Type-II Superconductors in High Magnetic Fields

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Abstract

Superconductivity in high magnetic fields has attracted considerable attention in recent years. The topic is important both for our fundamental understanding of superfluids and for numerous practical applications. In this thesis, we consider several effects originating from the interplay between the Landau level structure of the normal state quasiparticle spectrum, and the tendency of the quasiparticles to form Cooper pairs below the critical temperature.

A formalism designed to describe extreme type-II superconductors close to the upper critical field H_{c2} is developed. The theory which utilizes the selection rules coming from the symmetry properties of the vortex lattice, simplifies the algebra describing a superconductor in the mixed state significantly. We are, on the mean field level, able to include the quantizing effects of the magnetic field on the electron motion exactly. A main achievement is the exact calculation of the expansion coefficients giving the grand canonical potential of a superconductor in terms of a power series in the size of the order parameter. The result is an expression for the grand canonical potential in terms of a polynomial in a finite set of variables close to H_{c2}.

Using this formalism, a theory for the experimentally observed damped de Haas-van Alphen (dHvA) oscillations in the mixed state of a 2-dimensional (2D) superconductor is presented. The theory is compared with numerical results and the agreement is found to be good. A simple physical interpretation of the damping is provided. The dependence of the damping on a finite Zeeman term, temperature, and the magnetic field is considered. A comparison of the theory with experimental data for the quasi-2D superconductor κ-$(ET)_2Cu(NCS)_2$ yields good agreement.

The attenuation of a longitudinal sound wave in the mixed state is then calculated. In analogy with the dHvA effect, we predict that there should be damped oscillations in the sound attenuation in the mixed state as the external magnetic field is varied. Furthermore, the dependence of the oscillations on the sound frequency and temperature is shown to yield information on the low lying quasiparticle spectrum. Especially, the presense of gapless excitations due to the magnetic field makes the attenuation qualitatively different as compared to the attenuation in the Meissner state.

Some formal convergence properties of the Gor'kov theory for type-II superconductors close to H_{c2} are derived. We show that the theory is essentially a high temperature expansion; the convergence radius of the Gor'kov series is proportional to k_BT when there is a Landau level at the chemical potential.

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Contents

Chapter 1

Introduction

The relationship between external magnetic fields and superconductivity is both of practical importance and of fundamental interest as a physical phenomenon. It gives rise to a broad range of effects such as the Meissner effect (i.e. perfect diamagnetism), vortex structures and a number of different phases in the phase diagram. Indeed, with the discovery of the Meissner effect in 1933 [77], it became clear that a crucial problem to understand in superconductivity was that of perfect diamagnetism. Once this was understood, effects such as the infinite DC conductivity, discovered by Onnes [64], could also be explained. At the same time, this inherent property of superconductors can be used in practical applications, for example, to provide shielding from external fields.

Superconductors can, in general, be divided into two types according to their response to an external magnetic field. For type-I superconductors, it is energetically favorable to expel the magnetic field completely apart from a thin surface layer (Meissner effect) below an upper critical field H_c. Type-II superconductors allow a partial penetration of the external field in form of vortices. In the mean field approximation, these vortices form a regular lattice when the external field H is between the two critical fields $H_{c1} \leq H \leq H_{c2}$, as predicted theoretically by Abrikosov [1]. The superconductor is said to be in the so called *mixed state.* A wide range of phenomena arise from the tendency of the electrons to form Cooper pairs and the orbital frustration from the magnetic field. A thorough understanding of this mixed state is also very important from a practical point of view since type-I superconductors suffer from a small thermodynamic critical field H_c. This means that large currents (creating large fields) or large external fields will destroy the superconducting phase in type-I superconductors. Likewise, the Meissner phase in type-II superconductors is bounded by an even smaller critical field H_{c1} whereas H_{c2} can be very large (several Teslas). Hence, most technologically relevant materials are type-II superconductors operating in the mixed state.

Up to the late 1980's, the mixed state was (with a few noticeable exceptions) described in terms of Ginzburg-Landau theory [34, 107]. This theory has been successful in describing almost all physical phenomena for type-II superconductors. However, just over 20 years ago, magnetic oscillations in the free energy were observed in the layered superconductor 2H-$NbSe_2$ [49]. These oscillations which are called de-Haas-van Alphen (dHvA) oscillations, were later observed in a number of different type-II superconductors. From a theoretical point of view it is clear that such oscillations cannot be described by a semiclassical treatment such as Ginzburg-Landau theory which assumes that the bending of the electron orbit due to the magnetic field is negligible over the range of the electron mean free path. The oscillations are a pure quantum phenomenon originating in the quantization of the electron motion in a magnetic field, which becomes important when the mean free path of the electron is such that it can propagate coherently over many unit cells in the vortex lattice, and when the temperature T is sufficiently low such that $k_B T < \hbar\omega_c$, where $\omega_c = eH/mc$ is the cyclotron frequency. The occurrence of the dHvA oscillations in a wide range of superconductors seems to suggest that this effect is a fundamental property of a type-II superconductor in the mixed state. Furthermore, recent advances in Scanning Tunneling

Microscopy (STM) have enabled us to directly probe the quasiparticle levels bound in the vortex core [55, 57, 56], thus giving direct experimental evidence of the nature of the superconducting state in a magnetic field. These quasiparticle levels are completely ignored in the Ginzburg-Landau theory. Hence, an understanding of superconductivity in high magnetic fields based on the Ginzburg-Landau theory cannot be complete. A successful theory describing superconductors in high magnetic fields must include the quantum effects of the magnetic field from the beginning and should therefore be a generalization of the original BCS-theory [9]. The need for such a theory is further underlined by the high temperature (high T_c) superconductors, first discovered in the cuprates by Bednorz and Müller [13]. The normal state properties in these materials are unknown; the existence of a normal state Fermi surface is a highly controversial and debated issue. Since the dHvA measurements are a powerful tool in mapping out the Fermi surface, it is clearly of interest to carry out such experiments for high T_c materials. However, the high T_c materials are quasi 2-dimensional extreme type-II superconductors with a very high upper critical field ($H_{c2} \sim 10^2$T) at the low temperatures appropriate for dHvA measurements. This means that such experiments will be carried out in the mixed state of the high T_c's. Hence, even at the mean-field level, it is necessary to develop a microscopic theory for superconductivity in strong magnetic fields which goes beyond the traditional Ginzburg Landau treatment and includes the quantum effects due to the magnetic field from the beginning. Because of this, there has been a dramatic increase in the number of articles dealing with this issue since the late 1980's. Some theories have been in direct contradiction with each other, and there has been much debate, not least in connection with developing a consistent description of the dHvA oscillations in the mixed state.

This thesis examines theoretically several aspects of the interplay between a strong magnetic field and superconductivity. Specifically, I will present a theory for the dHvA oscillations described above. Furthermore, the effect of the magnetic field on the quasiparticle levels is treated within the context of sound attenuation. In addition, we examine some formal properties related to the validity of aspects of the theoretical formalism which is used to treat type-II superconductors close to H_{c2}. The thesis is structured as follows:

- **Chapter 2**. The traditional BCS theory, which has been hugely successful in describing weak coupling superconductors, is briefly outlined for an arbitrary external field. We discuss the effective interaction applicable as a first approximation to describe the attraction between the electrons. Then, the pairing hypothesis is described and the resultant pairing field is defined. The Bogoliubov-de Gennes (BdG) equations which diagonalize the corresponding mean field Hamiltonian, are introduced. These equations form a theoretical framework for much of the material presented in this thesis. The Green's function formalism used to describe weak coupling superconductors is presented. This formalism is very useful when developing a perturbation theory for type-II superconductors near H_{c2}. Finally, the validity of the mean field theory and the role of the fluctuations are discussed.

- **Chapter 3**. As this thesis is dealing with cases where the semiclassical approximation breaks down, this chapter develops further the formalism introduced in chapter 2 to specifically treat cases where the effect of the magnetic field must be included from the outset. We first consider the problem of two-electron scattering in a magnetic field. This will introduce a useful splitting of the Cooper pair motion into a center-of-mass motion and a relative motion. The symmetry of the vortex lattice is then introduced. This symmetry simplifies the mean field Hamiltonian and the corresponding BdG equations are then solved exactly in the limit of a very high magnetic field. A perturbative expansion of the grand canonical potential based on Green's functions is then developed. The symmetry of the vortex lattice reduces the necessary algebra significantly and we can solve the appropriate expansion integrals exactly.

A major result is the expression of the grand canonical potential in terms of a simple polynomial in a finite set of variables. The problem of self-consistency reduces to the trivial algebraic task of minimizing this polynomial; a fact that will be very useful when developing a self-consistent perturbative description of a type-II superconductor close to H_{c2}.

- **Chapter 4**. This chapter presents a theory for the dHvA oscillations in the mixed state of a type-II superconductor. We start by briefly sketching the well known theory of the dHvA oscillations in the normal state. Then, a perturbative theory for the oscillations in the mixed state is developed. We compare the predictions of this theory with an exact numerical solution of the BdG equations. The agreement is good close to H_{c2}. A physical interpretation of the presence of the dHvA oscillations in the mixed state is then presented. The effect of the electron spin and the difference between the case where the chemical potential is constant and the case where the number of particles is conserved is considered. Then, we simplify the analytical theory for the dHvA effect in order to make some predictions concerning the dependence of the oscillations on various quantities such as the temperature and the magnetic field. The agreement between these theoretical predictions and experimental data is found to be satisfactory. Finally, I briefly outline the main features of some of the alternative theories developed to describe the dHvA oscillations in the mixed state.

- **Chapter 5**. This chapter considers the problem of longitudinal sound attenuation for clean type-II superconductors in the mixed state. Since phonons interact with the quasiparticles, we can gain considerable information on the low lying density-of-states by considering this problem. The sound attenuation is shown to be an oscillatory function of the external magnetic field in analogy with the dHvA oscillations. We consider the two limits $\hbar\omega \gg k_BT$ and $\hbar\omega \ll k_BT$ where ω is the frequency of the sound wave. It turns out that the interpretation of the attenuation of the sound wave is somewhat more straightforward than the interpretation of the damped dHvA oscillations in the mixed state. The temperature dependence of the attenuation in the $\hbar\omega \ll k_BT$ limit is shown to yield information about the quasiparticle spectrum in the mixed state. The same is true for the frequency dependence in the $\hbar\omega \gg k_BT$ limit. This should make it possible to test some aspects of our theoretical understanding of type-II superconductors in high magnetic field by measuring the sound attenuation in the mixed state.

- **Chapter 6**. It has recently been suggested that perturbation (Gor'kov) theory should break down when describing type-II superconductors close to H_{c2} due to the large degeneracy of the normal state electron levels (Landau levels). The Gor'kov theory is a very important theoretical tool used by numerous authors to describe superconductors. If true, the break-down of the Gor'kov expansion for type-II superconductors would be a very important discovery. Also, it would invalidate much of the theory presented in this thesis! Thus, this chapter examines the convergence properties of the Gor'kov expansion in order to verify the existence of this break down. For zero temperature, it is shown that the Gor'kov expansion in fact is invalid and that there are non-perturbative terms in the expression for the ground state energy in the mixed state. For finite temperature however, it turns out that the non-perturbative terms for the appropriate thermodynamic potential cancel and that the Gor'kov theory is valid. We derive some criteria for the convergence of the Gor'kov series. These criteria essentially state that the Gor'kov theory is a high temperature expansion; the change of the quasiparticle levels as compared to the normal state levels must be of the order of k_BT or smaller for the Gor'kov expansion to be valid.

- **Chapter 7**. The results presented in the previous chapters are summarized. We also outline some future possible research projects which emerge naturally from the work described in this thesis.

