with spin-singlet Cooper-pairs with a zero

[3] This section is inspired by [9]

center-of-mass momentum. The Hamiltonian is given by

$$H^{mf}_{BCS,B} = \sum_{\mathbf{k}} (\xi_{\mathbf{k}\uparrow}\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow} + \xi_{-\mathbf{k}\downarrow}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}\downarrow} - \Delta_B\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow} - \Delta_B\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow}) \tag{24}$$

where

$$\xi_{\mathbf{k}\sigma} = 2t[\cos(ak_x) + \cos(ak_y)] - \mu + H_{z\sigma} = 2t[\cos(ak_x) + \cos(ak_y)] - \mu - \sigma\frac{1}{2}g\mu_B B \tag{25}$$

with

$$\sigma = \begin{cases} 1 & \text{for} \quad \uparrow \\ -1 & \text{for} \quad \downarrow . \end{cases} \tag{26}$$

The extra term in $\xi_{\mathbf{k}\sigma}$ in Eq. (25) is the Zeeman term where B is the size of the magnetic field. We focus on the case where the magnetic field is parallel to $\uparrow$ and antiparallel to $\downarrow$. The Hamiltonian can be written in matrix form choosing an advantageous basis

$$H^{mf}_{BCS,B} = \sum_{\mathbf{k}} \begin{pmatrix} \hat{c}^{\dagger}_{\mathbf{k}\uparrow} & \hat{c}_{-\mathbf{k}\downarrow} & \hat{c}_{\mathbf{k}\uparrow} & \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix} \begin{pmatrix} \xi_{\mathbf{k}\uparrow} & -\Delta_B & 0 & 0 \\ -\Delta_B & -\xi_{-\mathbf{k}\downarrow} & 0 & 0 \\ 0 & 0 & -\xi_{\mathbf{k}\uparrow} & \Delta_B \\ 0 & 0 & \Delta_B & \xi_{-\mathbf{k}\downarrow} \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}\uparrow} \\ \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \\ \hat{c}^{\dagger}_{\mathbf{k}\uparrow} \\ \hat{c}_{-\mathbf{k}\downarrow} \end{pmatrix}, \tag{27}$$

such that the Hamiltonian is block diagonal. If we denote the top, left block of the Hamiltonian H^{2x2}, it is clear that the bottom, right block is equal to $-H^{2x2}$. Thus it is sufficient to diagonalize only H^{2x2}. We now realize that the H^{2x2} can be written in terms of the BCS Hamiltonian without the magnetic field in Eq. (9),

$$H^{2x2} = H^{mf}_{BCS} + H_{z\uparrow}\mathbb{I}, \tag{28}$$

where $\mathbb{I}$ is the identity matrix. It is now trivial to see that the eigenenergies are just shifted by the amount $H_{z\uparrow}$ and that the eigenvectors must be of the same form as Eq. (10).

$$U^{\dagger}(H^{mf}_{BCS} + H_{z\uparrow}\mathbb{I})U = U^{\dagger}H^{mf}_{BCS}U + U^{\dagger}H_{z\uparrow}\mathbb{I}U \tag{29}$$

$$\begin{pmatrix} E_{\mathbf{k}\uparrow} & 0 \\ 0 & -E_{\mathbf{k}\downarrow} \end{pmatrix} = \begin{pmatrix} E_{\mathbf{k}} + H_{z\uparrow} & 0 \\ 0 & -E_{\mathbf{k}} + H_{z\uparrow} \end{pmatrix}, \tag{30}$$

where $E_{\mathbf{k}}$ is the eigenenergy from the BCS model without a magnetic field, see Eq. (14). From this argument we can conclude that we do not need any spin dependency on the elements of U. If we had kept the spin dependency on the elements of U the symmetries from demanding that $U^{\dagger}U = \mathbb{I}$, $UU^{\dagger} = \mathbb{I}$, $|det(U)| = 1$ would force us to draw the same conclusion. Calculating the eigenenergies of the Hamiltonian in Eq. (27) by bruteforce, we get

$$E_{\mathbf{k}\sigma} = \pm\frac{\xi_{\mathbf{k}\uparrow} - \xi_{-\mathbf{k}\downarrow}}{2} + \sqrt{\frac{(\xi_{\mathbf{k}\uparrow} + \xi_{-\mathbf{k}\downarrow})^2}{4} + \Delta_B^2}. \tag{31}$$

Without the spin dependency, this reduces to the eigenenergies of the system with no external magnetic field, see Eq. (14). Realizing that $H_{z\uparrow} = \frac{\xi_{\mathbf{k}\uparrow}-\xi_{-\mathbf{k}\downarrow}}{2}$ and that $\xi_{\mathbf{k}} = \frac{\xi_{\mathbf{k}\uparrow}+\xi_{-\mathbf{k}\downarrow}}{2}$, this reads

$$E_{\mathbf{k}\pm} = \pm H_{z\uparrow} + \sqrt{\xi_{\mathbf{k}}^2 + \Delta_B^2} = E_{\mathbf{k}} \pm H_{z\uparrow}, \tag{32}$$

which is exactly what we argued above. To diagonalize the Hamiltonian, we perform a rotation of the original $\hat{c}$-operators into $\hat{\gamma}$-operators as in section 3.1. The Bogoliubov transformation is given by

$$\begin{aligned} \hat{c}_{\mathbf{k}\uparrow} &= u_{\mathbf{k}}\hat{\gamma}_{\mathbf{k}\uparrow} + v_{\mathbf{k}}\hat{\gamma}^\dagger_{-\mathbf{k}\downarrow} \qquad & \hat{c}_{-\mathbf{k}\downarrow} &= u_{\mathbf{k}}\hat{\gamma}_{-\mathbf{k}\downarrow} - v_{\mathbf{k}}\hat{\gamma}^\dagger_{\mathbf{k}\uparrow} \\ \hat{c}^\dagger_{\mathbf{k}\uparrow} &= u_{\mathbf{k}}\hat{\gamma}^\dagger_{\mathbf{k}\uparrow} + v_{\mathbf{k}}\hat{\gamma}_{-\mathbf{k}\downarrow} \qquad & \hat{c}^\dagger_{-\mathbf{k}\downarrow} &= u_{\mathbf{k}}\hat{\gamma}^\dagger_{-\mathbf{k}\downarrow} - v_{\mathbf{k}}\hat{\gamma}_{\mathbf{k}\uparrow}. \end{aligned} \tag{33}$$

$u_{\mathbf{k}}$, $v_{\mathbf{k}}$ and Δ_B are assumed to be real. Following the same procedure as in section 3.1, the gap equation becomes

$$\begin{aligned} \Delta_B &= \frac{V}{N^2}\sum_{\mathbf{k}} \langle \hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow}\rangle \\ &= \frac{V}{N^2}\sum_{\mathbf{k}} \langle (u_{\mathbf{k}}\hat{\gamma}_{-\mathbf{k}\downarrow} - v_{\mathbf{k}}\hat{\gamma}^\dagger_{\mathbf{k}\uparrow})(u_{\mathbf{k}}\hat{\gamma}_{\mathbf{k}\uparrow} + v_{\mathbf{k}}\hat{\gamma}^\dagger_{-\mathbf{k}\downarrow})\rangle \\ &= \frac{V}{N^2}\sum_{\mathbf{k}} u_{\mathbf{k}}v_{\mathbf{k}}\left(1 - f(E_{\mathbf{k}\downarrow}) - f(E_{\mathbf{k}\uparrow})\right). \end{aligned} \tag{34}$$

From diagonalization and from demanding the transformation matrix U to be unitary, we obtain the following 4 equations

$$u_{\mathbf{k}}^2\xi_{\mathbf{k}\uparrow} - v_{\mathbf{k}}^2\xi_{-\mathbf{k}\downarrow} + 2u_{\mathbf{k}}v_{\mathbf{k}}\Delta_B = E_{\mathbf{k}\uparrow}, \tag{35}$$

$$v_{\mathbf{k}}^2\xi_{\mathbf{k}\uparrow} - u_{\mathbf{k}}^2\xi_{-\mathbf{k}\downarrow} - 2u_{\mathbf{k}}v_{\mathbf{k}}\Delta_B = -E_{-\mathbf{k}\downarrow}, \tag{36}$$

$$u_{\mathbf{k}}v_{\mathbf{k}}(\xi_{\mathbf{k}\uparrow} + \xi_{-\mathbf{k}\downarrow}) + \Delta_B(v_{\mathbf{k}}^2 - u_{\mathbf{k}}^2) = 0, \tag{37}$$

$$u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = \pm 1. \tag{38}$$

From these we can isolate $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$.

$$u_{\mathbf{k}} = \pm\sqrt{\frac{2\Delta_B^2 + E_{\mathbf{k}\uparrow}(\xi_{\mathbf{k}\uparrow} + \xi_{-\mathbf{k}\downarrow}) + \xi_{-\mathbf{k}\downarrow}^2 + \xi_{\mathbf{k}\uparrow}\xi_{-\mathbf{k}\downarrow} \pm K_1}{4\Delta_B^2 + (\xi_{\mathbf{k}\uparrow} + \xi_{-\mathbf{k}\downarrow})^2}}, \tag{39}$$

with

$$K_1 = 2\Delta_B\sqrt{\Delta_B^2 - E_{\mathbf{k}\uparrow}(E_{\mathbf{k}\uparrow} + \xi_{-\mathbf{k}\downarrow} - \xi_{\mathbf{k}\uparrow}) + \xi_{\mathbf{k}\uparrow}\xi_{-\mathbf{k}\downarrow}}, \tag{40}$$

and

$$v_{\mathbf{k}} = \pm\sqrt{\frac{2\Delta_B^2 - E_{-\mathbf{k}\downarrow}(\xi_{\mathbf{k}\uparrow} + \xi_{-\mathbf{k}\downarrow}) + \xi_{-\mathbf{k}\downarrow}^2 + \xi_{\mathbf{k}\uparrow}\xi_{-\mathbf{k}\downarrow} \pm K_2}{4\Delta_B^2 + (\xi_{\mathbf{k}\uparrow} + \xi_{-\mathbf{k}\downarrow})^2}}, \tag{41}$$

with

$$K_2 = 2\Delta_B \sqrt{\Delta_B^2 - E_{-\mathbf{k}\downarrow}(E_{-\mathbf{k}\downarrow} - \xi_{-\mathbf{k}\downarrow} + \xi_{\mathbf{k}\uparrow}) + \xi_{\mathbf{k}\uparrow}\xi_{-\mathbf{k}\downarrow}}. \tag{42}$$

Inserting that $E_{\mathbf{k}\uparrow} = H_{z\uparrow} + E_{\mathbf{k}}$, $E_{-\mathbf{k}\downarrow} = -H_{z\uparrow} + E$, $\xi_{\mathbf{k}\uparrow} = \xi_{\mathbf{k}} + H_{z\uparrow}$ and $\xi_{-\mathbf{k}\downarrow} = \xi_{\mathbf{k}} - H_{z\uparrow}$ these equations reduces to Eq. (14), which consolidate the fact that the Zeeman interaction does not affect the eigenvectors. The only difference it gives rise to is an extra eigenenergy and thereby a small modification of the gap equation. Thus, $u_{\mathbf{k}}v_{\mathbf{k}}$ is given by Eq. (15) and the gap equation becomes

$$\Delta_B = \frac{V}{N^2}\frac{\Delta_B}{2E_{\mathbf{k}}}\sum_{\mathbf{k}}(1 - f(E_{\mathbf{k}\downarrow}) - f(E_{\mathbf{k}\uparrow})). \tag{43}$$

Another way to find an expression for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ and thereby the gap equation is by looking at the commutator $[H^{mf}_{BCS,B}, \hat{c}_{\mathbf{k}\uparrow}]$. These calculations are to be found in appendix C. The same results are obtained with this method. Embedding the aforementioned adjustments in the script that solves the self-consistent gap equation and simulates its dependence of temperature, we see clearly an effect of the Zeeman interaction, see Fig. 2. It is indisputable that the magnetic field suppresses Δ_B and thereby the superconductivity, though the maximum Δ_B at $T = 0$ is not affected. We observe that Δ attenuates slowly at temperatures above 0.006 in Fig. 1. At the critical temperature this should go abruptly to zero. This is a numerical error due to the fact that N is too small.