Chapter 2

Formalism

2.1 Introduction

Superconductivity is a widespread phenomenon in nature. It is an example of a macroscopic quantum effect with observable consequences. Below a certain critical temperature T_c, the relevant particles forming a physical system condense into a phase which in many ways can be viewed as a macroscopic molecule. The particles can form a state characterized by a frictionless motion of the center-of-mass in much the same way as the electrons of atoms can form states with a non-zero angular momentum. The state of non-zero average motion gives rise to the remarkable effect of superconductivity. The condensation to the superfluid state appears on many energy scales in nature. Fig. 2.1 shows the transition temperature in different systems exhibiting superconductivity. As can be seen, it varies from one milliKelvin for ^{3}He to approximately 10^{13} Kelvin for the quark condensate. In condensed matter physics, superconductivity, a consequence of the condensation of the electrons, occurs in numerous systems such as many metals and alloys (e.g. Al and V_3Si), some of the quasi two-dimensional organic charge transfer salts $(ET)_nX$ where ET is the donor ion *bis(ethylenedithio)-tetrathiafulvalene*, and X is an inorganic anion such as $Cu(NCS)_2$, and in the now famous so-

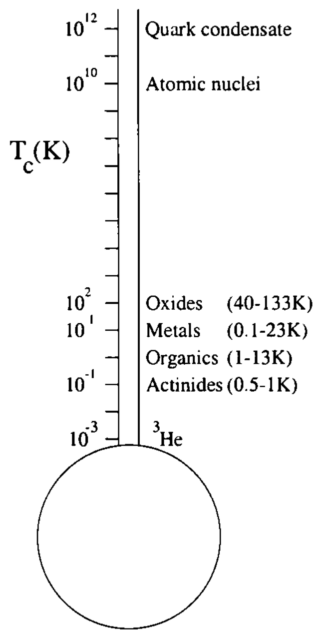


Figure 2.1: The critical temperature T_c for a wide range of systems

called high T_c materials such as YBCO. The list of superconducting materials stretches into the thousands and is ever increasing. Superconductivity represents a spectacular failure of Landau Fermi Liquid Theory and cannot be obtained in any finite order perturbation expansion [95] from the normal state. It therefore took almost fifty years to construct a theory for this non-Fermi liquid phenomenon. Furthermore, the mechanisms behind the new high T_c materials are still unknown.

In this chapter, we will briefly outline the traditional BCS theory for weak-coupling superconductivity. In section 2.2, we define the BCS Hamiltonian. Then in section 2.3, we introduce the generalized mean-field approximation leading to the introduction of the pairing field. In section 2.4, the Bogoliubov equations are introduced. Section 2.5 presents the Green's function formalism used to describe weak-coupling superconductors. These two sections form the framework of much of the theory developed later in this thesis. Finally in section 2.6, we will consider the validity of the mean-field approximation.

2.2 The BCS Hamiltonian

Superconductivity in condensed matter physics arises in general as a result of an effective attractive force between the electrons. In most cases, possibly excluding high T_c's, the organics, and other "exotic" superconductors, the attractive interaction is due to an overscreening effect from the phonons. It can be shown [98] that the effective interaction $V_{eff}(q)$ for a wave vector $\mathbf{q}$ and a frequency ω $(q = (\mathbf{q}, \omega))$ between two electrons in a metal within the jellium approximation has the form

$$V_{eff}(q) = \frac{V_c(q)\omega^2}{\omega^2 - \Omega_{ql}^2/\kappa(q) + i\delta}. \tag{2.1}$$

Here $\kappa(q)$ is the dielectric function of the electrons, $V_c(q) = 4\pi e^2/q^2\kappa(q)$ is the screened coulomb potential and Ω_{ql} is the bare longitudinal phonon frequency. This effective interaction between the electrons includes the screening due to electrons and phonons. We will not go into the details of the derivation and the approximations behind this effective interaction. They are not relevant for this thesis, which is based on a more simple effective interaction described below. The important point to note is that for $\omega < \omega_q$, where $\omega_q^2 = \Omega_{ql}^2/\kappa(q)$ is the dressed phonon frequency, the interaction is *attractive* due to the overscreening from the phonons. Hence, when the electrons do not differ too much in energy they attract each other. One can analyze the electron-phonon system using the interaction given above. This leads to the strong coupling theory as described by Eliashberg [41].

In this thesis, we will take a more modest approach and assume that the effective interaction between electrons close to the Fermi surface can be represented by an attractive contact potential $-g\delta(\mathbf{r})$ where g is the coupling strength. The phonon degrees of freedom are in some sense "integrated" out and we are left with the simple contact potential. This is the usual effective interaction used in the so-called weak coupling BCS-theory [10, 11]. The actual mechanism responsible for the attraction is unknown in materials such as the high T_c's or the organic transfer salts. For our purposes, it is therefore appropriate to take this more pragmatic approach and just assume that there is some sort of mechanism giving rise to an effective attraction between electrons close to the Fermi surface, and that such an interaction is well described by a contact potential. A problem with this interaction is that as it stands, it introduces divergencies in the theory. This is because it is effective for arbitrarily high energies. This is, of course, unphysical; the contact interaction should really be regarded as an effective low energy interaction. The standard way to renormalize this divergence is to introduce a physically motivated cutoff ω_D around the Fermi surface within which the interaction is effective [98]. Outside this range there is no interaction. Since the attraction for most materials is due to the phonons, ω_D is typically of the order of the Debye frequency. Using this approximation, the Hamiltonian of the electron system becomes

$$
\begin{aligned}
\hat{H} &= \hat{H}_0 + \hat{H}_I \\
&\sum_\sigma \int d^3r\, \psi_\sigma^\dagger(\mathbf{r})\mathcal{H}_{0,\sigma}\psi_\sigma(\mathbf{r}) - g\int d^3r\, \psi_\uparrow^\dagger(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r})\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}). \quad (2.2)
\end{aligned}
$$

Here

$$
\mathcal{H}_{0,\sigma} = \frac{(\mathbf{p} + \frac{e}{c}\mathbf{A})^2}{2m} + U_0(\mathbf{r}) - \mu_F + g^*\mu_B H\sigma_z/2 = \mathcal{H}_0 + g^*\mu_B H\sigma_z/2,
$$

where the momentum operator is $\mathbf{p} = -i\hbar\nabla$, the effective mass of the electron is m, μ_F is the chemical potential, and $\psi_\sigma(\mathbf{r})$ is the field operator for an electron with spin $\sigma = \pm 1$ along the z-direction. In this thesis, we take $e > 0$ so that the charge of the electron is $-e$. The electronic g-factor is denoted g^*, $\mu_B = e\hbar/2m_0c$ with m_0 taken to be the free electron mass, is the Bohr magneton. The magnetic field which points along the z-direction, is given by $\mathbf{H} = \nabla \times \mathbf{A}$. $U_0(\mathbf{r})$ denotes an external potential. Since the typical energy difference between a metal in the normal and in the superconducting phase is $\mathcal{O}(k_B T_c^2/T_F) \sim 10^{-8}$eV per electron ($T_F$ is the Fermi temperature) and the Coulomb and phonon interactions between electrons in the normal state lead to correlation energies of the order of 1eV, it is perhaps surprising that such a simple effective Hamiltonian as the one above should encapsulate the relevant physics of the problem [98]. However, one should regard the above Hamiltonian as describing the residual interaction between the quasiparticles. From Landau Fermi liquid theory, we know that the low lying excitations (which are the ones relevant for superconductivity) of the normal metal are well described as quasiparticles. Hence, it is assumed that the effects of the Coulomb and other interactions in the normal state are included in the effective mass m of the quasiparticle and that the effective Hamiltonian in Eq. (2.2) describes the effect of the weak residual attraction between the quasiparticles. Further justification for the introduction of the simple contact interaction is given in the standard books by Schrieffer [98] and de Gennes [34].

2.3 Pairing Theory

An essential step in the understanding of superconductivity was made by Cooper [28] when he studied a pair of interacting electrons above a Fermi sea of non-interacting electrons. The crucial result of his analysis is, that a bound state of the two electrons exists for an arbitrarily weak coupling. This result, which is in sharp contrast to the behaviour of two electrons interacting via a finite range potential in free space, suggests that the Fermi sea is unstable towards the pair formation of the electrons. In principle, the system will spontaneously form bound pairs of electrons until the pairs begin to overlap. If the condensation were to stop at this point, a Bose-Einstein condensation (BEC) approach might be appropriate. Instead, a quite different phenomenon takes place, namely a cooperative pairing condensation which involves a strong overlap of the pairs. In most superconductors there are $\sim 10^6$ pairs within a given volume of one electron pair. Hence, there is a massive overlap between the pairs; an independent pair approximation is totally invalid[1]. Due to this strong overlap, the Pauli principle is of utmost importance and there is a gap in the quasiparticle spectrum which does not appear in the BEC case. Describing superconductivity in terms of a Bose condensation of Cooper pairs is therefore incorrect for most superconductors with the possible exception of the high T_c materials. To reduce the complexity of the problem without losing the essential physics arising from the pairing correlations, the BCS theory makes the following substitution:

$$\psi_\sigma(\mathbf{r})\psi_{-\sigma}(\mathbf{r}) \to \langle\psi_\sigma(\mathbf{r})\psi_{-\sigma}(\mathbf{r})\rangle + [\psi_\sigma(\mathbf{r})\psi_{-\sigma}(\mathbf{r}) - \langle\psi_\sigma(\mathbf{r})\psi_{-\sigma}(\mathbf{r})\rangle] \tag{2.3}$$

Here $\langle \ldots \rangle$ means the thermal average. The fluctuation term in the brackets is now considered to be small. By substituting the above identity into the Hamiltonian and only keeping terms to first order in the fluctuation, it becomes

$$\begin{aligned} \hat{H}_{mean} = \sum_\sigma \int d^3r\, \psi^\dagger_\sigma(\mathbf{r})\mathcal{H}_{0,\sigma}\psi_\sigma(\mathbf{r}) \\ - \int d^3r\, [\Delta(\mathbf{r})\psi^\dagger_\downarrow(\mathbf{r})\psi^\dagger_\uparrow(\mathbf{r}) + c.c] + \frac{1}{g}\int d^3r\, |\Delta(\mathbf{r})|^2 \end{aligned} \tag{2.4}$$

where the order parameter is defined self-consistently as

$$\Delta(\mathbf{r}) = g\langle\psi_\uparrow(\mathbf{r})\psi_\downarrow(\mathbf{r})\rangle. \tag{2.5}$$

This approximation can be viewed as a Hartree-Fock theory generalized to include the essential pairing correlations between the electrons. These non-perturbative correlations are described by the order parameter $\Delta(\mathbf{r})$. The

[1]In the high T_c's, the size of the pairs is only a few times the lattice spacing. There is therefore only a few pairs overlapping a given pair in marked contrast with the systems described by BCS theory.

price one pays by the introduction of $\Delta(\mathbf{r})$ is the violation of particle conservation due to the non-zero value of the anomalous average $\langle\psi_\sigma\psi_{-\sigma}\rangle$. For macroscopic systems, it is easy to show that this causes no major problems in the sense that the relative fluctuation, $\langle(\hat{N}-\langle\hat{N}\rangle)^2\rangle/\langle\hat{N}\rangle$, in the number of particles, $\langle\hat{N}\rangle$, goes as $\langle\hat{N}\rangle^{-1/2}$ [107]. Thus, it is negligible for most systems. We note that the Hamiltonian in Eq. (2.4) ignores any dynamical interaction between the Cooper pairs. It is in some sense striking that BCS theory, which is based on such crude approximations, seems to work so well in many cases. The reason is that in real metals the pair-pair correlations are dominated by the Pauli-principle due to the strong overlap. One can therefore ignore the dynamical interactions between the pairs and concentrate on the correlations between the "mates" of the pairs. These correlations are well described by the effective Hamiltonian given in Eq. (2.4). Also, note we have ignored the usual Hartree-Fock terms $\langle\psi_\sigma^\dagger\psi_\sigma\rangle$ in $\hat{H}_{mean}$. This approximation is based on the assumption that these terms are the same in both the normal and the superconducting state and therefore do not affect the comparison between the two states [42].

It is interesting to note that the self-consistency condition given in Eq. (2.5) can be derived using the Gibbs variational principle. Take a Hermitian operator $\hat{\rho}$ with positive eigenvalues such that the trace $Tr(\hat{\rho}) = 1$. Define the function $\psi(\hat{\rho}) = Tr(\hat{H}\hat{\rho}) + \beta^{-1}Tr(\hat{\rho}\ln(\hat{\rho}))$ where $\hat{H}$ is the Hamiltonian for the system in question and $\beta = \frac{1}{k_BT}$. Minimize $\psi(\hat{\rho})$ by varying $\hat{\rho}$, subject to the condition $Tr(\hat{\rho}) = 1$. The operator $\tilde{\rho}$ that minimizes $\psi(\hat{\rho})$ is the density operator: that is, $\tilde{\rho} = \exp(-\beta\hat{H})/Tr(\exp(-\beta\hat{H}))$ and $\psi(\tilde{\rho})$ is the grand canonical potential for the system described by $\hat{H}$ [58]. This is the statistical mechanical analogue of the variational principle in quantum mechanics. By minimizing $\psi(\hat{\rho})$ within the subset of density operators of the form $\hat{\rho} = \exp(-\beta\hat{H}_{mean})/Tr(\exp(-\beta\hat{H}_{mean}))$ where $\hat{H}_{mean}$ is given by Eq. (2.4) with arbitrary $\Delta(\mathbf{r})$, one recovers the self-consistency condition given in Eq. (2.5). Based on physical arguments, we assert that the above subset of density operators describe superconductivity well [98]. We will in section 2.5 show that the above generalized mean field approximation can also be regarded as a stationary phase approximation to the free energy.