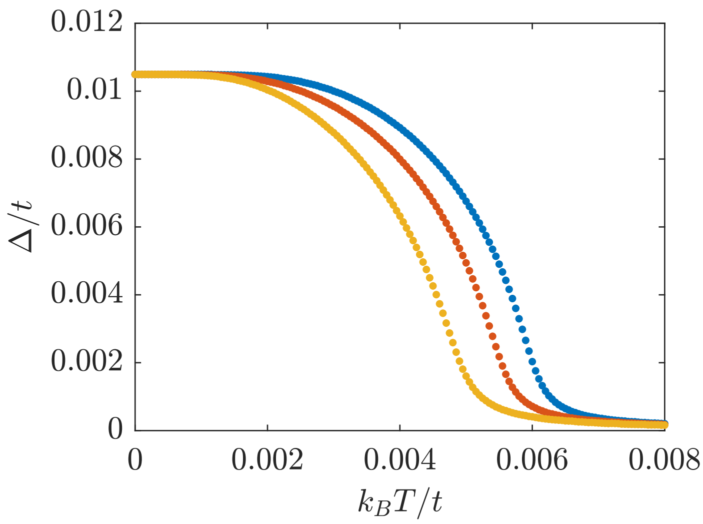


Fig. 2: The temperature dependence of the superconducting band gap Δ_B with increasing magnetic fields as a function of temperature. The blue curve is for $B = 0$, orange for $B = 0.007t$, yellow for $B = 0.01t$. For increasing magnetic fields there is a corresponding decreasing critical temperature.

Taking the limit $T \to 0$ of Eq. (43) it reduces to

$$\lim_{T\to 0} \Delta_B = \frac{V\Delta_B}{2E_{\mathbf{k}}}, \tag{44}$$

which is independent of the magnetic field. This consolidate the tendency plottet in Fig. 2. We know from Eq. (25) that a Zeeman field affects states differently depending on the spin of the state. Thus the application of a magnetic field increases the density of electrons with spins parallel to the applied field, in this case $\uparrow$, since the energy of these states are decreased, and the opposite is the case for spins antiparallel to the magnetic field, in this case $\downarrow$, see Fig. 3. Pairing time-reversal Cooper pairs in the presence of such a field means that the two bound electrons do not both have the energy corresponding to the Fermi surface. Since we have $E_{\mathbf{k}}$ in the denominator in Eq. (15) and thus in Eq. (34), moving away from the Fermi surface and thereby increasing $|E_{\mathbf{k}}|$ decreases the superconducting band gap. Thus, when we increase the magnetic field, the Cooper pairs are forced to be formed by electrons with an increasing difference in energy until this is no longer favourable and the superconductivity ceases to exist. This motivates Cooper pairs formed without time-reversal symmetry.

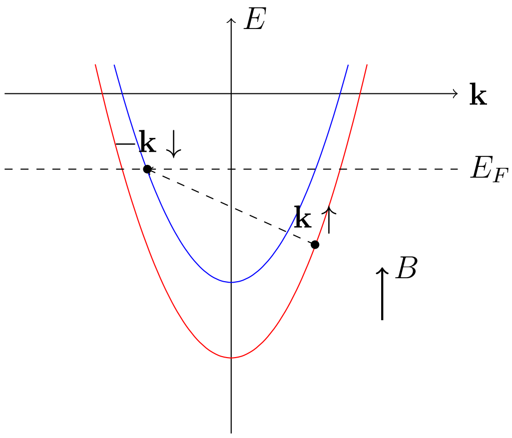
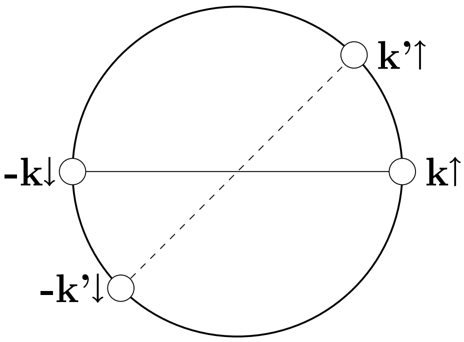
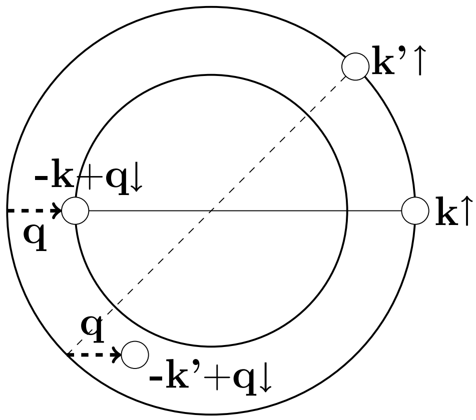


Fig. 3: The dispersion of the electrons in the presence of a magnetic field. The spin up states (red curve) will be pushed down in energy and the spin down states (blue curve) will be pushed up in energy by the magnetic field. To conserve the time reversal symmetry of the Cooper pairs, one of the bound electrons must have $E \neq E_F$. The BCS pairing is illustrated with a dashed line.

5 Fulde-Ferrell-Larkin-Ovchinnikov state



(a) $B = 0$



(b) $B \neq 0$

Fig. 4: The pairing states are illustrated with energy orthogonal to the paper. With no external magnetic field (a) the time-reversal Cooper pairs are formed $(-\mathbf{k}\downarrow, \mathbf{k}\uparrow)$. For a magnetic field applied orthogonal to the paper (b) the FFLO pairing state is depicted $(-\mathbf{k}+\mathbf{q}\downarrow, \mathbf{k}\uparrow)$. In this case the energy band is spin split due to the Zeeman interaction.

A new state, the FFLO state, was proposed by two different pairs of scientists, Fulde and Ferrel [10] and Larkin and Ovchinnikov [11] in the 1960s. The FFLO state was predicted theoretically to appear in superconductors at low temperature and at large magnetic fields but has not yet been conclusively observed experimentally. The two groups suggested two different modulations of the band gap Δ, the FF ansatz and the LO ansatz. They proposed that Cooper pairs could be formed by electrons from the two different spin bands, i.e., the pairing arising between state $(\mathbf{k}, \uparrow)$ at $(\mathbf{-k+q}, \downarrow)$ as illustrated in Fig. 4. Thus, the pairing state is formed with a finite center-of-mass momentum, $\mathbf{q}$, corresponding to the distance between the Fermi surfaces of the two spin bands. The fact that $\mathbf{q} \neq 0$ breaks the symmetry between the time-reversal Cooper pairs such that the energy of the coupled electrons is no longer degenerate, i.e., $\xi_{\mathbf{k}+\mathbf{q}/2\uparrow} \neq \xi_{-\mathbf{k}+\mathbf{q}/2\downarrow}$. The hypothesis is that transitioning the normal state into this pairing state can enhance the upper critical field [9]. Due to the fact that the FFLO state originates from paramagnetism, for the FFLO state to appear, it has to be the Pauli paramagnetic pair-breaking that is the dominating factor in suppressing the superconductivity [12], i.e., the Maki parameter described in section 4.1 must be high. For the FFLO state to be found it must hold that the superconductor is in the clean limit, i.e., when the electron mean free path l is much larger than the superconducting coherence length ξ_0 [13]. Further, previous studies have shown that we must be at very low temperatures and the magnetic field must be near the Clogston-Chandrasekhar limit [2]. These very stringent conditions, for the FFLO state to appear, makes it difficult to observe experimentally. One way to minimize the orbital effetcs is to investigate two-dimensional layered superconductors with an applied field parallel to the layers. This case is investigated with, e.g., the organic superconductor κ-(BEDT-TTF)$_2$Cu(NCS)$_2$ [14]. A high magnetic field phase diagram is obtained and due to the fact that magnetic order can be excluded in this organic material, Bergk et al. conclude that this could be a signature of the FFLO state. Another way to obtain a large Maki parameter is using heavy-fermion materials. A candidate for this is the compound $CeCoIn_5$, for which an anomaly in the specific heat in the vicinity of the superconducting critical field has been observed [15]. This anomaly, in addition to the fact that the phase transition changes from a second to a first order, could be due to the presence of a FFLO phase. This result is heavily debated and could also be explained by the presence of ordered local moments [16]. From a numerical study of the phase transition, in the case of a two-dimensional gas of heavy quasiparticles, the phase diagram in Fig. 5 can be obtained [2]. This is done for both spin dependent and independent masses. In this Fig. it is clear that the search for the FFLO state has to be localized to the region of low temperatures and high fields. Further, we see that the critical field is enhanced by the FFLO phase. The region, where the FFLO phase is present, is enhanced by a spin dependency on the masses. In both cases the phase transition changes from a second order to a first order as in previous studies. Despite the countless inconclusive evidence for the FFLO state there are no indisputable verification of the FFLO state, i.e., no thermodynamic or microscopic evidence have been reported so far. Conclusive evidence could be obtained using scanning tunneling microscopy that can detect the spatial variance in density of states of the quasiparticles [17]. Further, phase sensitive experiments measuring the tunnel effect between the FFLO state and the s-wave BCS state could provide an unambiguous approach to determine the existence of the FFLO state. In the following section, we will investigate if we can show that the FFLO phase does indeed exist using BCS theory to examine the free energy of the system.