2.4 The Bogoliubov-de Gennes equations

There are many ways of proceeding from the Hamiltonian defined in Eq. (2.4). Since it is quadratic in the field operators, a straightforward approach is to diagonalize the Hamiltonian by performing a suitable unitary transformation. This method was introduced independently by Bogoliubov [16] and Valatin [109]. It is described in detail by de Gennes [34] in its general form, when the order parameter varies in space. The Hamiltonian can be diagonalized by writing the field operators as

$$\begin{aligned} \psi_\uparrow(\mathbf{r}) &= \sum_n [\gamma_{n\uparrow} u_n(\mathbf{r}) - \gamma_{n\downarrow}^\dagger v_n^*(\mathbf{r})] \\ \psi_\downarrow(\mathbf{r}) &= \sum_n [\gamma_{n\downarrow} u_n(\mathbf{r}) + \gamma_{n\uparrow}^\dagger v_n^*(\mathbf{r})] \end{aligned} \tag{2.6}$$

Here, the γ's are new fermion operators satisfying the usual commutation rules $\gamma_{n\sigma}^\dagger \gamma_{m\sigma'} + \gamma_{m\sigma'} \gamma_{n\sigma}^\dagger = \delta_{nm}\delta_{\sigma\sigma'}$ etc. If the Bogoliubov wave functions $u_n(\mathbf{r})$ and $v_n(\mathbf{r})$ satisfy the *Bogoliubov-de Gennes* (BdG) equations

$$\begin{aligned} E_n u_n(\mathbf{r}) &= \mathcal{H}_0 u_n(\mathbf{r}) + \Delta(\mathbf{r}) v_n(\mathbf{r}) \\ E_n v_n(\mathbf{r}) &= -\mathcal{H}_0^* v_n(\mathbf{r}) + \Delta(\mathbf{r})^* u_n(\mathbf{r}) \end{aligned} \tag{2.7}$$

then the Hamiltonian is diagonalized; i.e. it is on the form

$$\hat{H}_{mean} = E_g + \sum_{n\sigma} E_{n\sigma} \gamma_{n\sigma}^\dagger \gamma_{n\sigma} \tag{2.8}$$

where $E_{n\sigma} = E_n + g^* \mu_B H \sigma_z / 2$. The BdG equations have the property that if (u_n, v_n) is a solution with energy E_n then $(-v_n^*, u_n^*)$ is a solution with energy

$-E_n$. By choosing only the positive energy solutions, we ensure that E_g is the ground state energy for the Hamiltonian. The BdG equations above contain, within the mean field approximation, all possible effects for any value of the magnetic field in the presence or absence of impurities (described by the external potential $U_0(\mathbf{r})$). They are, however, very difficult to solve in the general case. Since the above system of equations is hermitian, the solutions satisfy the orthogonality conditions

$$\begin{aligned} \int d^3r \left[u_n(\mathbf{r})^* u_m(\mathbf{r}) + v_n(\mathbf{r})^* v_m(\mathbf{r})\right] &= \delta_{nm} \\ \int d^3r \left[u_n(\mathbf{r}) v_m(\mathbf{r}) - v_n(\mathbf{r}) u_m(\mathbf{r})\right] &= 0 \end{aligned} \tag{2.9}$$

and the completeness relations

$$\begin{aligned} \sum_n [u_n(\mathbf{r}) u_n(\mathbf{r}')^* + v_n(\mathbf{r})^* v_n(\mathbf{r}')] &= \delta(\mathbf{r}' - \mathbf{r}) \\ \sum_n [u_n(\mathbf{r}) v_n(\mathbf{r}')^* - v_n(\mathbf{r})^* u_n(\mathbf{r}')] &= 0. \end{aligned} \tag{2.10}$$

The self-consistency condition reads

$$\Delta(\mathbf{r}) = g\langle\psi_\uparrow\psi_\downarrow\rangle = g\sum_n v_n(\mathbf{r})^* u_n(\mathbf{r})[1 - f(E_{n\uparrow}) - f(E_{n\downarrow})] \tag{2.11}$$

where $f(E) = 1/[1 + \exp(\beta E)]$ is the Fermi function. The above set of equations serve as a convenient general starting point to investigate superconductors with a spatially varying order parameter in an external potential $U_0(\mathbf{r})$; we will use them throughout the thesis. They can be solved exactly in some special cases and are, in general, well-suited for a numerical calculation. One such case where the BdG equations can be solved analytically, arises when there is no external potential and no magnetic field. One then obtains the well-known solutions $u_{\mathbf{k}}(\mathbf{r}) = u_k e^{i\mathbf{kr}}$ and $v_{\mathbf{k}}(\mathbf{r}) = v_k e^{i\mathbf{kr}}$ with $u_k^2 = \frac{1}{2}(1 + \xi(k)/E(k))$, $v_k^2 = \frac{1}{2}(1 - \xi(k)/E(k))$, $\xi(k) = k^2/2m - \mu_F$

and $E(k) = (\xi^2 + \Delta^2)^{1/2}$ [98]. The order parameter is determined by $1 = \frac{g}{2}\sum_{\mathbf{k}} \tanh(\beta E(k)/2)/E(k)$ (ignoring spin). From here, we recover all the well-known results of the BCS theory for a homogeneous system in no external magnetic field.

2.5 The Partition Function

It is sometimes convenient to solve the problem using standard many-body methods based on Green's functions. This is especially true when we cannot solve the BdG equations exactly but need to do some perturbative calculations. In this case, the Green's function technique is very powerful. Another case where the Green's functions come in useful, is in the calculation of various responses of the superconductor to external probes. The formalism outlined in this section is also a natural starting point if one wants to go beyond mean field theory. We start by noting that the partition function

$$\mathcal{Z} \equiv Tr(e^{-\beta\hat{H}}) \tag{2.12}$$

can be written as a functional integral [80]:

$$\mathcal{Z} = \int_{\psi_\sigma(\mathbf{r},\beta)=-\psi_\sigma(\mathbf{r},0)} \mathcal{D}(\psi^*_\sigma(\mathbf{r},\tau)\psi_\sigma(\mathbf{r},\tau))e^{-\int d^4x\,\mathcal{L}(\mathbf{r},\tau)}. \tag{2.13}$$

Here $\mathcal{D}(\psi^*_\sigma(\mathbf{r},\tau)\psi_\sigma(\mathbf{r},\tau))$ denotes functional integration over the electron fields which are Grassman variables, τ is imaginary time, and $\int d^4x = \int_0^\beta d\tau \int d^3r$. The Lagrangian is given by

$$\mathcal{L}(\mathbf{r},\tau) = \sum_\sigma \psi^*_\sigma(\mathbf{r},\tau)\partial_\tau\psi_\sigma(\mathbf{r},\tau) + H(\psi^*_\sigma(\mathbf{r},\tau),\psi_\sigma(\mathbf{r},\tau)) \tag{2.14}$$

where $H(\psi^*_\sigma(\mathbf{r},\tau),\psi_\sigma(\mathbf{r},\tau))$ is the effective Hamiltonian given by Eq. (2.2). The standard trick to introduce pairing in this formalism is to use the following identity:

$$e^{|a|^2} = \frac{1}{\pi}\int dx\, dx^*\, e^{-(|x|^2+ax^*+a^*x)}. \tag{2.15}$$

The functional form of this identity used to introduce the pairing correlations is written

$$e^{g\int d^4x\, \psi_\uparrow^*\psi_\downarrow^*\psi_\downarrow\psi_\uparrow} = \frac{1}{N}\int \mathcal{D}(\Delta(\mathbf{r},\tau)\Delta(\mathbf{r},\tau)^*)e^{-\int d^4x[|\Delta|^2/g+\Delta^*\psi_\downarrow\psi_\uparrow+\Delta\psi_\uparrow^*\psi_\downarrow^*]}. \tag{2.16}$$

The pairing field $\Delta(\mathbf{r},\tau)$ is complex and it has Bose statistics (i.e. $\Delta(\mathbf{r},\beta) = \Delta(\mathbf{r},0)$). The normalization constant is $\int \mathcal{D}(\Delta\Delta^*)\exp(-\int d^4x\, |\Delta|^2/g)$ and will not be important in the following. Using this identity, the partition function becomes

$$\begin{aligned} \mathcal{Z} &= \int \mathcal{D}(\Delta\Delta^*)\mathcal{Z}(\Delta,\Delta^*) \\ \mathcal{Z}(\Delta,\Delta^*) &= e^{-\int d^4x\,|\Delta|^2/g} \\ &\times \int \mathcal{D}(\psi_\sigma^*\psi_\sigma)e^{-\int d^4x \sum_\sigma[\psi_\sigma^*(\partial_\tau+\mathcal{H}_{0,\sigma})\psi_\sigma+\Delta^*\psi_\downarrow\psi_\uparrow+\Delta\psi_\uparrow^*\psi_\downarrow^*]}. \end{aligned} \tag{2.17}$$

The integral over the electron fields is now Gaussian and can be done analytically. Hence, the introduction of these so-called auxiliary (pairing) fields enables us to integrate out the electronic degrees of freedom and we are left with the collective degrees of freedom described by the pairing field. This method was first used by Stratonovich [103] and Hubbard [59] and is therefore called the Hubbard-Stratonovich transformation. Here, we will approximate the partition function by the saddle point approximation. To do so, one puts

$$\mathcal{Z} \simeq \mathcal{Z}(\tilde{\Delta},\tilde{\Delta}^*) \tag{2.18}$$

where $\tilde{\Delta}(\mathbf{r},\tau)$ is determined by the condition $\delta\ln\mathcal{Z}(\Delta,\Delta^*)/\delta\Delta|_{\tilde{\Delta}} = 0$. This condition gives $\Delta(\mathbf{r}) = g\langle\psi_\uparrow(\mathbf{r})\psi_\downarrow(\mathbf{r})\rangle$ and we recover mean field theory. Mean field theory is therefore equivalent to a saddle point approximation to the partition function. However, the choice of the auxilary fields is largely arbitrary. One could just as well have obtained standard Hartree-Fock theory by another choice of fields. The choice of the auxiliary field should be guided by the physics of the problem which in this case is the pairing interactions. Ignoring spin for the moment and using Wick's theorem for the above quadratic integral, we get:

$$\begin{pmatrix} \partial_\tau + \mathcal{H}_0 & \Delta(\mathbf{r}) \\ \Delta(\mathbf{r})^* & \partial_\tau - \mathcal{H}_0 \end{pmatrix} \begin{pmatrix} \mathcal{G}(\mathbf{r}\tau, \mathbf{r}'\tau') & \mathcal{F}(\mathbf{r}\tau, \mathbf{r}'\tau') \\ \mathcal{F}^\dagger(\mathbf{r}\tau, \mathbf{r}'\tau') & -\mathcal{G}(\mathbf{r}'\tau', \mathbf{r}\tau) \end{pmatrix} = -\delta^4(r - r')\mathbf{1}. \tag{2.19}$$

Here $\delta^4(r-r') = \delta^3(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau')$ and $\mathbf{1}$ is a 2×2 unit matrix. The Green's functions are defined as [42]

$$\begin{aligned} \mathcal{G}(\mathbf{r}\tau, \mathbf{r}'\tau') &\equiv -\langle T_\tau \psi_\uparrow(\mathbf{r}\tau), \psi_\uparrow^\dagger(\mathbf{r}'\tau')\rangle \\ \mathcal{F}(\mathbf{r}\tau, \mathbf{r}'\tau') &\equiv -\langle T_\tau \psi_\uparrow(\mathbf{r}\tau), \psi_\downarrow(\mathbf{r}'\tau')\rangle \\ \mathcal{F}^\dagger(\mathbf{r}\tau, \mathbf{r}'\tau') &\equiv -\langle T_\tau \psi_\downarrow^\dagger(\mathbf{r}\tau), \psi_\uparrow^\dagger(\mathbf{r}'\tau')\rangle. \end{aligned} \tag{2.20}$$

The operator T_τ denotes time-ordering with respect to the argument τ; and $\psi(\tau) \equiv \exp(\mathcal{H}_{mean}\tau/\hbar)\psi\exp(-\mathcal{H}_{mean}\tau/\hbar)$. Eq. (2.19) are the celebrated Gor'kov equations. They are used as a starting point for the treatment of superconductors using Green's functions within the mean-field approach [42]. It is easy to show that they are equivalent to the BdG equations derived in section 2.4. In the case of zero magnetic field and no external potential, these equations can readily be solved. We recover the well known results stated at the end of section 2.4. For a general magnetic field and external potential, the Gor'kov equations cannot be solved exactly. It is then fruitful to return to Eq. (2.18) which, as it stands, is suitable for a perturbative expansion in the order parameter. This expansion will obviously only be valid close to the transition line $H_{c2}(T)$ where the order parameter is small. Such an expansion will form the basis for many of the analytical results presented in this thesis.