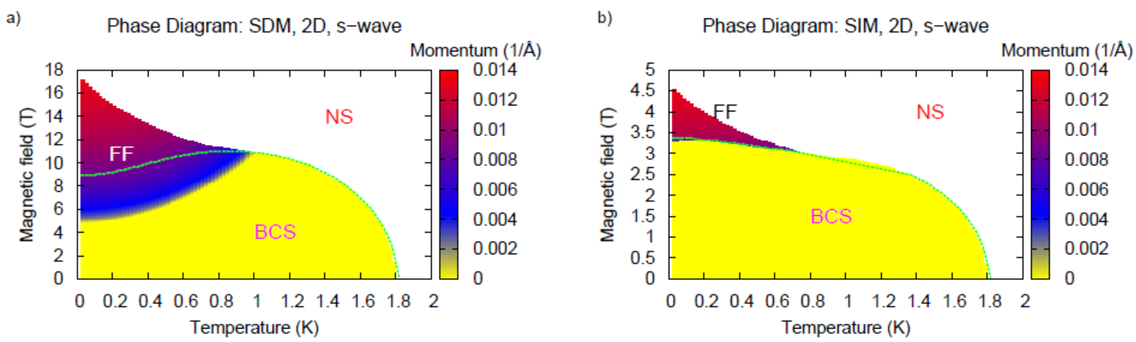


Fig. 5: Phase diagram for the two-dimensional correlated gas with s-wave symmetry in the SM case (a) and the SIM case (b). SDM: spin dependent masses. SIM: spin independent masses. These plots are from [2]. The white area represent the normal phase, the yellow region is the s-wave BCS phase with $\mathbf{q} = 0$ and blue-red region corresponds to the FF phase with $\mathbf{q} \neq 0$. The green line represents the BCS critical field.

5.1 Modulation of the Gap Equation by a Zeeman Interaction, $\mathbf{q} \neq 0$

The ansatz Fulde og Ferrell proposed is a modulation of the band gap of a plane wave form [18]

$$\Delta(r) = \Delta_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}}, \qquad \text{where} \qquad \Delta_{\mathbf{q}} \in \mathbb{R}, \tag{45}$$

such that the phase of the superconducting gap now oscillates spatially with the wave vector $\mathbf{q}$. Investigating the Hamiltonian in real space and evaluating the Fourier transformation with this modulation of the band gap, the Hamiltonian in reciprocal space becomes

$$H = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}\sigma} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} - \frac{V}{N^2} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \hat{c}^{\dagger}_{\mathbf{k}+\mathbf{q}/2\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \hat{c}_{-\mathbf{k}'+\mathbf{q}/2\downarrow} \hat{c}_{\mathbf{k}'+\mathbf{q}/2\uparrow}, \tag{46}$$

where $\xi_{\mathbf{k}\sigma}$ is defined in Eq. (25). We can no longer, as we did above, neglect the constant term, since we are interested in calculating the free energy. Thus, a constant shift in the energy is now of great importance. Defining the superconducting gap

$$\Delta_{\mathbf{q}} \equiv \frac{V}{N^2} \sum_{\mathbf{k}} \langle \hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \hat{c}_{\mathbf{k}+\mathbf{q}/2\uparrow} \rangle = \frac{V}{N^2} \sum_{\mathbf{k}} \langle \hat{c}^{\dagger}_{\mathbf{k}+\mathbf{q}/2\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \rangle \tag{47}$$

and using the mean-field expansion

$$\begin{aligned} \hat{c}^{\dagger}_{\mathbf{k}+\mathbf{q}/2\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow} &= \langle \hat{c}^{\dagger}_{\mathbf{k}+\mathbf{q}/2\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \rangle \hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \\ + \hat{c}^{\dagger}_{\mathbf{k}+\mathbf{q}/2\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \langle \hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \rangle &- \langle \hat{c}^{\dagger}_{\mathbf{k}+\mathbf{q}/2\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \rangle \langle \hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \rangle \end{aligned} \tag{48}$$

we can, as in previous sections, rewrite H

$$H = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}\sigma} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} (\Delta_{\mathbf{q}} \hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \hat{c}_{\mathbf{k}+\mathbf{q}/2\uparrow} + \Delta_{\mathbf{q}} \hat{c}^{\dagger}_{\mathbf{k}+\mathbf{q}/2\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}+\mathbf{q}/2\downarrow}) + \frac{N^2}{V} \Delta^2_{\mathbf{q}}. \tag{49}$$

Contrary to preceding sections, we are no longer neglecting the third constant term in the mean-field expansion. This leads to the last term in H. As long as we are summing over all $\mathbf{k}$'s in the Brillouin zone, we can always shift the summation and obtain an equivalent result. Thus, writing

$$\begin{aligned} H = \sum_{\mathbf{k}} (&\xi_{\mathbf{k}+\mathbf{q}/2\uparrow} \hat{c}^{\dagger}_{\mathbf{k}+\mathbf{q}/2\uparrow} \hat{c}_{\mathbf{k}+\mathbf{q}/2\uparrow} + \xi_{-\mathbf{k}+\mathbf{q}/2\downarrow} \hat{c}^{\dagger}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \\ &- \Delta_{\mathbf{q}} \hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \hat{c}_{\mathbf{k}+\mathbf{q}/2\uparrow} - \Delta_{\mathbf{q}} \hat{c}^{\dagger}_{\mathbf{k}+\mathbf{q}/2\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}+\mathbf{q}/2\downarrow}) + \frac{N^2}{V} \Delta^2_{\mathbf{q}} \end{aligned} \tag{50}$$

with

$$\xi_{\mathbf{k},\mathbf{q}\sigma} = \xi_{\mathbf{k},\mathbf{q}} - \mu - \sigma \frac{1}{2} g \mu_B B, \quad \xi_{\mathbf{k},\mathbf{q}} = 2t(\cos(a[k_x + q_x/2]) + \cos(ak_y)) \tag{51}$$

makes it possible to write the Hamiltonian on a simple matrix form. To begin with we focus on the case where $\mathbf{q} = (q_x, 0)$.

$$H = \sum_{\mathbf{k}} \begin{pmatrix} \hat{c}^\dagger_{\mathbf{k}+\mathbf{q}/2\uparrow} & \hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \end{pmatrix} \begin{pmatrix} \xi_{\mathbf{k}+\mathbf{q}/2\uparrow} & -\Delta_{\mathbf{q}} \\ -\Delta_{\mathbf{q}} & -\xi_{-\mathbf{k}+\mathbf{q}/2\downarrow} \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}+\mathbf{q}/2\uparrow} \\ \hat{c}^\dagger_{-\mathbf{k}+\mathbf{q}/2\downarrow} \end{pmatrix} + \sum_{\mathbf{k}} \xi_{-\mathbf{k}+\mathbf{q}/2\downarrow} + \frac{N^2}{V}\Delta^2_{\mathbf{q}}. \tag{52}$$

Due to the fact that $\hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow}\hat{c}^\dagger_{-\mathbf{k}+\mathbf{q}/2\downarrow} = 1 - \hat{c}^\dagger_{-\mathbf{k}+\mathbf{q}/2\downarrow}\hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow}$, see Eq. (4), we must add $\xi_{-\mathbf{k}+\mathbf{q}/2\downarrow}$. The eigenenergies of the matrix is given by

$$E_{\mathbf{k},\mathbf{q},\sigma} = E_{\mathbf{k},\mathbf{q}} + \sigma \xi^{(a)}_{\mathbf{k},\mathbf{q}} \tag{53}$$

with

$$E_{\mathbf{k},\mathbf{q}} = \sqrt{\xi^{(s)2}_{\mathbf{k},\mathbf{q}} + \Delta^2_{\mathbf{q}}}, \quad \xi^{(s)}_{\mathbf{k},\mathbf{q}} = \frac{\xi_{\mathbf{k}+\mathbf{q}/2\uparrow} + \xi_{-\mathbf{k}+\mathbf{q}/2\downarrow}}{2}, \quad \xi^{(a)}_{\mathbf{k},\mathbf{q}} = \frac{\xi_{\mathbf{k}+\mathbf{q}/2\uparrow} - \xi_{-\mathbf{k}+\mathbf{q}/2\downarrow}}{2}. \tag{54}$$

This has exactly the same shape as Eq. (31). We can now use the Bogoliubov transformation with the same form as in previous sections

$$\begin{pmatrix} \hat{c}_{\mathbf{k}+\mathbf{q}/2\uparrow} \\ \hat{c}^\dagger_{-\mathbf{k}+\mathbf{q}/2\downarrow} \end{pmatrix} = U \begin{pmatrix} \hat{\gamma}_{\mathbf{k}+\mathbf{q}/2\uparrow} \\ \hat{\gamma}^\dagger_{-\mathbf{k}+\mathbf{q}/2\downarrow} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k},\mathbf{q}} & v_{\mathbf{k},\mathbf{q}} \\ -v_{\mathbf{k},\mathbf{q}} & u_{\mathbf{k},\mathbf{q}} \end{pmatrix} \begin{pmatrix} \hat{\gamma}_{\mathbf{k}+\mathbf{q}/2\uparrow} \\ \hat{\gamma}^\dagger_{-\mathbf{k}+\mathbf{q}/2\downarrow} \end{pmatrix} \tag{55}$$

to diagonalize the Hamiltonian. For clarity we define $H_{const.} \equiv \sum_{\mathbf{k}} \xi_{-\mathbf{k}+\mathbf{q}/2\downarrow} + \frac{N^2}{V}\Delta^2_{\mathbf{q}}$.

$$\begin{aligned} H &= \sum_{\mathbf{k}} \begin{pmatrix} \hat{c}^\dagger_{\mathbf{k}+\mathbf{q}/2\uparrow} & \hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \end{pmatrix} UU^\dagger \begin{pmatrix} \xi_{\mathbf{k}+\mathbf{q}/2\uparrow} & -\Delta_{\mathbf{q}} \\ -\Delta_{\mathbf{q}} & -\xi_{-\mathbf{k}+\mathbf{q}/2\downarrow} \end{pmatrix} UU^\dagger \begin{pmatrix} \hat{c}_{\mathbf{k}+\mathbf{q}/2\uparrow} \\ \hat{c}^\dagger_{-\mathbf{k}+\mathbf{q}/2\downarrow} \end{pmatrix} + H_{const.} \\ &= \sum_{\mathbf{k}} \begin{pmatrix} \hat{\gamma}^\dagger_{\mathbf{k}+\mathbf{q}/2\uparrow} & \hat{\gamma}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \end{pmatrix} \begin{pmatrix} E_{\mathbf{k},\mathbf{q},\uparrow} & 0 \\ 0 & -E_{\mathbf{k},\mathbf{q},\downarrow} \end{pmatrix} \begin{pmatrix} \hat{\gamma}_{\mathbf{k}+\mathbf{q}/2\uparrow} \\ \hat{\gamma}^\dagger_{-\mathbf{k}+\mathbf{q}/2\downarrow} \end{pmatrix} + H_{const.} \\ &= \sum_{\mathbf{k}\sigma} E_{\mathbf{k},\mathbf{q},\sigma}\gamma^\dagger_{\mathbf{k},\mathbf{q},\sigma}\gamma_{\mathbf{k},\mathbf{q}\sigma} + \sum_{\mathbf{k}}(\xi_{-\mathbf{k}+\mathbf{q}/2\downarrow} - E_{\mathbf{k},\mathbf{q},\downarrow}) + \frac{N^2}{V}\Delta^2_{\mathbf{q}}. \end{aligned} \tag{56}$$

The constant term $\sum_{\mathbf{k}} E_{\mathbf{k},\mathbf{q},\downarrow}$ comes from $\hat{\gamma}_{-\mathbf{k}+\mathbf{q}/2\downarrow}\hat{\gamma}^\dagger_{-\mathbf{k}+\mathbf{q}/2\downarrow} = 1 - \hat{\gamma}^\dagger_{-\mathbf{k}+\mathbf{q}/2\downarrow}\hat{\gamma}_{-\mathbf{k}+\mathbf{q}/2\downarrow}$. From the diagonalization we can obtain expressions for $u_{\mathbf{k},\mathbf{q}}$ and $v_{\mathbf{k},\mathbf{q}}$. The transformation matrix is still unitary such that $u^2_{\mathbf{k},\mathbf{q}} + v^2_{\mathbf{k},\mathbf{q}} = 1$.

$$u_{\mathbf{k},\mathbf{q}} = \sqrt{\frac{1}{2}\left(1 + \frac{\xi_{\mathbf{k}+\mathbf{q}/2\uparrow} + \xi_{-\mathbf{k}+\mathbf{q}/2\downarrow}}{2E_{\mathbf{k},\mathbf{q}}}\right)} = \sqrt{\frac{1}{2}\left(1 + \frac{\xi^{(s)}_{\mathbf{k},\mathbf{q}}}{E_{\mathbf{k},\mathbf{q}}}\right)}, \quad v_{\mathbf{k},\mathbf{q}} = \sqrt{\frac{1}{2}\left(1 - \frac{\xi^{(s)}_{\mathbf{k},\mathbf{q}}}{E_{\mathbf{k},\mathbf{q}}}\right)}. \tag{57}$$

Removing the spin dependency and setting $\mathbf{q} = 0$, this reduces to the original $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$, see Eq. (14). Multiplying $u_{\mathbf{k},\mathbf{q}}$ and $v_{\mathbf{k},\mathbf{q}}$ we obtain

$$u_{\mathbf{k},\mathbf{q}}v_{\mathbf{k},\mathbf{q}} = \frac{\Delta_{\mathbf{q}}}{2E_{\mathbf{k},\mathbf{q}}}. \tag{58}$$

We can now use the Bogoliubov transformation to rewrite the gap equation with the same procedure as in section 3.1.

$$\Delta_{\mathbf{q}} = \frac{V}{N^2}\sum_{\mathbf{k}}\langle(u_{\mathbf{k},\mathbf{q}}\hat{\gamma}_{-\mathbf{k}+\mathbf{q}/2\downarrow} - v_{\mathbf{k},\mathbf{q}/2}\hat{\gamma}^\dagger_{\mathbf{k}+\mathbf{q}/2\uparrow})(u_{\mathbf{k},\mathbf{q}}\hat{\gamma}_{\mathbf{k}+\mathbf{q}/2\uparrow} + v_{\mathbf{k},\mathbf{q}}\hat{\gamma}^\dagger_{-\mathbf{k}+\mathbf{q}/2\downarrow})\rangle \tag{59}$$

$$= \frac{V}{N^2}\sum_{\mathbf{k}} u_{\mathbf{k},\mathbf{q}}v_{\mathbf{k},\mathbf{q}}(\langle\hat{\gamma}_{-\mathbf{k}+\mathbf{q}/2\downarrow}\hat{\gamma}^\dagger_{-\mathbf{k}+\mathbf{q}/2\downarrow}\rangle - \langle\hat{\gamma}^\dagger_{\mathbf{k}+\mathbf{q}/2\uparrow}\hat{\gamma}_{\mathbf{k}+\mathbf{q}/2\uparrow}\rangle) \tag{60}$$

$$= \frac{V}{N^2}\sum_{\mathbf{k}} u_{\mathbf{k},\mathbf{q}}v_{\mathbf{k},\mathbf{q}}(1 - f(E_{\mathbf{k},\mathbf{q},\downarrow}) - f(E_{\mathbf{k},\mathbf{q},\uparrow})) \tag{61}$$

$$= \frac{V}{N^2}\sum_{\mathbf{k}} \frac{\Delta_{\mathbf{q}}}{2E_{\mathbf{k},\mathbf{q}}}(1 - f(E_{\mathbf{k},\mathbf{q},\downarrow}) - f(E_{\mathbf{k},\mathbf{q},\uparrow})). \tag{62}$$

For $\mathbf{q} = 0$ this reduces to Eq. (43).

5.2 Minimizing the Free Energy

From the Hamiltonian in Eq. 56 we can obtain an expression for the partition function, Z. The last three terms in are just constants, such that they will contribute to the free energy in the same way they are in the Hamiltonian since $Z = \sum e^{-\beta E}$ [19] and $\mathcal{F} = -\frac{1}{\beta}\ln Z$, where $\beta \equiv 1/k_BT$. Thus, we will only calculate the partition function for the two first terms which we will denote H_1. This calculation is fairly simple due to the fact that $\hat{\gamma}^\dagger_{\mathbf{k},\mathbf{q},\sigma}\hat{\gamma}_{\mathbf{k},\mathbf{q},\sigma} = \hat{n}_{\mathbf{k},\mathbf{q},\sigma}$ just counts the number of quasiparticles in the given state.

$$\begin{aligned}
Z_1 &= \sum_i e^{-\beta H_1} = \sum_{i,j} e^{-\beta\left(\sum_{\mathbf{k}} E_{\mathbf{k},\mathbf{q},\uparrow}\hat{n}_{i,\mathbf{k},\mathbf{q},\uparrow} + E_{\mathbf{k},\mathbf{q},\downarrow}\hat{n}_{j,\mathbf{k},\mathbf{q},\downarrow}\right)} = \sum_{i,j}\prod_{\mathbf{k}} e^{-\beta\left(E_{\mathbf{k},\mathbf{q},\uparrow}\hat{n}_{i,\mathbf{k},\mathbf{q},\uparrow} + E_{\mathbf{k},\mathbf{q},\downarrow}\hat{n}_{j,\mathbf{k},\mathbf{q},\downarrow}\right)} \\
&= \prod_{\mathbf{k}}\left(e^{-\beta E_{\mathbf{k},\mathbf{q},\uparrow}} + e^{-\beta E_{\mathbf{k},\mathbf{q},\downarrow}} + e^0 + e^{-\beta(E_{\mathbf{k},\mathbf{q},\uparrow}+E_{\mathbf{k},\mathbf{q},\downarrow})}\right) \\
&= \prod_{\mathbf{k}}\left(1 + e^{-\beta E_{\mathbf{k},\mathbf{q},\uparrow}}\right)\left(1 + e^{-\beta E_{\mathbf{k},\mathbf{q},\downarrow}}\right), \\
\mathcal{F}_1 &= -\frac{1}{\beta}\ln(Z_1) = \sum_{\mathbf{k}} \ln\left(\left(1 + e^{-\beta E_{\mathbf{k},\mathbf{q},\uparrow}}\right)\left(1 + e^{-\beta E_{\mathbf{k},\mathbf{q},\downarrow}}\right)\right) \\
&= -\frac{1}{\beta}\sum_{\mathbf{k}\sigma}\ln\left(1 + e^{-\beta E_{\mathbf{k},\mathbf{q},\sigma}}\right).
\end{aligned} \tag{63}$$

The free energy functional of the total Hamiltonian thereby becomes

$$\mathcal{F} = -\frac{1}{\beta}\sum_{\mathbf{k}\sigma}\ln(1 + e^{-\beta E_{\mathbf{k},\mathbf{q},\sigma}}) + \sum_{\mathbf{k}}(\xi_{-\mathbf{k}+\mathbf{q}/2\downarrow} - E_{\mathbf{k},\mathbf{q},\downarrow}) + \frac{N^2\Delta^2_{\mathbf{q}}}{V}. \tag{64}$$

We will now minimize the free energy with respect to $\Delta_{\mathbf{q}}$, i.e., finding a $\Delta_{\mathbf{q}}$ for which $\frac{\partial \mathcal{F}}{\partial \Delta_{\mathbf{q}}} = 0$ is true.

$$
\begin{aligned}
\frac{\partial \mathcal{F}}{\partial \Delta_{\mathbf{q}}} &= \frac{\partial}{\partial \Delta_{\mathbf{q}}} \left(\sum_{\mathbf{k}} \left(-\frac{1}{\beta} \left(\ln \left[1 + e^{-\beta E_{\mathbf{k},\mathbf{q},\uparrow}} \right] + \ln \left[1 + e^{-\beta E_{\mathbf{k},\mathbf{q},\downarrow}} \right] \right) - E_{\mathbf{k},\mathbf{q},\downarrow} \right) + \frac{N^2 \Delta_{\mathbf{q}}^2}{V} \right) \\
&= \frac{2N^2 \Delta_{\mathbf{q}}}{V} + \sum_{\mathbf{k}} \left(-\frac{1}{\beta} \left[\frac{-\beta \Delta_{\mathbf{q}} e^{-\beta E_{\mathbf{k},\mathbf{q},\uparrow}}}{E_{\mathbf{k},\mathbf{q}}(1 + e^{-\beta E_{\mathbf{k},\mathbf{q},\uparrow}})} + \frac{-\beta \Delta_{\mathbf{q}} e^{-\beta E_{\mathbf{k},\mathbf{q},\downarrow}}}{E_{\mathbf{k},\mathbf{q}}(1 + e^{-\beta E_{\mathbf{k},\mathbf{q},\downarrow}})} \right] - \frac{\Delta_{\mathbf{q}}}{E_{\mathbf{k},\mathbf{q}}} \right) \\
&= \frac{2N^2 \Delta_{\mathbf{q}}}{V} + \sum_{\mathbf{k}} \Delta_{\mathbf{q}} \left(\frac{f(E_{\mathbf{k},\mathbf{q},\uparrow}) + f(E_{\mathbf{k},\mathbf{q},\downarrow}) - 1}{E_{\mathbf{k},\mathbf{q}}} \right) = 0, \\
\Delta_{\mathbf{q}} &= \frac{V}{2N^2} \sum_{\mathbf{k}} \left(\frac{1 - f(E_{\mathbf{k},\mathbf{q},\uparrow}) - f(E_{\mathbf{k},\mathbf{q},\downarrow})}{E_{\mathbf{k},\mathbf{q}}} \right) \Delta_{\mathbf{q}}.
\end{aligned}
\tag{65}
$$

This is exactly what we found using our Bogoliubov transformation in Eq. (62). Thus, solving the self-consistent gap equation is equivalent to minimizing the free energy. If we had not assumed that $\Delta_{\mathbf{q}}$ was real, we would have to minimize with respect to both $\Delta_{\mathbf{q}}$ and $\Delta_{\mathbf{q}}^*$. The same gap equation would be obtained. To consolidate this result we can investigate it numerically. For simplicity we set $B = 0, \mathbf{q} = 0$. First, we choose a specific temperature for which we solve the self-consistent gap equation. Secondly, we find the normalized free energy $\mathcal{F}/N^2$ for a range of Δ's at the same temperature and then find the minima of these free energies. These minima do in fact correspond to $\pm\Delta_{\mathbf{q}=0}$ found from self consistency. These saddle points are illustrated in Fig. 6.