2.6 Validity of the Mean Field approximation

Before embarking on developing further the mean field theory for superconductors in high magnetic fields, we will briefly consider the fluctuations away from the mean field approximation. In general, below a certain upper critical dimension d_c, the fluctuations will dominate the behavior of a physical system close to the phase transition lines. The critical dimension for the universality class to which the Ginzburg-Landau theory belongs is $d_c = 4$. Unfortunately, experimental systems tend to have spatial dimensions less then 4! Thus, there will be a region around the phase transition line where mean field theory is invalid. Using simple dimensional analysis, one can show [80, 44] that the temperature region, called the Ginzburg region, in which one expects the mean field theory to begin to break down is determined by

$$\Delta t \equiv |T - T_c|/T = \left(\frac{k_B}{\Delta C \xi^D}\right)^{\frac{2}{4-D}}. \tag{2.21}$$

Here, D is the dimension of the system, ΔC is the discontinuity of the specific heat per unit volume at T_c, and ξ is the correlation length. This expression enables us to understand why mean field theory works so well for normal 3D weak coupling superconductors. Here the correlation length is of the order of the size of a Cooper pair $\xi \sim 10^3$Å and ΔC is several joule/cm^3 [80]. This gives $t \sim 10^{-15}$, which means that mean field theory is valid apart from an unobservably small region around the phase transition line. For high T_c's where $\xi \sim 10$Å or for highly anisotropic or essentially 2D materials, the critical region can be much larger. One can observe several new phases such as "pancake" vortices, entangled, and disentangled vortex liquids [31] in these systems; the theory for this kind of vortex physics is currently being actively investigated [14].

Chapter 3

Superconductivity at high magnetic fields

3.1 Introduction

A superconductor in no external magnetic field and no external potential is characterized by the pairing of electrons with opposite momenta $\mathbf{k}$ and -$\mathbf{k}$[1]. Because the time-reversed states are degenerate in energy, the pairing instability is greatest for this choice of pairing. When a superconductor is subjected to an external magnetic field, the Hamiltonian is no longer real due to the substitution $-i\hbar\nabla \to -i\hbar\nabla + \mathbf{A}e/c$ and the time-reversal symmetry is broken [106]. It is not possible to form a translationally invariant superconducting state. For low external fields, it is useful to think of the external field as "frustrating" the order parameter by inducing currents perpendicular to the field as it couples to the transverse momentum of the electrons. The superconductor sets up screening currents corresponding to a spatially varying order parameter. The response of the superconductor to an external magnetic field can, on the mean-field level, be separated into two cases as mentioned in the introduction. For type-I superconductors, it is energetically

[1]This is not true if the superconductor is in a current carrying state.

favorable below a certain field H_{c1} to expel the external field completely in the bulk of the superconductor. From a microscopic point of view, this arises because the transverse supercurrents induced by the external field screen the field completely in the bulk of the material. Type-II superconductors are different since they allow partial penetration of the magnetic field below an upper critical field H_{c2}. This is energetically favorable due to the fact that the coherence length ξ, which measures the length scale of the variation of the order parameter, is smaller than the penetration depth λ of the magnetic field. By allowing the field to penetrate partially, the superconductor can benefit both from the superconducting condensation energy and from the free energy $-BH/8\pi^2$ associated with a magnetic field. The order parameter becomes nonuniform; it forms the so-called *vortices* of screening currents surrounding nodal lines of the order parameter where the magnetic field is high and the density of the superconducting electrons is low. Each vortex contains a flux quantum $\Phi_0 \equiv hc/2e$ ($h = 2\pi\hbar$). To minimize the energy, the vortices form a regular array. Microscopically, this happens because the Cooper pairs acquire less transverse momentum in the presence of the magnetic field as compared to the type-I case. The screening of the external field is therefore not complete. When the field is lowered below a lower critical field H_{c1}, the currents screen the field completely and the superconductor enters the Meissner state[2]. Using Ginzburg-Landau theory, one can derive the result [107] that for $\kappa \equiv \lambda/\xi > 1/\sqrt{2}$ and $H_{c1} < H < H_{c2}$, the free energy is lowered by allowing a partial penetration of the field; hence the superconductor is of type-II. For $\kappa < 1/\sqrt{2}$ the superconductor is of type-I. The state of the superconductor for $H_{c1} < H < H_{c2}$ is often called the *mixed* state. In Fig. 3.1, we illustrate the phase diagram for the two types of superconductors. In Fig. 3.2, we sketch the structure of an isolated vortex for a type-II superconductor when $\lambda \gg \xi$. Up to the beginning of the 90's, the

[2]This simple picture is only true within mean-field theory where fluctuations of the order parameter are ignored as described in section 2.6.

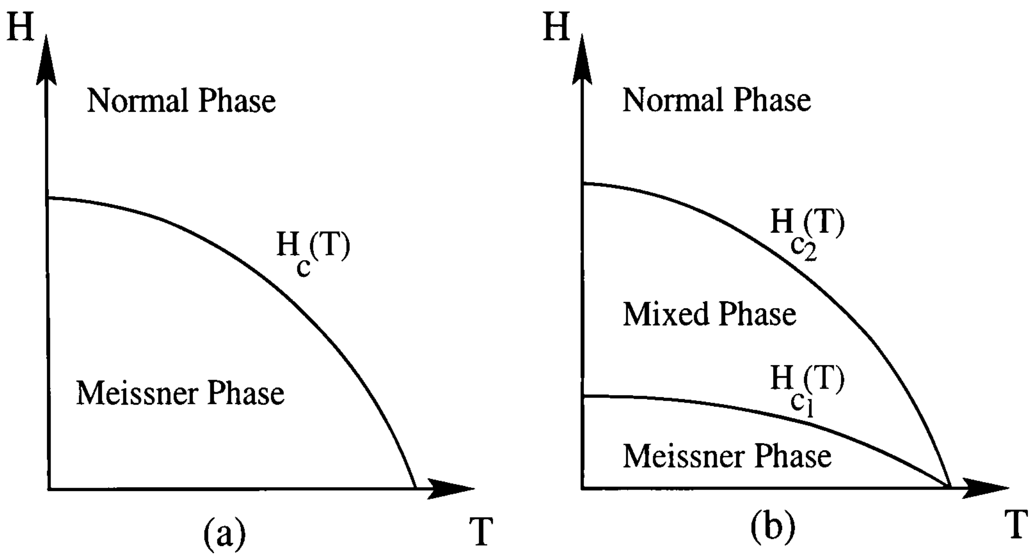


Figure 3.1: The mean-field phase diagrams for type-I (a) and type-II (b) superconductors.

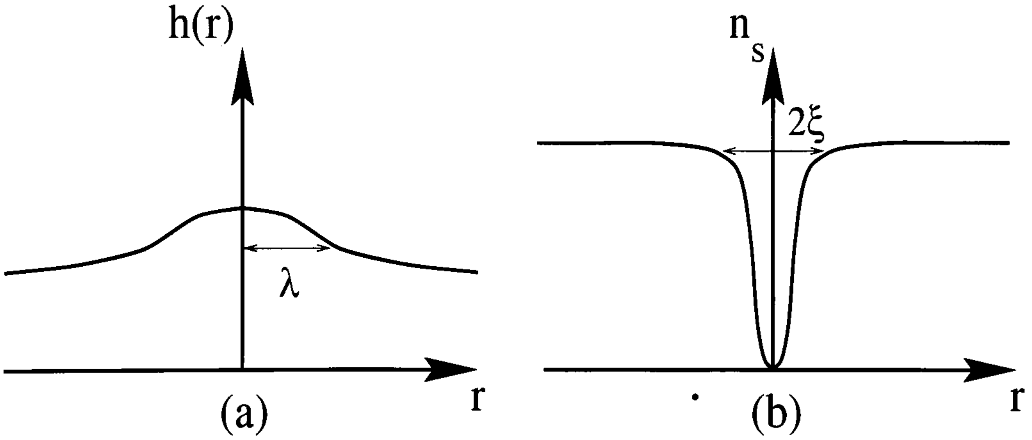


Figure 3.2: Structure of an isolated vortex. (a) The microscopic magnetic field $h(\mathbf{r})$ is maximum at the center of the vortex and decreases going outwards because of the screening from the supercurrents in a region of radius $\sim \lambda$. (b) The density of superconducting electrons n_s is reduced in a core region of radius $\sim \xi$.

effect of a magnetic field on a superconductor was typically described within Ginzburg-Landau theory which is based on a semiclassical approximation for the treatment of the magnetic field [42]. This approximation breaks down if the electron states are not localized and there is a non-zero average field $H = \nabla \times \mathbf{A}$. In this case, $\mathbf{A} \propto L$ where L is the system size; since the electron states are not localized, even a weak magnetic field cannot be treated perturbatively. The discrete nature of the Landau levels become important and the semiclassical approximation breaks down when the temperature is sufficiently low and the material clean enough such that $k_B T \ll \hbar\omega_c$ and $\omega_c/2\pi \gg \tau^{-1}$, where τ is the impurity scattering lifetime.

As large parts of this thesis deal with cases where the semiclassical approximation breaks down, we will in this chapter outline the theoretical formalism developed in order to include the quantum effects of the average magnetic field exactly from the outset. In section 3.2, we consider the problem of two-electron scattering in a high magnetic field. This leads us to a useful splitting of the two particle motion into the center-of-mass (COM) and the relative motion. The symmetries of the vortex lattice will be used in sections 3.3-3.5 to simplify the Hamiltonian and the corresponding BdG equations. We will then examine the solutions of the resultant BdG equations in the limit of a very high magnetic field. The perturbative expansion of the grand canonical potential in $\Delta(\mathbf{r})$ is considered in section 3.7. Again, the use of the symmetries of the system enables us to simplify the problem considerably; the expansion can be expressed as a simple polynomial in a finite set of variables describing the amplitude of Cooper pairing with different COM kinetic energies. Self-consistency reduces in this language to the simple algebraic problem of minimizing this polynomial. The perturbative expansion is then used in section 3.7.4 to examine the transition temperature T_c in different COM kinetic energy channels.

3.2 Two particle scattering in a magnetic field

We start by considering a pair of electrons in a magnetic field. As is well known, free electrons in a constant external magnetic field reside in discrete energy levels (Landau levels) [65]. The presence of the Landau levels gives rise to many interesting phenomena in the theory of normal metals and, as we shall see, in superconductors as well. Since Ginzburg-Landau theory which is based on a semiclassical treatment of the effect of the magnetic field, completely ignores the quantizing effect of the magnetic field, it is necessary to develop a more microscopic formalism to describe these phenomena. Consider an electron moving in a magnetic field $\mathbf{H}$ pointing in the z-direction. In the Landau gauge $\mathbf{A} = (0, Hx, 0)$ which is used throughout the thesis, the eigenstates of the single particle Hamiltonian can be chosen to be [65]

$$\phi_{N,k,k_z}(\mathbf{r}) = \frac{1}{\sqrt{L_y L_z}} e^{-iky} \phi_N\left(\frac{x - kl^2}{l}\right) e^{ik_z z} = \phi_{N,k}(x,y) \frac{e^{ik_z z}}{L_z} \tag{3.1}$$

where $\phi_N(x) = (2^N N! \sqrt{\pi} l)^{-1/2} H_N(x) e^{-\frac{1}{2}x^2}$ with H_N being a Hermite polynomial of order N, and $l^2 = \hbar c/eH$ is the magnetic length squared. The size of the system is $L_x \times L_y \times L_z$. The energy $E_N(k_z)$ of such a state is $E_N(k_z) = \hbar\omega_c(N + 1/2) + \hbar^2 k_z^2/2m$ with $\omega_c = eH/mc$. We have ignored the Zeeman effect for simplicity. Since the energy does not depend on k, each energy level (Landau level) has a degeneracy of $L_x L_y / 2\pi l^2$ for a single spin value. The motion along the z-direction is unaltered by the magnetic field and we will, for notational simplicity, ignore this degree of freedom until chapter 5.

We will treat the case of extreme type-II superconductors ($\kappa \gg 1$), where the magnetic field can to a good approximation be considered as constant in space. The problem of superconductivity in a magnetic field then reduces to the case of pairing between electrons residing in different Landau levels around the Fermi level. Most physical systems such as the high T_c

materials, the organics and the A15 compounds (eg. $NbSe_2$) have $\kappa \gg 1$ making the case of $\kappa \gg 1$ experimentally relevant. A simple two-particle state of non-interacting electrons in two Landau levels can be written as $\psi(\mathbf{r}_1, \mathbf{r}_2) = \phi_{N_1,k_1}(\mathbf{r}_1)\phi_{N_2,k_2}(\mathbf{r}_2)$. The energy of such a state is $(N_1+N_2+1)\hbar\omega_c$. As we are going to consider electrons interacting through the contact potential $-g\delta(\mathbf{r}_1 - \mathbf{r}_2)$ which only depends on the relative coordinate between the electrons, it is convenient to move to a picture describing the two particle state in terms of center-of-mass (COM) and relative coordinates. This transformation, which of course is trivial in the case of zero external field, was given by MacDonald *et al.* [67] in the case of electrons in an external magnetic field. It reads

$$\phi_{N_1,K+k/2}(\mathbf{r}_1)\phi_{N_1,K-k/2}(\mathbf{r}_2) = \sum_{j=0}^{N_1+N_2} B_j^{N_1,N_2} \phi^R_{j,K}(\mathbf{R})\phi^r_{N_1+N_2-j,k}(\mathbf{r}) \tag{3.2}$$

where $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ are the COM and relative coordinates respectively. The expressions for the COM and relative wave functions are identical to Eq. (3.1) except that the magnetic lengths are $l^R = l/\sqrt{2}$ and $l^r = \sqrt{2}l$. The coefficients $B_j^{N_1,N_2}$ are given by

$$\begin{aligned} B_j^{N,M} &= \left(\frac{j!(N+M-j)!N!M!}{2^{N+M}}\right)^{1/2} \times \\ &\sum_{m=\max(0,j-N)}^{\min(j,M)} \frac{(-1)^{M-m}}{(j-m)!(N+m-j)!(M-m)!m!} \end{aligned} \tag{3.3}$$

The coefficients give the amplitude for having kinetic energy $\hbar\omega_c(j+1/2)$ in the COM motion and $\hbar\omega_c(N_1+N_2-j+1/2)$ in the relative motion.

Superconductivity is, as pointed out by Cooper [28], associated with an instability with respect to pair formation due to the attractive interaction between the electrons. One way to examine this instability is to consider the scattering of two electrons interacting via the attractive effective interaction in the presence of the Fermi sea. To derive an expression for the critical temperature in high magnetic fields, MacDonald *et al.* [67] looked at the scattering of two electrons residing in the electron states $|\phi_{N_1,K+k/2}\rangle$ and $|\phi_{N_2,K-k/2}\rangle$, into the states $|\phi_{N_1',K+k'/2}\rangle$ and $|\phi_{N_2',K-k'/2}\rangle$ in the ladder approximation. The instability towards pair formation manifests itself as a divergence of the particle-particle ladder graphs for the electron-electron scattering amplitude [98]. Since the interaction only depends on the relative coordinate and hence is diagonal in the COM energy, it turns out that the scattering amplitude separates into different channels corresponding to different values of the conserved COM kinetic energy. The critical temperature T_c for the channel with the lowest COM kinetic energy has the highest T_c when more than one Landau level is occupied[94, 68]. We will return in more detail to this point in section 3.7.4. The main conclusion one can draw from the analysis above is that the superconducting pairing can be separated into instabilities at different COM kinetic energies. Since T_c is highest for the minimum COM kinetic energy, it is to be expected that the superconducting order parameter will mainly be formed by Cooper pairs with minimum COM kinetic energy.

3.3 Symmetries

In order to set up an appropriate theory for a physical problem, it is always prudent to take advantage of the symmetries of the problem. In the present case, the relevant symmetries are described by the magnetic translation group [115]. The relevant property of this group for the present problem is that the single-particle Hamiltonian for an electron in a uniform magnetic field does *not* commute with the ordinary translation operator perpendicular to the applied field, since the vector potential $\mathbf{A}$ depends on $\mathbf{r}$. Instead, it commutes with an operator that translates and gauge transforms. Denoting $\mathcal{T}g_{\Delta x}$ as the operator which translates by Δx

and gauge transforms in the x-direction (and likewise for the y-direction), we have $[\mathcal{H}_0, \mathcal{T}g_{\Delta x}] = [\mathcal{H}_0, \mathcal{T}g_{\Delta y}] = 0$. It is then natural to look for single particle eigenfunctions of $\mathcal{H}_0$ which obey this symmetry. However, since $[\mathcal{T}g_{\Delta x}, \mathcal{T}g_{\Delta y}] = 0$ only when $\Delta x \Delta y = nhc/eH = n2\Phi_0/H$ (n is an integer), we cannot find eigenfunctions of $\mathcal{H}_0$ which are also eigenfunctions for $\mathcal{T}g_{\Delta x}$ and $\mathcal{T}g_{\Delta y}$ for general Δx and Δy. Instead, we can look for eigenfunctions of $\mathcal{T}g_{\Delta x=a_x}$ and $\mathcal{T}g_{\Delta y=2\pi l^2/a_x}$ since then $\Delta x \Delta y = nhc/eH = 2\Phi_0/H$. This constraint gives rise to the Aharanov-Bohm effect [2]. In the superconducting case, the above symmetry properties can be directly generalized to the case of the Gor'kov equations [94]. One obtains from the symmetry properties of the Gor'kov equations that the order parameter can only be an eigenfunction of both $\mathcal{T}g_{\Delta x}$ and $\mathcal{T}g_{\Delta y}$ if $\Delta x \Delta y = nhc/2eH = n\Phi_0/H$. This leads directly to the famous flux quantization condition, i.e. the fact that each vortex must inclose an integer number of Φ_0.

3.4 The vortex lattice Hamiltonian

Experimentally, one observes that the vortices formed in the mixed state form a regular array; i.e. the vortex lattice[3]. On the mean-field level, this configuration of the vortices comes from the fact that the superconductor is minimizing the free energy. Within Ginzburg-Landau theory, one can show [1] that this minimization leads to a regular array of the vortices. It turns out that the symmetry of the lattice that gives the lowest free energy is triangular [107]. The same conclusion for the order parameter is reached within the more microscopic BCS theory as we will describe in section 3.5. Thus, one expects that in order to develop a theory for type-II superconductors in the mixed state, it will be beneficial to use a set of basis states which obey the appropriate symmetries of the magnetic translation group

[3]Again, we disregard systems for which the region in phase-space where fluctuations are dominant is large.

such that the vortex lattice can readily be formed. Furthermore, from section 3.2, we must expect the condensation of the electrons into different COM kinetic energy channels to emerge from the theory as well. A convenient set of orthogonal basis states which has the desired symmetry properties, was introduced by Norman *et al.* [84]:

$$\phi_{N\mathbf{k}}(\mathbf{r}) = \sqrt{\frac{a_x}{L_x}} \sum_t e^{ik_x a_x t} e^{i\pi t^2/4} \phi_{N,-k_y+ta_x/l^2}(\mathbf{r}). \tag{3.4}$$

The magnetic Brillouin zone (MBZ) is defined by $\mathbf{k} = (k_x, k_y)$ where $k_x \in [0, \frac{2\pi}{a_x}[$ with $\Delta k_x = \frac{2\pi}{L_x}$ and $k_y \in [0, a_x/l^2[$ with $\Delta k_y = \frac{2\pi}{L_y}$. The advantage of using this set of basis functions becomes apparent once we assume that the order parameter has the following translational-gauge transformation symmetries:

$$\begin{aligned} \Delta(x, y + a_y) &= \Delta(x, y) \\ e^{2ia_x(y+a_y/2)/l^2} \Delta(x + a_x, y + a_y/2) &= e^{i\pi/2} \Delta(x, y). \end{aligned} \tag{3.5}$$

with $a_y \equiv \pi l^2/a_x$. This symmetry, combined with the symmetry properties of the basis states defined in Eq. (3.4), results in the following selection rule:

$$\int d^3r\, \Delta(\mathbf{r}) \phi^*_{M\mathbf{k}}(\mathbf{r}) \phi^*_{N\mathbf{k}'}(\mathbf{r}) \propto \delta_{\mathbf{k},-\mathbf{k}'}. \tag{3.6}$$

This selection rule states that the pairing of electrons in the single particle states defined in Eq. (3.4), is restricted to pairs with opposite quantum numbers $\mathbf{k}$ and -$\mathbf{k}$. Equation (3.5) implies that $|\Delta(\mathbf{r})|$ forms a vortex lattice. The selection rule given in Eq. (3.6) simplifies both the subsequent numerical and analytical analysis significantly, since we can now treat the pairing problem for each $\mathbf{k}$ independently. In the $\phi_{N\mathbf{k}}(\mathbf{r})$ basis, the mean-field Hamiltonian with the assumed translationally symmetric order parameter becomes:

$$\begin{aligned}
\hat{H}_{mean} &= \hat{H}_0 + \hat{H}_1 \\
\hat{H}_0 &= \sum_{\sigma} \int d^3r\, \psi_\sigma^\dagger(\mathbf{r}) \mathcal{H}_{0,\sigma} \psi_\sigma(\mathbf{r}) \\
\hat{H}_1 &= \sum_{\substack{NM \\ \mathbf{k}}} \int d\mathbf{r}\, [\Delta(\mathbf{r}) w(N) w(M) \phi^*_{M\mathbf{k}}(\mathbf{r}) \phi^*_{N-\mathbf{k}}(\mathbf{r}) \hat{a}^\dagger_{M\mathbf{k}\uparrow} \hat{a}^\dagger_{N-\mathbf{k}\downarrow} \\
&\quad + c.c.].
\end{aligned} \tag{3.7}$$

Note that this Hamiltonian explicitly shows that pairing only arises between electrons with vectors **k** and -**k**. This, of course, is a direct consequence of the assumed vortex lattice symmetry. There is another new feature in the Hamiltonian as compared to the conventional BCS-Hamiltonian: we have introduced some the functions $w(N)$. These weight functions are introduced to get a smoother and hence more physically realistic cut-off in the pairing interaction around the Fermi level. This is achieved using a model where the pairing interaction between Landau levels N and M is scaled by $W(N)W(M)$ as in Eq. (3.7). The weight function is chosen to be Gaussian, i.e. $w(N) \propto e^{-(\xi_N/0.5\hbar\omega_D)^2}$ where ω_D is the pairing width and $\xi_N = (N+1/2)\hbar\omega_c - \mu_F$. This slight generalisation of the BCS Hamiltonian was introduced by Norman *et al.* [84], although they used a different weight function. The order parameter is now defined as

$$\Delta(\mathbf{r}) \equiv g \sum_{\substack{NM \\ \mathbf{k}}} w(N) w(M) \phi_{N\mathbf{k}}(\mathbf{r}) \phi_{M-\mathbf{k}}(\mathbf{r}) \langle a_{N\mathbf{k}\uparrow} a_{M-\mathbf{k}\downarrow} \rangle. \tag{3.8}$$

This definition of the order parameter differs from Eq. (2.5) through the presence of the weight functions. It is important to introduce this redefinition once the weight functions are introduced; otherwise the self-consistency condition will *not* be equivalent to minimizing the thermodynamic potential within the subset of density operators described by $\hat{H}_{mean}$ as mentioned in section (2.3) or to the saddle point approximation of the partition function as described in section (2.5). Also, it is easily checked that $\phi_{N\mathbf{k}}(\mathbf{r})\phi_{M-\mathbf{k}}(\mathbf{r})$ has the right symmetry properties as defined in Eq. (3.5). This means that the assumed symmetry of $\Delta(\mathbf{r})$ is self-consistent since the corresponding selection rule leads to a pairing with the right symmetry.

3.5 The Bogoliubov de-Gennes equations in a magnetic field

In this section, we will expand the BdG equations in the basis set $\phi_{N\mathbf{k}}(\mathbf{r})$ introduced in Eq. (3.4). The idea is to use the symmetry properties of the vortex lattice to write the BdG equations in as simple a form as possible. This will facilitate subsequent numerical and analytical analysis significantly.