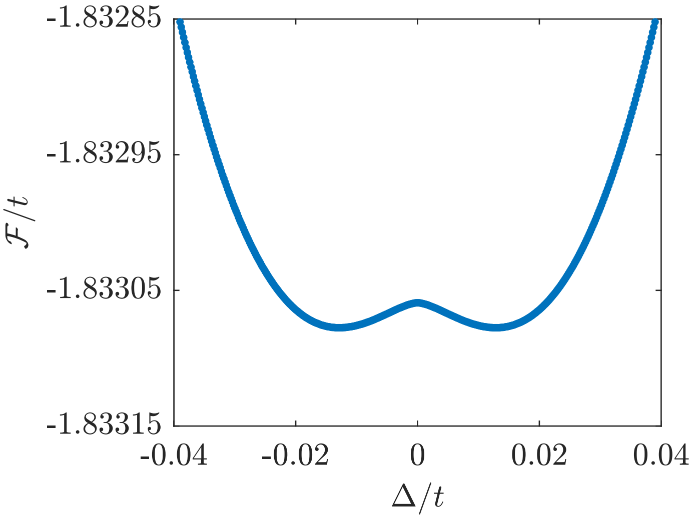


Fig. 6: Free energy as a function of Δ. The two minima correspond to $\pm\Delta_{\mathbf{q}=0}$ found from self-consistency.

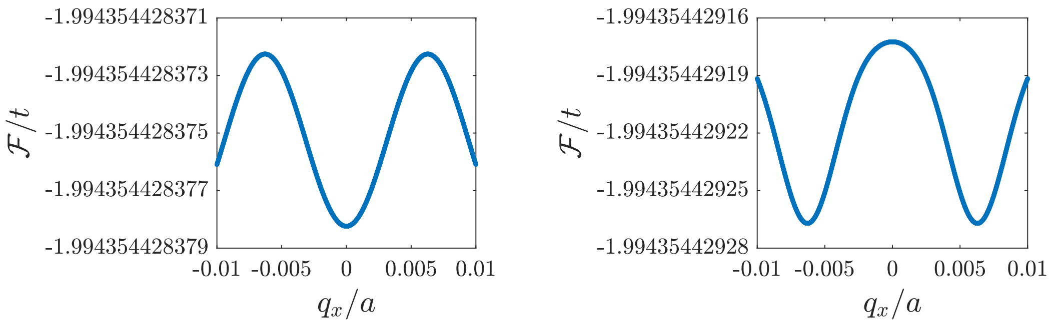
For $T \to 0$, it should be true that $\mathcal{F} = \langle H \rangle$. This is a way to check whether the free energy functional is correct. For $T \to 0$, the free energy functional in Eq. (64) becomes

$$\lim_{T\to 0} \mathcal{F} = \sum_{\mathbf{k}} (\xi_{-\mathbf{k}+\mathbf{q}/2\downarrow} - E_{\mathbf{k},\mathbf{q},\downarrow}) + \frac{N^2 \Delta_{\mathbf{q}}^2}{V}. \tag{66}$$

For $T \to 0$, the expectation value of the diagonalized Hamiltonian in Eq. (56)

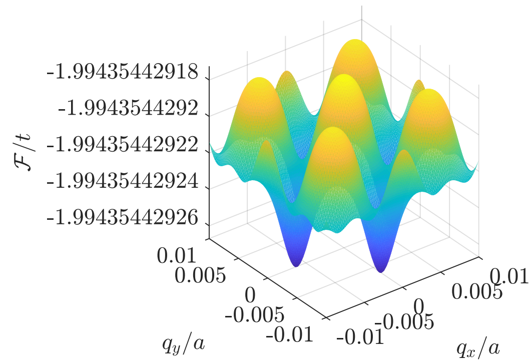
$$\begin{aligned}
\lim_{T\to 0} \langle H \rangle &= \sum_{\mathbf{k}\sigma} (E_{\mathbf{k},\mathbf{q},\sigma} \langle \hat{\gamma}^\dagger_{\mathbf{kq}\sigma} \hat{\gamma}_{\mathbf{kq}\sigma} \rangle - \Delta_{\mathbf{q}} \sum_{\mathbf{k}} (\cancelto{0}{\langle \hat{\gamma}^\dagger_{\mathbf{k}+\mathbf{q}/2\uparrow} \hat{\gamma}^\dagger_{-\mathbf{k}+\mathbf{q}/2\downarrow} \rangle} + \cancelto{0}{\langle \hat{\gamma}_{-\mathbf{k}+\mathbf{q}/2\downarrow} \hat{\gamma}_{\mathbf{k}+\mathbf{q}/2\uparrow} \rangle}) \\
&\quad + \sum_{\mathbf{k}} (\xi_{-\mathbf{k}+\mathbf{q}/2\downarrow} - E_{\mathbf{k},\mathbf{q},\downarrow}) + \frac{N^2 \Delta_{\mathbf{q}}^2}{V} \\
&= \sum_{\mathbf{k}} (E_{\mathbf{k},\mathbf{q},\uparrow} \cancelto{0}{f(E_{\mathbf{k},\mathbf{q},\uparrow})} + E_{\mathbf{k},\mathbf{q},\downarrow} \cancelto{0}{f(E_{\mathbf{k},\mathbf{q},\downarrow})} + \sum_{\mathbf{k}} (\xi_{-\mathbf{k}+\mathbf{q}/2\downarrow} - E_{\mathbf{k},\mathbf{q},\downarrow}) + \frac{N^2 \Delta_{\mathbf{q}}^2}{V} \\
&= \sum_{\mathbf{k}} (\xi_{-\mathbf{k}+\mathbf{q}/2\downarrow} - E_{\mathbf{k},\mathbf{q},\downarrow}) + \frac{N^2 \Delta_{\mathbf{q}}^2}{V}.
\end{aligned} \tag{67}$$

This is a strong indicator that Eq. (64) is correct. As we would expect we get the same result calculating $\langle H \rangle$ given in the basis of the $\hat{c}$-operators, see Eq. (50). This is checked in Appendix D. We can now numerically solve the self-consistent gap equation and insert this in the expression of the free energy. Doing this for a range of q_x's for $B = 0$, we see that the free energy is minimum at $q_x = 0$, see Fig. 7. This suggests that the FFLO state is not favourable in the absence of a magnetic field, which is what we would expect. Calculating each term in Eq. (64), we find that the first term is very flat and approximately zero as expected. The last term proportional to $\Delta_{\mathbf{q}}$ maximizes the free energy at $\mathbf{q} = 0$ whereas the term $\sum_{\mathbf{k}} (\xi_{-\mathbf{k}+\mathbf{q}/2\downarrow} - E_{\mathbf{k},\mathbf{q}\downarrow})$ minimizes the free energy at $q_x = 0$. The latter dominates such that the total free energy is mimimized at $q_x = 0$.

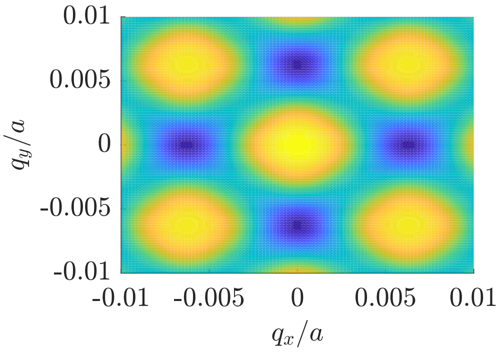


(a) $B = 0$ (b) $B \neq 0$

Fig. 7: Free energy as a function of q_x for $T \to 0$ with $B = 0$ (a) and a B-field just below the Clogston-Chandrasekhar limit (b).



(a)



(b)

Fig. 8: The free energy as a function of q_x and q_y with a magnetic field above the critical field and a temperature just above absolute zero (a). The minima is symmetric around zero (b). It is clear that the free energy is minimzed if either q_x or q_y is zero.