As shown in section 3.4, the advantage of using this basis set is that in the presence of the vortex lattice we only have pairing between states with magnetic momenta $\mathbf{k}$ and $-\mathbf{k}$. Thus, the BdG equations split into a set of equations for each $\mathbf{k}$. Expanding the Bogoliubov wave functions for a given $\mathbf{k}$ as $u^{\eta}_{\mathbf{k}}(\mathbf{r}) = \sum_N u^{\eta}_{N\mathbf{k}}\phi_{N\mathbf{k}}(\mathbf{r})$ and $v^{\eta}_{\mathbf{k}}(\mathbf{r}) = \sum_N v^{\eta}_{N\mathbf{k}}\phi^*_{N-\mathbf{k}}(\mathbf{r})$, the BdG equations defined in section 2.4 for the Hamiltonian given by Eq. (2.4) become [84]:

$$
\begin{aligned}
(\xi_N - E^{\eta}_{\mathbf{k}})u^{\eta}_{N\mathbf{k}} + \sum_M F_{\mathbf{k}NM}v^{\eta}_{M\mathbf{k}} &= 0 \\
(-\xi_N - E^{\eta}_{\mathbf{k}})v^{\eta}_{N\mathbf{k}} + \sum_M F^*_{\mathbf{k}MN}u^{\eta}_{M\mathbf{k}} &= 0 \quad .
\end{aligned}
\tag{3.9}
$$

where $E^{\eta}_{\mathbf{k}}$ is the the quasiparticle energy corresponding to the Bogoliubov wave functions $u^{\eta}_{\mathbf{k}}(\mathbf{r})$ and $v^{\eta}_{\mathbf{k}}(\mathbf{r})$. We have defined $\xi_N \equiv (N + 1/2)\hbar\omega_c - \mu_F$. Using the inverse of the unitary transformation given in Eq. (2.6), i.e. $a_{N\mathbf{k}\uparrow} = \sum_\eta [u^{\eta}_{N\mathbf{k}}\gamma^{\eta}_{\mathbf{k}\uparrow} - v^{\eta}_{N-\mathbf{k}}{}^*\gamma^{\eta}{}^{\dagger}_{-\mathbf{k}\downarrow}]$ and $a_{N-\mathbf{k}\downarrow} = \sum_\eta [u^{\eta}_{N-\mathbf{k}}\gamma^{\eta}_{-\mathbf{k}\downarrow} + v^{\eta}_{N\mathbf{k}}{}^*\gamma^{\eta}{}^{\dagger}_{\mathbf{k}\uparrow}]$, we obtain from Eq. (3.8):

$$\Delta(\mathbf{r}) = \frac{g a_x}{\sqrt{L_y l L_x}} \sum_j \Delta_j \sum_t e^{it^2\pi/2} \phi_{j,\sqrt{2}ta_x/l^2}(\sqrt{2}\mathbf{r}). \tag{3.10}$$

The self-consistency arises through the parameters Δ_j which are determined via the solutions to the BdG equations:

$$\Delta_j = \sum_{\mathbf{k}\eta}[1 - f(E^\eta_{\mathbf{k}\uparrow}) - f(E^\eta_{\mathbf{k}\downarrow})] \sum_{NM} B_j^{NM} w(N) w(M) u^\eta_{\mathbf{k}N} v^{\eta *}_{\mathbf{k}M} \chi^*_{N+M-j}(\mathbf{k}) \tag{3.11}$$

with $E^\eta_{\mathbf{k}\sigma} = E^\eta_{\mathbf{k}} + g^* \mu_B H \sigma/2$. Here

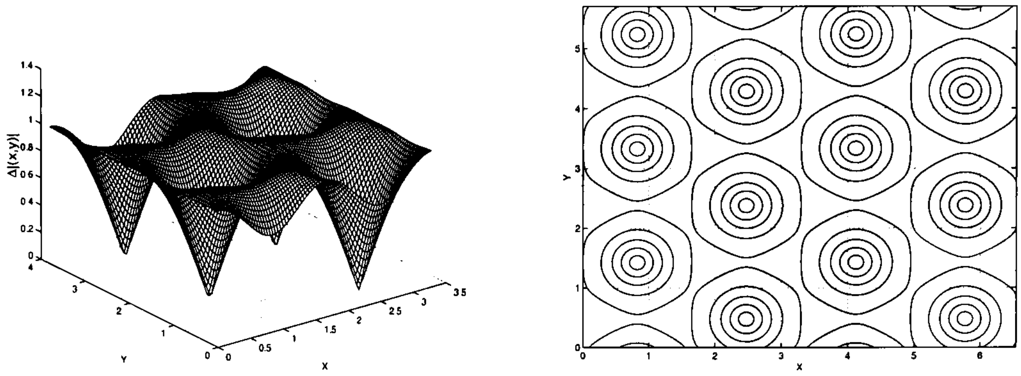
$$\chi_j(\mathbf{k}) = \sqrt{l} \sum_t e^{2ik_x a_x t} e^{-it^2\pi/2} \phi_j[\sqrt{2}(k_y l + t a_x/l)]. \tag{3.12}$$

The appearance of the weight functions $w(N)$ in this formula is a direct result of the redefinition of the order parameter in Eq. (3.8). The matrix element $F_{\mathbf{k}NM}$ which is the $\mathbf{k}$-dependent pairing self-energy in the Landau level representation, is given by:

$$F_{\mathbf{k}NM} = \frac{g a_x}{\sqrt{2 L_x L_y l}} \sum_{j=0}^{N+M} B_j^{NM} \Delta_j \chi_{N+M-j}(\mathbf{k}). \tag{3.13}$$

Thus, by using the symmetry of the vortex lattice, we have split the BdG equations into a set of equations for each magnetic momentum $\mathbf{k}$ in the MBZ. These equations are however still linked through the self-consistent determination of the order parameter which contains contributions from all $\mathbf{k}$, as can be seen from Eq. (3.11). For each $\mathbf{k}$, the BdG equations describe the problem of pairing of electrons in the same and in different Landau levels. The sums over the Landau levels are restricted to levels within ω_D of the Fermi level and each level is weighted by a factor $w(N)$. So the problem of describing a weak coupling extreme type-II superconductor in a strong external magnetic field can be reduced to that of a $2N_L \times 2N_L$ matrix diagonalization for each $\mathbf{k}$, with N_L being the number of Landau levels within the pairing width. Another major advantage of using the symmetry of the vortex lattice is that the order parameter is given by a finite set of parameters Δ_j where $0 \leq j \leq 2N_{max}$, with N_{max} being the highest Landau level participating in the pairing. So within this formalism, self-consistency has been reduced to the determination of this set of parameters. The Δ_j's give the amplitude for electron pairing with COM kinetic energy $(j+1/2)\hbar\omega_c$ thus linking up with the remarks in section 3.2. They are also directly related to the Landau level expansion of the Ginzburg-Landau order parameter[34, 107] as can be seen directly from Eq. (3.10). The Landau level functions in the expansion given in Eq. (3.10) correspond to a magnetic length of $l/\sqrt{2}$. This suggests that the order parameter can be described as being formed by electron pairs of charge $2e$ residing in "bosonic Landau levels". However, such language, which is used by some authors[92], is somewhat misleading as one in general cannot regard the Cooper pairs as bosons as emphasized in section 2.3. From Ginzburg-Landau theory, we know that near the phase transition line $H_{c2}(T)$ the order parameter is very well described by only the lowest Landau level wave function. Therefore, we conclude that close to $H_{c2}(T)$ we have $\Delta_0 \gg \Delta_{j\neq 0}$. However, deeper into the mixed state, we must expect that many Δ_j's contribute to the order parameter.

Up till now, we have not specified the value of a_x which was introduced in Eq. (3.4). Varying this free parameter corresponds to changing the translational symmetry of the vortex lattice. For instance, for $a_x = (\sqrt{3}\pi/2)^{1/2}l$, the lattice has triangular symmetry; for $a_x = \sqrt{\pi/2}l$ the order parameter forms a square lattice. Thus, a_x determines the geometry of the vortex lattice. From Ginzburg-Landau theory, we expect [107] that the triangular lattice gives the lowest value of the grand canonical potential. Within the more microscopic theory outlined in this chapter, the only way to decide which symmetry is the correct one is to evaluate the grand potential for each solution with a



(a) (b)

Figure 3.3: The triangular vortex lattice. The size $|\Delta(\mathbf{r})|$ of the order parameter is depicted in Fig. (a) as a 3D plot, whereas Fig. (b) shows the same in terms of a contour plot to highlight the triangular symmetry. The centers of the concentric circles are the zeroes of the order parameter.

given symmetry. The configuration of the vortices which gives the lowest energy is then the correct one. The energy for various vortex lattices has been calculated both by the present author [19] and by Norman *et al.* [84]. In every calculation, it has turned out that the triangular vortex lattice gives the lowest energy in agreement with Ginzburg-Landau theory. So for the rest of this thesis, we will work with a triangular vortex lattice corresponding to $a_x = (\sqrt{3}\pi/2)^{1/2} l$. The triangular lattice has six-fold rotational symmetry in addition to the translational symmetry. This additional symmetry introduces even more simplifications in the algebra. It can be shown [84, 19] that one need only consider the $\mathbf{k}$'s in an irreducible triangle defined by a triangle with vertices $\Gamma = (a_y/4, a_x/2)$, $M = (3a_y/4, a_x/2)$ and $K = (3a_y/4, a_x/6)$. The area of this triangle is 1/24 of the area of the full MBZ. Also, Ryan and Rajagopal have shown [94] that for a triangular symmetry, Δ_j is different from zero only for $j = 0, 6, 12 \ldots$. The triangular vortex lattice, given by Eq. (3.10) with $a_x = (\sqrt{3}\pi/2)^{1/2} l$ and only $\Delta_0 \neq 0$, is plotted in Fig. 3.3.

An important property of the formalism stated above is the presence of the zeroes in $\Delta(\mathbf{r})$. When we have triangular symmetry, it is easy to show that

$$\Delta(\mathbf{r}) = 0 \quad \text{for} \quad \mathbf{r} = (-a_x/2, a_y/4) + n_1\mathbf{R_1} + n_2\mathbf{R_2} \tag{3.14}$$

where n_1 and n_2 are integers and $\mathbf{R_1} = (0, a_y)$ and $\mathbf{R_2} = (a_x, a_y/2)$ are vectors spanning the vortex lattice. These zeroes constitute the centers of the vortices as illustrated in Fig. 3.3. As can be seen from Eqs. (3.10) and (3.12), the expressions for $\Delta(\mathbf{r})$ and $\mathcal{X}(\mathbf{k})$ are very similar. It is therefore not surprising that there is a direct link between the zeroes of the order parameter in real space and the zeroes of $\mathcal{X}(\mathbf{k})$ and thus the $\mathbf{k}$-dependent pairing self-energy $F_{\mathbf{k}NM}$. Specifically, we have:

$$\mathcal{X}_j(\mathbf{k}) = 0 \quad \text{for} \quad \mathbf{k} = (a_y/4l^2, a_x/2l^2) + n_1\mathbf{K_1} + n_2\mathbf{K_2} \tag{3.15}$$

where $\mathbf{K_1} = a_y/l^2$ and $\mathbf{K_2} = a_x/l^2$. These zeroes of the pairing self-energies have important consequences for various thermodynamic and transport properties as will be discussed in chapter 5.

Once a self-consistent solution to the BdG equations is obtained, one can of course calculate various thermodynamic quantities and also a number of transport coefficients within the linear response approximation. As we have seen, the assumed symmetry of the order parameter makes it much easier to find such a solution. In the language of section 2.3 and section 2.5, one can say that finding self-consistent solutions to the BdG equations assuming a regular vortex lattice corresponds to minimizing the grand potential within the mean-field approximation, using only a subset of density operators $\hat{\rho}$ describing systems with translational (and rotational) symmetry. This requirement on the functional form of $\Delta(\mathbf{r})$, which is formed by products of single particle states, restricts the electrons to form pairs of opposite magnetic momenta $\mathbf{k}$ and $-\mathbf{k}$. We end up with a set of functions $\Delta(\mathbf{r})$ which can be characterized by a finite discrete set of parameters Δ_j. Again, the assumption that the triangular symmetry gives the *global* minimum for the mean-field approximation to the grand potential is based both on Ginzburg-Landau theory and on several calculations for various a_x using the formalism outlined above.

3.6 Solutions at a very high magnetic field

3.6.1 The quantum limit

The BdG equations take a particularly simple form when we are in the quantum limit (QL). The quantum limit is defined as the case of high magnetic fields and/or low electron densities, such that all the electrons reside in the lowest $N = 0$ Landau level. In 2D, this limit is achieved for external fields H and densities n_σ such that $eH/2\pi\hbar c \geq n_\sigma$ where $n_\sigma = N_\sigma/L_xL_y$ is the density of electrons with spin σ. In this section, we will treat this limit to gain some feeling for the formalism developed in section (3.5). Also, some of the results from the QL will be used later as a starting point for the development of analytical theories. In the QL, Eq. (3.9) reduces to a simple 2×2 matrix for each $\mathbf{k}$ which can be solved analytically [3, 37, 81, 94]. The quasiparticle energy is

$$E_{\mathbf{k}}^{N} = \sqrt{\xi_N^2 + |F_{\mathbf{k}NN}|^2} \tag{3.16}$$

and the corresponding Bogoliubov functions are given by

$$\left.\begin{array}{l} |U_{\mathbf{k}}^{N}(\mathbf{r})|^2 \\ |V_{\mathbf{k}}^{N}(\mathbf{r})|^2 \end{array}\right\} = \frac{1}{2}\left(1 \pm \frac{\xi_N}{E_{\mathbf{k}}^{N}}\right)|\phi_{N\pm\mathbf{k}}(\mathbf{r})|^2. \tag{3.17}$$

Here, we have $N = 0$ since the electrons are confined to the lowest Landau level. This solution looks very much like the normal BCS solution in zero external magnetic field [107]. The Cooper pairs are formed by electrons in states of opposite magnetic momenta. However, contrary to the $H = 0$ case, these states are not related by a time-reversal operation, since time-reversal symmetry does not exist for $H \neq 0$. More importantly, the energy gap $\Delta(\mathbf{k}) \equiv |F_{\mathbf{k}00}|$ is no longer constant but depends on the magnetic momentum $\mathbf{k}$. Significantly, as $\Delta(\mathbf{k}) \propto \chi_0(\mathbf{k})$, we get gapless superconductivity for the points defined by Eq. (3.15). The consequence of such gapless points will be considered in chapter 5. The above solution can in some ways be considered as a simple limit in which to study superconductivity in high magnetic fields. The corresponding critical temperature turns out to be an *increasing* function of the magnetic field [104]. This behaviour is a direct consequence of the increased degeneracy of the Landau level with increasing magnetic field. Based on these results, Tešanović *et al.* [92] proposed the existence of a new superconducting state for very high magnetic fields. This state could possibly exist *without* the system being superconducting for $H = 0$, the idea simply being that the increasing degeneracy of the lowest Landau level makes the system unstable towards the formation of Cooper pairs. However, there has been some debate whether a superconducting state in such high magnetic fields is physically reasonable [82, 93, 97, 105] and there is still no experimental verification of such a state.

3.6.2 The quantum limit approximation

The QL solution has also served as an inspiration to obtain approximate solutions for the BdG equations in the general case, when several Landau levels participate in the pairing. It is then tempting to assume that when we are close to the transition line, such that the matrix elements in Eq. (3.9) are sufficiently small ($\hbar\omega_c \gg |F_{\mathbf{k}NM}|$), the Cooper pairs are only formed by electrons belonging to the same Landau level. Hence, one ignores all off-diagonal terms in Eq. (3.9) which is equivalent to setting $F_{\mathbf{k}NM} \propto \delta_{NM}$. The solution of the BdG equations then again reduces to the diagonalization of a 2×2 matrix for each $\mathbf{k}$ in each Landau level. The solution is given by Eq. (3.16) and (3.17) where N is now the index of a Landau level within the pairing width. This approximation which is called the quantum limit approximation (QLA), has formed the basis of several calculations [24, 37, 38, 40, 92]. However, one has to be careful when using this approximation. This is most apparent in 2D when the chemical potential μ_F is either at a Landau level such that $n_F = \frac{\mu_F}{\hbar\omega_c} - 1/2 = n$ (n integer)or exactly between two Landau levels ($n_F = n + 1/2$). For $n_F = n$, we have exact degeneracy between an electron in a Landau level $n_F + m$ and a hole in the level $n_F - m$, i.e. $\xi_{n_F+m} = -\xi_{n_F-m}$; for $n_F = n + 1/2$, we have $\xi_{n_F+m+1/2} = -\xi_{n_F-m-1/2}$. A major effect of the self-consistent pairing field is then to mix these two degenerate excitations strongly. The Cooper pairs are mainly formed by mixing the hole level with Landau level index $n = n_F - m$ (or $n_F - m - 1/2$) and an electron in the Landau level $n_F + m$ (or $n_F + m + 1/2$). This mixing is caused by the off-diagonal matrix element $F_{\mathbf{k}n_F+m,n_F-m}$ (or $F_{\mathbf{k}n_F+m+1/2,n_F-m-1/2}$) and the diagonal approximation is clearly invalid.

3.7 The Gor'kov expansion of the grand canonical potential

3.7.1 The expansion

In much of this thesis, we will be calculating various properties of the mixed state very close to the phase transition line $H_{c2}(T)$. Since the order parameter is small close to H_{c2}, it is natural to use a perturbation theory in $\Delta(\mathbf{r})$ as a basis for analytical calculations. The formalism outlined in section 2.5 provides a natural starting point for such a theory. The grand canonical potential is given by $\Omega = -k_B T \ln(\mathcal{Z})$ [80]. From Eq. (2.18), we know that within the mean-field approximation the partition function for a system with the Hamiltonian of Eq. (3.7) can be written as:

$$\begin{aligned}
\mathcal{Z}_S &= \int \mathcal{D}(\psi_\sigma^* \psi_\sigma) e^{-\int d^4x \sum_\sigma [\psi_\sigma^*(\partial_\tau + \mathcal{H}_{0,\sigma})\psi_\sigma + \Delta^* \tilde{\psi}_\downarrow \tilde{\psi}_\uparrow + \Delta \tilde{\psi}_\uparrow^* \tilde{\psi}_\downarrow^* + |\Delta|^2/g]} \\
&= \mathcal{Z}_0 e^{-\int d^4x |\Delta|^2/g} \langle e^{-\int d^4x [\Delta^* \tilde{\psi}_\downarrow \tilde{\psi}_\uparrow + \Delta \tilde{\psi}_\uparrow^* \tilde{\psi}_\downarrow^*]} \rangle_0 . \qquad (3.18)
\end{aligned}$$

Here $\mathcal{Z}_0 = Tr(e^{-\beta \hat{H}_0})$ and the thermal average of an operator in the non-interacting system is written

$$\langle \hat{O} \rangle_0 \equiv Tr(e^{-\beta \hat{H}_0} \hat{O}) / \mathcal{Z}_0 . \qquad (3.19)$$

Owing to the presence of the weight functions in Eq. (3.7), we have introduced the modified field operator:

$$\tilde{\psi}_\sigma(\mathbf{r}) \equiv \sum_{N,\mathbf{k}} w(N) \phi_{N,\mathbf{k}}(\mathbf{r}) \hat{a}_{N,\mathbf{k}\sigma} \qquad (3.20)$$

where $\hat{a}^+_{N,\mathbf{k}\sigma}$ creates a particle in the state of spin σ and wave function $\phi(\mathbf{r})_{N\mathbf{k}}$. A perturbation theory in $\Delta(\mathbf{r})$ could be obtained by expanding the exponentials in Eq. (3.18) in a power series. However, it turns out that it is much more convenient to expand the grand canonical potential $\Omega_S = -k_B T \ln(\mathcal{Z}_S)$ since it follows from the linked cluster theorem, that we then only have to consider a subset of the perturbation terms; these are the so-called connected graphs [80]:

$$\Omega_S - \Omega_N = -k_B T \sum (\text{all connected graphs}) \qquad (3.21)$$

where $\Omega_N = -k_B T \ln \mathcal{Z}_0$. In that way we obtain to fourth order in the order parameter:

$$\Omega_S - \Omega_N = \Omega_2 + \Omega_4 \qquad (3.22)$$

where

$$\Omega_2 = \frac{1}{g}\int d^2r\,|\Delta(\mathbf{r})|^2 - \frac{1}{\beta}\int d^2r_1 d^2r_2\,\Delta(\mathbf{r}_1)\Delta^*(\mathbf{r}_2)K_2(\mathbf{r}_1,\mathbf{r}_2) \tag{3.23}$$

$$\Omega_4 = \frac{1}{2\beta}\int d^2r_1\ldots d^2r_4\,K_4(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)\Delta(\mathbf{r}_1)\Delta(\mathbf{r}_2)\Delta^*(\mathbf{r}_3)\Delta^*(\mathbf{r}_4). \tag{3.24}$$

The kernels are given by [23]:

$$\begin{aligned} K_2(\mathbf{r}_1,\mathbf{r}_2) &= \frac{1}{\hbar^2}\sum_\nu \tilde{\mathcal{G}}^0_\uparrow(\mathbf{r}_2,\mathbf{r}_1,-\omega_\nu)\tilde{\mathcal{G}}^0_\downarrow(\mathbf{r}_2,\mathbf{r}_1,\omega_\nu) \\ K_4(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4) &= \frac{1}{\hbar^4}\sum_\nu \tilde{\mathcal{G}}^0_\downarrow(\mathbf{r}_4,\mathbf{r}_1,\omega_\nu)\tilde{\mathcal{G}}^0_\uparrow(\mathbf{r}_3,\mathbf{r}_1,-\omega_\nu) \\ &\times\; \tilde{\mathcal{G}}^0_\downarrow(\mathbf{r}_3,\mathbf{r}_2,\omega_\nu)\tilde{\mathcal{G}}^0_\uparrow(\mathbf{r}_4,\mathbf{r}_2,-\omega_\nu) \end{aligned} \tag{3.25}$$

where $\omega_\nu = (2\nu+1)\pi k_B T/\hbar$ (ν integer) are the fermionic Matsubara frequencies. Because we are using a smooth pairing cutoff in our Hamiltonian, we have instead of the Green's function for the normal state $\mathcal{G}^0_\sigma(\mathbf{r}_2,\mathbf{r}_1,\omega_\nu)$, the following function in our kernels:

$$\tilde{\mathcal{G}}^0_\sigma(\mathbf{r}_2,\mathbf{r}_1,\omega_\nu) = \sum_{N\mathbf{k}} \frac{\phi_{N\mathbf{k}}(\mathbf{r}_2)\phi^*_{N\mathbf{k}}(\mathbf{r}_1)}{i\omega_\nu - \xi_{N\sigma}/\hbar} w^2(N) \tag{3.26}$$

with $\xi_{n\sigma} = \xi_n + g^*\sigma\hbar\omega_c\frac{m}{4m_0}$. The appropriate Feynman graphs for Ω_S are presented in Fig. (3.4).

Equations (3.22)-(3.25) represent the desired perturbation expansion of the grand canonical potential in the size of the order parameter. It is often called the Gor'kov expansion since it was derived by Gor'kov in his microscopic derivation of the Ginzburg-Landau theory [47]. We expect this expansion to give a good description of the mixed state close to H_{c2} where $\Delta(\mathbf{r})$ is small. In chapter 6, We will examine when this perturbation series in $\Delta(\mathbf{r})$ is

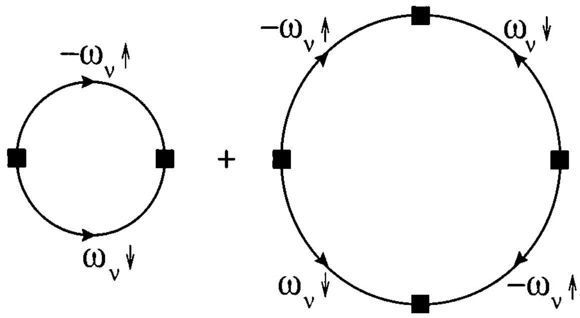


Figure 3.4: The contributions to Ω_S to fourth order. The arrowed lines are the electron propagators with a given Matsubara frequency and spin. The filled squares with outgoing and incoming arrows are the $\Delta(\mathbf{r})$ and $\Delta^*(\mathbf{r})$ respectively.

convergent. It turns out to be a high temperature expansion with the small parameter essentially being $\Delta(\mathbf{r})/k_B T$.