We will now investigate if there is a region with low temperatures and magnetic fields close to the critical field for which the FFLO state is favourable. We can investigate this in the same approach as above, i.e., find the free energy for a range of q_x's. For the FFLO state to be favourable, we would expect the minima of the free energy to be present at a $\mathbf{q} \neq 0$. Let us first theoretically investigate whether the gap equation and the free energy functional is inversion symmetric, i.e., invariant under the exchange $\mathbf{q} \to -\mathbf{q}$, see Eq. (64). If this is true we would expect two minima symmetrical around $\mathbf{q} = 0$.

$$\mathcal{F}_{\mathbf{q}\to-\mathbf{q}} = -\frac{1}{\beta}\sum_{\mathbf{k}\sigma} \ln\left[1+\exp\left(-\beta E_{\mathbf{k},-\mathbf{q},\sigma}\right)\right] + \sum_{\mathbf{k}} (\xi_{-\mathbf{k}-\mathbf{q}/2\downarrow} - E_{\mathbf{k},-\mathbf{q}\downarrow}) + \frac{N^2\Delta_{\text{-}\mathbf{q}}^2}{V}. \tag{68}$$

All terms dependent of $\mathbf{q}$ have an explicit $\mathbf{q}$-dependence in either $\xi_{\mathbf{k}-\mathbf{q}/2\uparrow}$, $\xi_{\mathbf{k}-\mathbf{q}/2\downarrow}$ or both. We can now change the dummy index to $\mathbf{k}' = \mathbf{k} - \mathbf{q}$. The only impact from this change is that the sum must be shifted. This will have no consequences since we are still summing over the Brillouin zone even if we shift the sum. Thus, the free energy and the gap equation is inversion symmetric. With a given temperature close to absolute zero, we can determine the superconducting gap with $B = 0$, $\mathbf{q} = 0$ and thereby find the critical field in the Pauli limit using Eq. (23). This allow us to choose a field just above that limit. Further, we must have a relatively large N to avoid finite size effects. We choose $N = 5000$ such that the number of sites in the lattice is $N^2 = 25 \cdot 10^6$. In the presence of this field, we can now once more calculate the free energy for different q_x's. We find that the free energy is no longer minimized at $\mathbf{q}_x = 0$, see Fig. 7. This indicates that the FF phase is favorable at this specific magnetic field. Further, it is indeed symmetric around zero as predicted. This motivates for the LO ansatz where the phase is a superposition of the two minima.

$$\Delta(x) = \Delta_{-\mathbf{q}} e^{-i\mathbf{q}_x\cdot\mathbf{x}} + \Delta_{\mathbf{q}} e^{i\mathbf{q}_x\cdot\mathbf{x}} = \Delta_{\mathbf{q}} e^{-i\mathbf{q}_x\cdot\mathbf{x}} + \Delta_{\mathbf{q}} e^{i\mathbf{q}_x\cdot\mathbf{x}} = 2\Delta_{\mathbf{q}} \cos\left(\mathbf{q}_x\cdot\mathbf{x}\right). \tag{69}$$

Varying the magnetic field slightly such that it is still near the critical field we see that the q_x, for which the free energy is minimized, is shifted. This confirms that these

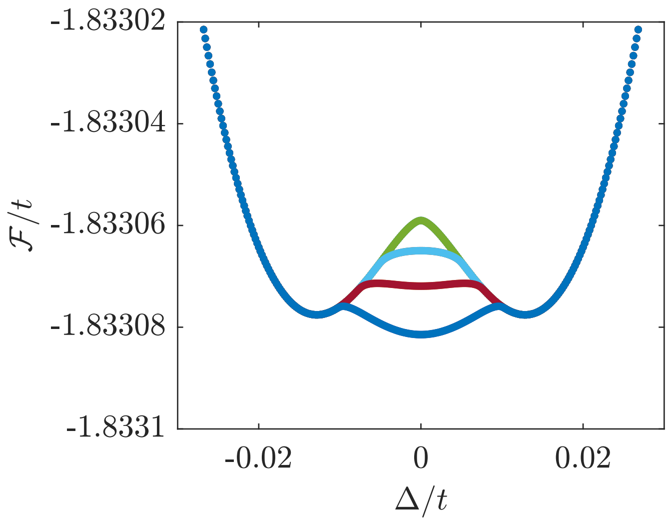


Fig. 9: Free energy as a function of the superconducting gap for increasing magnetic fields. We observe a first order transition from the FFLO state to the normal state.

two are correlated. The fact that the order parameter Δ is different from zero for a field above the critical field is itself a strong indicator of the presence of the FFLO phase. With the same high magnetic field, we can once more calculate the free energy numerically, varying both q_x and q_y to investigate if it is favourable to have a modulation of the band gap both in the x-direction and the y-direction. We find that it is in fact favourable to have either q_x or q_y equal to zero, see Fig. 8. Thus the superconducting gap will have a striped modulation in real space.

The phase transition from the FFLO phase to the normal phase can be investigated through the free energy, see Fig. 9. As the magentic field is increased the local maxima at $\Delta = 0$ becomes a minima. At the critical field this minima becomes smaller than the two minima at $\Delta \neq 0$. This transition is thus a first order transition.

6 Conclusion

Throughout this thesis, we have used BCS theory to investigate how a Zeeman interaction affects the superconducting band gap in two-dimensional type II superconductors. First, we explored the simplest case with no perturbations for superconductors consisting of time-reversal Copper pairs. A self-consistent equation for the superconducting band gap was obtained theoretically. This was solved numerically, and the temperature dependence was simulated. We found that the band gap decreases with increasing temperatures until it reaches zero. This shows how superconductivity is supressed by thermal fluctuations until it is completely destroyed at the critical temperature. In the presence of an external magnetic field, we investigated how the self-consistent gap equation for Δ_B was modified by a Zeeman interaction neglecting the orbital effects, i.e., for a system with a large Maki parameter. Due to the fact that the states are affected differently according to the spin of the state, we had to introduce a spin-dependency which lead to a small modification of the gap equation. Simulating the temperature dependence of the gap equation showed that the critical temperature is decreased in the presence of an external magnetic field. The maximum value of Δ_B was not affected by the applied magnetic field. Subsequently we reviewed the FFLO state. The purpose was to investigate whether it could be favourable to pair electrons with a non-zero center-of-mass momentum. To do this, we examined the free energy functional. We showed, theoretically and numerically, that minimizing the free energy is equivalent to solving the self-consistent gap equation. Further, we solved the self-consistent gap equation numerically and determined the free energy for a range of q_x's. In the absence of a magnetic field, we showed that the FFLO state is not favourable. At low temperatures and magnetic fields near the Clogston-Chandrasekhar limit, we found that the FFLO state was indeed favourable. Varying both q_x and q_y we found that the free energy was minimal if the modulation of the gap was restricted to only either the x-direction or the y-direction. The phase transition from the FFLO state to the normal state is a first order transition. We could also observe both theoretically and numerically that the free energy functional and the gap equation is symmetric under the exchange $\mathbf{q} \to -\mathbf{q}$. This motivates for the LO phase. In further research it would be of great interest to examine if, using the LO ansatz rather than the FF ansatz, would modify the free energy. Could this be a more favorable state? Further, the transition between the FF state and the depaired state could be investigated. Is this a first order phase transition? This could be done examining the free energy as a function of $\Delta_{\mathbf{q}=0}$ with increasing magnetic fields. The Maki parameter could be investigated numerically by adding vortices and investigating when the orbital effects would make the FFLO phase unfavourable. In the presence of orbital contributions a potential correlation between the Maki parameter and which state, the FF or the LO, is more favorable. Further, we could examine how the plot of the superconducting band gap as function of temperature is modified by the FFLO phase.

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Appendices

A An investigation of the anti-commutators for the $\hat{\gamma}$-operators

We want to investigate if the same anti-commutator relations apply for the quasiparticles as for the original c-operators. If this is true, these new $\hat{\gamma}$-operators must describe fermions. From the Bogoliubov transformation in Eq. (10) we have that

$$\hat{\gamma}_{\mathbf{k}\uparrow} = u_{\mathbf{k}}\hat{c}_{\mathbf{k}\uparrow} - v_{\mathbf{k}}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}, \quad \hat{\gamma}^{\dagger}_{\mathbf{k}\uparrow} = u_{\mathbf{k}}\hat{c}^{\dagger}_{\mathbf{k}\uparrow} - v_{\mathbf{k}}\hat{c}_{-\mathbf{k}\downarrow}. \tag{70}$$

From the second quantization representation we had the following anti-commutator relations for the c-operators

$$\{\hat{c}_{\nu j}, \hat{c}^{\dagger}_{\nu k}\} = \delta_{\nu j \nu k}, \quad \{\hat{c}^{\dagger}_{\nu j}, \hat{c}^{\dagger}_{\nu k}\} = 0, \quad \{\hat{c}_{\nu j}, \hat{c}_{\nu k}\} = 0. \tag{71}$$

Let us investigate the first relation.

$$\begin{aligned}\{\hat{\gamma}_{\mathbf{k}\uparrow}, \hat{\gamma}^{\dagger}_{\mathbf{k}\uparrow}\} &= \{(u_{\mathbf{k}}\hat{c}_{\mathbf{k}\uparrow} - v_{\mathbf{k}}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}), (u_{\mathbf{k}}\hat{c}^{\dagger}_{\mathbf{k}\uparrow} - v_{\mathbf{k}}\hat{c}_{-\mathbf{k}\downarrow})\} \\ &= u_{\mathbf{k}}^2\{\hat{c}_{\mathbf{k}\uparrow}, \hat{c}^{\dagger}_{\mathbf{k}\uparrow}\} + v_{\mathbf{k}}^2\{\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}, \hat{c}_{-\mathbf{k}\downarrow}\} - u_{\mathbf{k}}v_{\mathbf{k}}[\{\hat{c}_{\mathbf{k}\uparrow}, \hat{c}_{-\mathbf{k}\downarrow}\} + \{\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}, \hat{c}^{\dagger}_{\mathbf{k}\uparrow}\}] \\ &= u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1.\end{aligned} \tag{72}$$

$$\begin{aligned}\{\hat{\gamma}_{\mathbf{k}\uparrow}, \hat{\gamma}_{\mathbf{k}\uparrow}\} &= \{(u_{\mathbf{k}}\hat{c}_{\mathbf{k}\uparrow} - v_{\mathbf{k}}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}), (u_{\mathbf{k}}\hat{c}_{\mathbf{k}\uparrow} - v_{\mathbf{k}}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow})\} \\ &= u_{\mathbf{k}}^2\{\hat{c}_{\mathbf{k}\uparrow}, \hat{c}_{\mathbf{k}\uparrow}\} + v_{\mathbf{k}}^2\{\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}, \hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\} - u_{\mathbf{k}}v_{\mathbf{k}}[\{\hat{c}_{\mathbf{k}\uparrow}, \hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\} + \{\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}, \hat{c}_{\mathbf{k}\uparrow}\}] \\ &= 0.\end{aligned} \tag{73}$$

$$\begin{aligned}\{\hat{\gamma}^{\dagger}_{\mathbf{k}\uparrow}, \hat{\gamma}^{\dagger}_{\mathbf{k}\uparrow}\} &= \{(u_{\mathbf{k}}\hat{c}^{\dagger}_{\mathbf{k}\uparrow} - v_{\mathbf{k}}\hat{c}_{-\mathbf{k}\downarrow}), (u_{\mathbf{k}}\hat{c}^{\dagger}_{\mathbf{k}\uparrow} - v_{\mathbf{k}}\hat{c}_{-\mathbf{k}\downarrow})\} \\ &= u_{\mathbf{k}}^2\{\hat{c}^{\dagger}_{\mathbf{k}\uparrow}, \hat{c}^{\dagger}_{\mathbf{k}\uparrow}\} + v_{\mathbf{k}}^2\{\hat{c}_{-\mathbf{k}\downarrow}, \hat{c}_{-\mathbf{k}\downarrow}\} - u_{\mathbf{k}}v_{\mathbf{k}}[\{\hat{c}^{\dagger}_{\mathbf{k}\uparrow}, \hat{c}_{-\mathbf{k}\downarrow}\} + \{\hat{c}_{-\mathbf{k}\downarrow}, \hat{c}^{\dagger}_{\mathbf{k}\uparrow}\}] \\ &= 0.\end{aligned} \tag{74}$$

The $\hat{\gamma}$-operators do in fact represent fermions.

B Density of States in a Superconductor

The states are filled up to the Fermi level in the normal state where there is a finite density of states. Let us investigate what happens with the density of states when the material becomes superconducting. One way to calculate the density of states is to count the number of states N up to an energy E and thereafter take the derivative with respect to this energy.

$$N_s(E) = \frac{dN(E)}{dE} = \frac{dN}{d\xi}\frac{d\xi}{dE} = N_n(\xi)\frac{d\xi}{dE}, \tag{75}$$

where $N_s(E)$ is the density of states in the superconducting state and $N_n(E)$ is the density of states in the normal state. Since we are interested in what happens near the Fermi surface and $\Delta \ll E_F$, it is a good approximation to assume that the density of states in the normal state are constant in this range, i.e., $N_n(\xi) = N_n(0)$, [20]. This leads to the simple result

$$\frac{N_s(E)}{N(0)} = \frac{d\xi}{dE} = \begin{cases} \frac{E}{\sqrt{E^2-\Delta^2}} & \text{for} \quad E > |\Delta| \\ 0 & \text{for} \quad E < |\Delta| \end{cases}, \tag{76}$$

where we have used the energy given in (14). From this we see explicitly that a gap with the size 2Δ opens up around the Fermi level in the electron density of states. This gap arises from the pairing of electrons into Cooper pairs. Thus 2Δ corresponds to the energy demanded to break up a Cooper pair, e.g., by thermal fluctuations or a magnetic field. The density of states diverges near the edges of the superconducting gap, when $E = \pm\Delta$. This is due to the fact that all the states inside the gap in the normal state are pushed out of this range of energies for temperatures below the critical temperature. This causes them to pile up near the edges, see Fig. 10. These are the van Hove singularities of the superconducting energy spectrum. At $T = 0K$ all occupied states will have energies below $E_F - \Delta$, but as the temperature is increased, Cooper pairs will be broken resulting in normal electrons occupying states above $E_F + \Delta$.

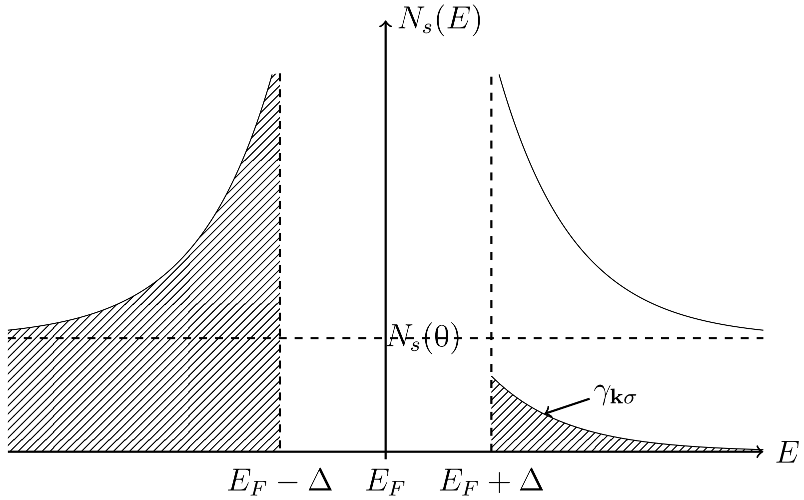

Fig. 10: Density of states as a function of energy at a temperature $0K < T < T_c$ in a BCS superconductor. The shaded area represents the occupied states. At $T = 0$ all electrons are paired in Cooper pairs and there will only be occupied states below the Fermi surface. As the temperature is increased the Cooper pairs will be broken by, e.g., thermal fluctuations resulting in normal electrons occupying states above $E_F + \Delta$.

C Alternative deriviation of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$

To consolidate the results from section 3, we will look at the commutator between H and $c_{\mathbf{k}\sigma}$. We assume that we do need the spin dependency on the elements of U.

$$[H^{mf}_{BCS,B}, \hat{c}_{\mathbf{k}\uparrow}] = \sum_{\mathbf{k}'}(\xi_{\mathbf{k}'\uparrow}[\hat{c}^{\dagger}_{\mathbf{k}'\uparrow}\hat{c}_{\mathbf{k}'\uparrow}, \hat{c}_{\mathbf{k}\uparrow}] + \xi_{-\mathbf{k}'\downarrow}[\hat{c}^{\dagger}_{-\mathbf{k}'\downarrow}\hat{c}_{-\mathbf{k}'\downarrow}, \hat{c}_{\mathbf{k}\uparrow}] - \Delta_B[\hat{c}^{\dagger}_{\mathbf{k}'\uparrow}\hat{c}^{\dagger}_{-\mathbf{k}'\downarrow}, \hat{c}_{\mathbf{k}\uparrow}] - \Delta_B[\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow}, \hat{c}_{\mathbf{k}\uparrow}]). \tag{77}$$

Now we can use the identity $[\hat{A}\hat{B}, \hat{C}] = \hat{A}\{\hat{B}, \hat{C}\} - \{\hat{A}, \hat{C}\}\hat{B}$ [3] and the anti commutator relations we found previously, see Eq. (4).

$$[H^{mf}_{BCS,B}, \hat{c}_{\mathbf{k}\uparrow}] = \sum_{\mathbf{k}'} -\xi_{\mathbf{k}'\uparrow}\hat{c}_{\mathbf{k}'\uparrow}\delta_{\mathbf{k}\mathbf{k}'} + \Delta_B\hat{c}^{\dagger}_{-\mathbf{k}'\downarrow}\delta_{\mathbf{k}'\mathbf{k}} = -\xi_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow} + \Delta_B\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\delta_{\mathbf{k}'\mathbf{k}} \tag{78}$$

Now we can insert the Bogoliubov transformation given in Eq. (33).

$$[H^{mf}_{BCS,B}, \hat{c}_{\mathbf{k}\uparrow}] = -\xi_{\mathbf{k}\uparrow}(u_{\mathbf{k}\uparrow}\hat{\gamma}_{\mathbf{k}\uparrow} + v_{\mathbf{k}\uparrow}\hat{\gamma}^{\dagger}_{-\mathbf{k}\downarrow}) + \Delta_B(u_{-\mathbf{k}\downarrow}\hat{\gamma}^{\dagger}_{-\mathbf{k}\downarrow} - v_{-\mathbf{k}\downarrow}\hat{\gamma}_{\mathbf{k}\uparrow}). \tag{79}$$

The commutation relation can also be calculated using the fact that the quasiparticle operators diagonalize the Hamiltonian, i.e., $H = \sum_{\mathbf{k}\sigma} E_{\mathbf{k}\sigma}\gamma^\dagger_{\mathbf{k}\sigma}\gamma_{\mathbf{k}\sigma}$.

$$
\begin{aligned}
[H^{mf}_{BCS,B}, \hat{c}_{\mathbf{k}\uparrow}] &= [\sum_{\mathbf{k}'\sigma} E_{\mathbf{k}'\sigma}\hat{\gamma}^\dagger_{\mathbf{k}'\sigma}\hat{\gamma}_{\mathbf{k}'\sigma}, (u_{\mathbf{k}\uparrow}\hat{\gamma}_{\mathbf{k}\uparrow} + v_{\mathbf{k}\uparrow}\hat{\gamma}^\dagger_{-\mathbf{k}\downarrow})] && (80)\\
&= \sum_{\mathbf{k}'\sigma} E_{\mathbf{k}'\sigma}(u_{\mathbf{k}\uparrow}[\hat{\gamma}^\dagger_{\mathbf{k}'\sigma}\hat{\gamma}_{\mathbf{k}'\sigma}, \hat{\gamma}_{\mathbf{k}\uparrow}] + v_{\mathbf{k}\uparrow}[\hat{\gamma}^\dagger_{\mathbf{k}'\sigma}\hat{\gamma}_{\mathbf{k}'\sigma}, \hat{\gamma}^\dagger_{-\mathbf{k}\downarrow}]) && (81)\\
&= \sum_{\mathbf{k}'\sigma} E_{\mathbf{k}'\sigma}(-u_{\mathbf{k}\uparrow}\hat{\gamma}_{\mathbf{k}'\sigma}\delta_{\mathbf{k}'\mathbf{k}\sigma\uparrow} + v_{\mathbf{k}\uparrow}\hat{\gamma}^\dagger_{\mathbf{k}'\sigma}\delta_{\mathbf{k}'\mathbf{k}\sigma\uparrow}) && (82)\\
&= -E_{\mathbf{k}\uparrow}u_{\mathbf{k}\uparrow}\hat{\gamma}_{\mathbf{k}\uparrow} + E_{-\mathbf{k}\downarrow}v_{-\mathbf{k}\downarrow}\hat{\gamma}^\dagger_{-\mathbf{k}\downarrow}. && (83)
\end{aligned}
$$

Combining Eq. (79) and Eq. (83) we get the two following equations in the left column. The same procedure can be applied to $[H^{mf}_{BCS,B}, \hat{c}_{-\mathbf{k}\downarrow}]$ and from this we get the equations in the right column.

$$
\begin{aligned}
u_{\mathbf{k}\uparrow}E_{\mathbf{k}\uparrow} &= v_{-\mathbf{k}\downarrow}\Delta_B + u_{\mathbf{k}\uparrow}\xi_{\mathbf{k}\uparrow} \qquad & u_{-\mathbf{k}\downarrow}E_{-\mathbf{k}\downarrow} &= v_{\mathbf{k}\uparrow}\Delta_B + u_{-\mathbf{k}\downarrow}\xi_{-\mathbf{k}\downarrow}\\
v_{\mathbf{k}\uparrow}E_{-\mathbf{k}\downarrow} &= u_{-\mathbf{k}\downarrow}\Delta_B - v_{\mathbf{k}\uparrow}\xi_{\mathbf{k}\uparrow} \qquad & v_{-\mathbf{k}\downarrow}E_{\mathbf{k}\uparrow} &= u_{\mathbf{k}\uparrow}\Delta_B - v_{-\mathbf{k}\downarrow}\xi_{-\mathbf{k}\downarrow}
\end{aligned} \tag{84}
$$

Calculating $[H^{mf}_{BCS,B}, \hat{c}^\dagger_{\mathbf{k}\uparrow}]$ and $[H^{mf}_{BCS,B}, \hat{c}^\dagger_{-\mathbf{k}\downarrow}]$, we obtain the same equations as above. Combining these equations with $u^2_{\mathbf{k}} + v^2_{\mathbf{k}} = 1$ allows us to find analytical expressions for the elements of U.

$$
\begin{aligned}
u_{\mathbf{k}\uparrow} &= \pm\frac{\Delta_B}{\sqrt{\Delta_B^2 + (E_{\mathbf{k}\uparrow} - \xi_{\mathbf{k}\uparrow})^2}} \qquad & v_{\mathbf{k}\uparrow} &= \pm\frac{\Delta_B}{\sqrt{\Delta_B^2 + (E_{-\mathbf{k}\downarrow} + \xi_{\mathbf{k}\uparrow})^2}}\\
u_{-\mathbf{k}\downarrow} &= \pm\frac{\Delta_B}{\sqrt{\Delta_B^2 + (E_{-\mathbf{k}\downarrow} - \xi_{-\mathbf{k}\downarrow})^2}} \qquad & v_{-\mathbf{k}\downarrow} &= \pm\frac{\Delta_B}{\sqrt{\Delta_B^2 + (E_{\mathbf{k}\uparrow} + \xi_{-\mathbf{k}\downarrow})^2}}
\end{aligned} \tag{85}
$$

Inserting $E_{\mathbf{k}\uparrow} = B + E_{\mathbf{k}}$, $E_{-\mathbf{k}\downarrow} = -B + E$, $\xi_{\mathbf{k}\uparrow} = \xi_{\mathbf{k}} + B$ and $\xi_{-\mathbf{k}\downarrow} = \xi_{\mathbf{k}} - B$, we find that $u_{\mathbf{k}\uparrow}$, $u_{-\mathbf{k}\downarrow}$ reduces to $u_{\mathbf{k}}$ and $v_{\mathbf{k}\uparrow}$, $v_{-\mathbf{k}\downarrow}$ reduces to $v_{\mathbf{k}}$ in Eq. (14). Thus we obtain the same result as from the diagonalization of the Hamiltonian and we observe once more that we do not need the spin dependency on the elements of U.

D The expectation value of the nondiagonalized FFLO Hamiltonian for $T \to 0$

We want to investigate if the expectation value of the nondiagonalized FFLO Hamiltonian in Eq. (50) is the same as the expectation value of the diagonalized FFLO Hamiltonian in Eq. (56) $T \to 0$. This is a way to control that we have not made any mistakes in the diagonalization process.

$$
\begin{aligned}
\langle H\rangle =& \sum_{\mathbf{k}}[\xi_{\mathbf{k}+\mathbf{q}/2\uparrow}\langle \hat{c}^{\dagger}_{\mathbf{k}+\mathbf{q}/2\uparrow}\hat{c}_{\mathbf{k}+\mathbf{q}/2\uparrow}\rangle + \xi_{-\mathbf{k}+\mathbf{q}/2\downarrow}\langle \hat{c}^{\dagger}_{-\mathbf{k}+\mathbf{q}/2\downarrow}\hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow}\rangle \\
&\quad - \Delta_{\mathbf{q}}(\langle \hat{c}^{\dagger}_{\mathbf{k}+\mathbf{q}/2\uparrow}\hat{c}^{\dagger}_{-\mathbf{k}+\mathbf{q}/2\downarrow}\rangle + \langle \hat{c}_{-\mathbf{k}+\mathbf{q}/2\downarrow}\hat{c}_{\mathbf{k}+\mathbf{q}/2\uparrow}\rangle)] + \frac{N^2\Delta_{\mathbf{q}}^2}{V} \\
=& \sum_{\mathbf{k}}[\xi_{\mathbf{k}+\mathbf{q}/2\uparrow}\langle(u_{\mathbf{k}}\hat{\gamma}^{\dagger}_{\mathbf{k}+\mathbf{q}/2\uparrow} + v_{\mathbf{k}}\hat{\gamma}_{-\mathbf{k}+\mathbf{q}/2\downarrow})(u_{\mathbf{k}}\hat{\gamma}_{\mathbf{k}+\mathbf{q}/2\uparrow} + v_{\mathbf{k}}\hat{\gamma}^{\dagger}_{-\mathbf{k}+\mathbf{q}/2\downarrow})\rangle \\
&\quad + \xi_{-\mathbf{k}+\mathbf{q}/2\downarrow}\langle(u_{\mathbf{k}}\hat{\gamma}^{\dagger}_{-\mathbf{k}+\mathbf{q}/2\downarrow} - v_{\mathbf{k}}\hat{\gamma}_{\mathbf{k}+\mathbf{q}/2\uparrow})(u_{\mathbf{k}}\hat{\gamma}_{-\mathbf{k}+\mathbf{q}/2\downarrow} - v_{\mathbf{k}}\hat{\gamma}^{\dagger}_{\mathbf{k}+\mathbf{q}/2\uparrow})\rangle \\
&\quad - \Delta_{\mathbf{q}}(\langle(u_{\mathbf{k}}\hat{\gamma}^{\dagger}_{\mathbf{k}+\mathbf{q}/2\uparrow} + v_{\mathbf{k}}\hat{\gamma}_{-\mathbf{k}+\mathbf{q}/2\downarrow})(u_{\mathbf{k}}\hat{\gamma}^{\dagger}_{-\mathbf{k}+\mathbf{q}/2\downarrow} - v_{\mathbf{k}}\hat{\gamma}_{\mathbf{k}+\mathbf{q}/2\uparrow})\rangle \\
&\quad + \langle(u_{\mathbf{k}}\hat{\gamma}_{-\mathbf{k}+\mathbf{q}/2\downarrow} - v_{\mathbf{k}}\hat{\gamma}^{\dagger}_{\mathbf{k}+\mathbf{q}/2\uparrow})(u_{\mathbf{k}}\hat{\gamma}_{\mathbf{k}+\mathbf{q}/2\uparrow} + v_{\mathbf{k}}\hat{\gamma}^{\dagger}_{-\mathbf{k}+\mathbf{q}/2\downarrow})\rangle)] + \frac{N^2\Delta_{\mathbf{q}}^2}{V}
\end{aligned}
\tag{86}
$$

Here we have used the Bogoliubov transformation given in Eq. (55). We will now use $\langle\hat{\gamma}^{\dagger}_{\mathbf{k},\mathbf{q}\sigma}\hat{\gamma}^{\dagger}_{\mathbf{k},\mathbf{q}\sigma} = 0\rangle$, $\langle\hat{\gamma}_{\mathbf{k},\mathbf{q}\sigma}\hat{\gamma}_{\mathbf{k},\mathbf{q}\sigma} = 0\rangle$ and $\langle\hat{\gamma}^{\dagger}_{\mathbf{k},\mathbf{q}\sigma}\hat{\gamma}_{\mathbf{k}',\mathbf{q}\sigma'}\rangle = \delta_{\mathbf{k}\mathbf{k}'\sigma\sigma'}f(E_{\mathbf{k},\mathbf{q},\sigma})$.

$$
\begin{aligned}
\lim_{T\to 0}\langle H\rangle =& \sum_{\mathbf{k}}[\xi_{\mathbf{k}+\mathbf{q}/2\uparrow}(u_{\mathbf{k}}^2\cancelto{0}{f(E_{\mathbf{k},\mathbf{q},\uparrow})} + v_{\mathbf{k}}^2(1 - \cancelto{0}{f(E_{\mathbf{k},\mathbf{q},\downarrow})})) \\
&\quad + \xi_{-\mathbf{k}+\mathbf{q}/2\downarrow}(u_{\mathbf{k}}^2\cancelto{0}{f(E_{\mathbf{k},\mathbf{q},\downarrow})} + v_{\mathbf{k}}^2(1 - \cancelto{0}{f(E_{\mathbf{k},\mathbf{q},\uparrow})})) \\
&\quad - \Delta_{\mathbf{q}}(-u_{\mathbf{k}}v_{\mathbf{k}}\cancelto{0}{f(E_{\mathbf{k},\mathbf{q},\uparrow})} + u_{\mathbf{k}}v_{\mathbf{k}}(1 - \cancelto{0}{f(E_{\mathbf{k},\mathbf{q},\downarrow})}) \\
&\quad + u_{\mathbf{k}}v_{\mathbf{k}}(1 - \cancelto{0}{f(E_{\mathbf{k},\mathbf{q},\downarrow})}) - u_{\mathbf{k}}v_{\mathbf{k}}\cancelto{0}{f(E_{\mathbf{k},\mathbf{q},\uparrow})})] + \frac{N^2\Delta_{\mathbf{q}}^2}{V} \\
=& \sum_{\mathbf{k}}[v_{\mathbf{k}}^2(\xi_{\mathbf{k}+\mathbf{q}/2\uparrow} + \xi_{-\mathbf{k}+\mathbf{q}/2\downarrow} - 2u_{\mathbf{k}}v_{\mathbf{k}}\Delta_{\mathbf{q}})] + \frac{N^2\Delta_{\mathbf{q}}^2}{V} \\
=& \sum_{\mathbf{k}}\left[2v_{\mathbf{k}}^2\xi^{(s)}_{\mathbf{k},\mathbf{q}} - \frac{\Delta_{\mathbf{q}}^2}{E_{\mathbf{k},\mathbf{q}}}\right] + \frac{N^2\Delta_{\mathbf{q}}^2}{V} = \sum_{\mathbf{k}}\left[\xi^{(s)}_{\mathbf{k},\mathbf{q}}\left(1 - \frac{\xi^{(s)}_{\mathbf{k},\mathbf{q}}}{E_{\mathbf{k},\mathbf{q}}}\right) - \frac{\Delta_{\mathbf{q}}^2}{E_{\mathbf{k},\mathbf{q}}}\right] + \frac{N^2\Delta_{\mathbf{q}}^2}{V} \\
=& \sum_{\mathbf{k}}\left[\xi^{(s)}_{\mathbf{k},\mathbf{q}} - \frac{(\xi^{(s)2}_{\mathbf{k},\mathbf{q}} + \Delta_{\mathbf{q}}^2)}{E_{\mathbf{k},\mathbf{q}}}\right] + \frac{N^2\Delta_{\mathbf{q}}^2}{V} = \sum_{\mathbf{k}}\left[\xi_{-\mathbf{k}+\mathbf{q}/2} - E_{\mathbf{k},\mathbf{q},\downarrow}\right] + \frac{N^2\Delta_{\mathbf{q}}^2}{V}
\end{aligned}
\tag{87}
$$

In the last steps we have used that $f(E_{\mathbf{k},\mathbf{q},\sigma}) \to 0$ for $T \to 0$. Further we have used Eq. (53), (54) and (58) and the fact that $\xi^{(s)}_{\mathbf{k},\mathbf{q}} - E_{\mathbf{kq}} = \xi_{-\mathbf{k}+\mathbf{q}/2\downarrow} - E_{\mathbf{k},\mathbf{q},\downarrow}$. We do get the same result as in Eq. (66) and (67).