3.7.2 Self-consistency and minimization of Ω_S

In the formalism outlined in section (3.7.1), nothing has been said about how to determine the size and form of the order parameter $\Delta(\mathbf{r})$. All that is given is how to compute $\Omega_S - \Omega_N$ once $\Delta(\mathbf{r})$ is known. But from sections (2.3) and (2.5), we know that mean-field theory is equivalent to a saddle point approximation of the partition function and hence the grand canonical potential. Thus, an elegant result of the Gor'kov expansion is the fact that self-consistency in this formalism amounts to the somewhat simpler problem of minimizing Ω_S with respect to $\Delta(\mathbf{r})$. We saw that the gap equation can be derived by putting $\delta \ln \mathcal{Z}(\Delta, \Delta^*)/\delta\Delta|_{\bar{\Delta}} = 0 \Leftrightarrow \delta\Omega_S/\delta\Delta(\mathbf{r}) = 0$. From Eq. (3.22)-(3.25), we obtain to third order in $\Delta(\mathbf{r})$:

$$\frac{1}{g}\Delta^*(\mathbf{r}) = \frac{1}{\beta}\int d^2r_1\, \Delta^*(\mathbf{r}_1) K_2(\mathbf{r}, \mathbf{r}_1)$$
$$-\frac{1}{\beta}\int d^2r_1 d^2r_2 d^2r_3\, K_4(\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)\Delta(\mathbf{r}_1)\Delta^*(\mathbf{r}_2)\Delta^*(\mathbf{r}_3). \tag{3.27}$$

This non-linear integral equation for $\Delta(\mathbf{r})$ is in general very hard to solve. It forms the basis for the derivation of the Ginzburg-Landau theory which essentially states that Eq. (3.27), under certain conditions which constitute a semiclassical approximation, can be rewritten as a simpler differential equation, i.e. the Ginzburg-Landau equation. But as explained in section 3.1, these conditions are not fulfilled in the case of strong external magnetic fields. We therefore have to consider Eq. (3.27) in all its complexity. There have been some attempts to solve this equation for special cases. Most progress has been made in the case of the quantum limit as defined in section (3.6). In this case, the Landau level sum for the modified Green's function in Eq. (3.26) reduces to one term, and Tešanović *et al.* [104] managed to find a set of solutions to Eq. (3.27). The solutions are characterized by an order parameter which formes a regular lattice with one flux quantum Φ_0 per lattice cell. However, as mentioned in section (3.6), there has been some doubt whether this limit has any physical relevance. Thus, it is desirable to try to solve Eq. (3.27) for the much harder case where several Landau levels participate in the pairing.

3.7.3 The vortex lattice solution

To make any progress in developing an analytical theory based on the Gor'kov expansion for superconductors in high magnetic fields, we must address the question of solving Eq. (3.27) when several Landau levels participate in the pairing. There have been some attempts to solve this equation using various approximations. Using a semiclassical approach in addition to various other types of approximations, Maniv *et al.* [72, 116] have provided an approximate solution to Eq. (3.27). As they do not seem to use the simplifications coming from the symmetry of the order parameter to their fullest extent, their calculation is long and rather complicated. From their solution they calculate several observables. Unfortunately, as we shall see in more detail in section (4.10.2), their results seem to be unphysical and do not agree with exact numerical solutions of the BdG equations nor with experimental observations.

Not surprisingly, a solution is much easier to find if one uses the symmetries and the formalism of section (3.5) extensively. Assuming that the order parameter forms a vortex lattice and therefore can be written in the form of Eq. (3.10), the Gor'kov expansion of the grand canonical potential will reduce to a polynomial expansion of $\Omega_S - \Omega_N$ in the parameters Δ_j. It turns out that using the formalism of section (3.5) and especially Eq. (3.6) one is able to solve the integrals in the Gor'kov expansion given by Eq. (3.23)-(3.25) *exactly* [23]. We obtain to fourth order:

$$\Omega_S - \Omega_N = \sum_j \alpha_j(T,H)\Delta_j^2 + \sum_{j_1\cdots j_4} \gamma_{j_1\cdots j_4}(T,H)\Delta_{j_1}\cdots\Delta_{j_4} \tag{3.28}$$

where

$$\begin{aligned}\alpha_j(T,H) &= \frac{g a_x}{\sqrt{2} l L_x L_y}\left[1 - \frac{g}{4\pi l^2}\sum_{n_1,n_2} B_j^{n_1\, n_2\, 2}\right.\\ &\times \left. w^2(n_1)w^2(n_2)\frac{\tanh(\beta\xi_{n_1\downarrow}/2)+\tanh(\beta\xi_{n_2\uparrow}/2)}{2(\xi_{n_1\downarrow}+\xi_{n_2\uparrow})}\right]\end{aligned} \tag{3.29}$$

and

$$\begin{aligned}\gamma_{j_1\cdots j_4}(T,H) &= \frac{g^4 a_x^4}{8L_x^4 L_y^4 l^4}\sum_{n_1\ldots n_4} w^2(n_1)w^2(n_2)w^2(n_3)w^2(n_4)f(n_1,n_2,n_3,n_4)\\ &\times B_{j_1}^{n_1 n_4} B_{j_2}^{n_3 n_2} B_{j_3}^{n_1 n_2} B_{j_4}^{n_3 n_4}\, \Xi_{n_1+n_2-j_3,\, n_3+n_4-j_4}^{n_1+n_4-j_1,\, n_2+n_3-j_2}.\end{aligned} \tag{3.30}$$

Here

$$
\begin{aligned}
f(n_1,n_2,n_3,n_4) = &\left[(e^{-\beta\xi_{n_1\downarrow}}+1)(\xi_{n_1\downarrow}+\xi_{n_2\uparrow})(-\xi_{n_1\downarrow}+\xi_{n_3\downarrow})(\xi_{n_1\downarrow}+\xi_{n_4\uparrow})\right]^{-1} \\
&+\left[(e^{\beta\xi_{n_2\uparrow}}+1)(\xi_{n_2\uparrow}+\xi_{n_1\downarrow})(\xi_{n_2\uparrow}+\xi_{n_3\downarrow})(\xi_{n_2\uparrow}-\xi_{n_4\uparrow})\right]^{-1} \\
&+\left[(e^{-\beta\xi_{n_3\downarrow}}+1)(-\xi_{n_3\downarrow}+\xi_{n_1\downarrow})(\xi_{n_3\downarrow}+\xi_{n_2\uparrow})(\xi_{n_3\downarrow}+\xi_{n_4\uparrow})\right]^{-1} \\
&+\left[(e^{\beta\xi_{n_4\uparrow}}+1)(\xi_{n_4\uparrow}+\xi_{n_1\downarrow})(\xi_{n_4\uparrow}-\xi_{n_2\uparrow})(\xi_{n_4\uparrow}+\xi_{n_3\uparrow})\right]^{-1}
\end{aligned}
\tag{3.31}
$$

and

$$
\begin{aligned}
&\Xi^{j_1,j_2}_{j_3,j_4} = \\
&\frac{L_xL_y}{4\pi a_x}\sum_j B_j^{j_1j_2}B_j^{j_3j_4}\sum_{h_1h_2} e^{-i\pi(h_1^2-h_2^2)}\left[\phi_{j_1+j_2-j}\left(\frac{2h_1a_x}{l}\right)\phi_{j_3+j_4-j}\left(\frac{2h_2a_x}{l}\right)\right. \\
&\qquad \left. + e^{-i\pi(h_1-h_2)}\phi_{j_1+j_2-j}\left(\frac{2h_1a_xl+a_x}{l}\right)\phi_{j_3+j_4-j}\left(\frac{2h_2a_x+a_x}{l}\right)\right].
\end{aligned}
\tag{3.32}
$$

To the best of my knowledge, Eqs. (3.28)-(3.32) represent the first exact quantum-mechanical solutions for the expansion coefficients of $\Omega_S-\Omega_N$ to fourth order in $\Delta(\mathbf{r})$ away from the quantum limit. The reason that we have been able to calculate the expansion coefficients exactly is that the selection rule given by Eq. (3.6) simplifies the relevant integrals significantly. The assumed symmetry of the vortex lattice enables the development of a powerful algebra which makes integrals involving $\Delta(\mathbf{r})$ much easier to solve. Indeed, one could in principle calculate the expansion coefficients for any order of $\Delta(\mathbf{r})$ exactly. To examine the convergence properties of the Gor'kov expansion, we have calculated the expansion coefficients for $\Omega_S-\Omega_N$ up to and including the eighth order term in $\Delta(\mathbf{r})$ [23]. But, as usual, the algebra gets more cumbersome with increasing order and most of the essential physics is contained within the first two terms given by Eq. (3.29)-(3.30). The result given by Eq. (3.28) is a multidimensional polynomial in Δ_j where the coefficients depend on the temperature T and the external field H. A very important result of this section is that the self-consistency inherent in the mean-field approximation is now reduced to a much simpler *algebraic* problem: the minimization with respect to the Δ_j's of the multidimensional polynomial in Eq. (3.28). This will form the basis for much of the analytical results presented in the following chapters.

3.7.4 The transition temperature

We will now examine the transition temperature T_c in the different COM channels. Since the order parameter is very small close to T_c, we know that the perturbation theory developed in section 3.7 should describe this transition regime well[4]. In this formalism, the transition to the mixed state occurs when the quadratic term for $\Omega_S - \Omega_N$ given by Eq. (3.23) becomes negative. The system can then lower its energy by forming a non-zero order parameter. Thus, we can determine T_c by finding where the quadratic term changes sign. From Eq. (3.23), we obtain

$$\frac{1}{g}\Delta^*(\mathbf{r}) = \frac{1}{\beta}\int d^2r_1\,\Delta^*(\mathbf{r}_1)K_2(\mathbf{r},\mathbf{r}_1). \tag{3.33}$$

This is, of course, just the linear term in the self-consistency condition given by Eq. (3.27). Equation (3.33) is in general simpler to solve than Eq. (3.27). In 1966, Rajagopal and Vasudevan [90, 91] provided a solution of this equation. These papers constitute, to my knowledge, the first calculations of the properties of the mixed state taking into account the quantizing effect of the external magnetic field. Using the formalism developed in section 3.4, we can relatively easily find a solution to the integral equation given by Eq. (3.33). It turns out that a $\Delta(\mathbf{r})$ of the form given by Eq. (3.10) with only one $\Delta_j \neq 0$ is an eigenfunction to the integral operator $K_2(\mathbf{r},\mathbf{r}_1)$ in Eq. (3.33) with eigenvalue λ_j. Thus, T_c for this Δ_j can be derived by setting $\lambda_j = \beta/g$. Equivalently, the desired equation can simply be derived by looking at the

[4]Again, this is true within mean-field theory.

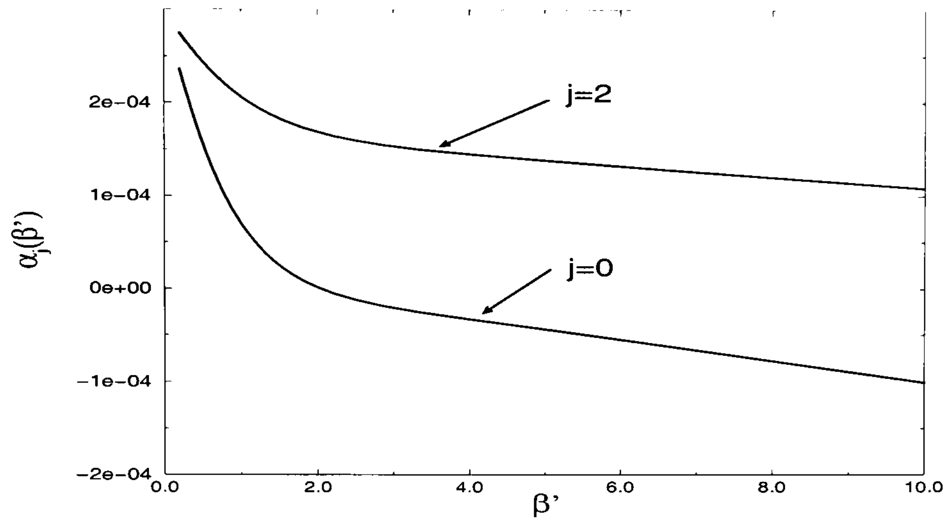


Figure 3.5: α_j as a function of $\beta' \equiv \hbar\omega_c/k_BT$ for $n_F = 12$, $g/\hbar\omega_c l^2 = 8$ and $\omega_D = 5$. We get $T_c(j=0) \simeq \frac{\hbar\omega_c}{2k_B}$. T_c for $j=2$ is not depicted on this plot.

sign change of the quadratic terms of $\Omega_S - \Omega_N$ as given in Eq. (3.29). When α_j becomes negative, it is energetically favorable to form Cooper pairs with COM kinetic energy $(j + 1/2)\hbar\omega$. From Eq. (3.29), we immediately obtain:

$$\frac{1}{g} = \frac{1}{4\pi l^2} \sum_{n_1,n_2} B_j^{n_1\, n_2\, 2} w^2(n_1) w^2(n_2) \frac{\tanh(\beta\xi_{n1\downarrow}/2) + \tanh(\beta\xi_{n2\uparrow}/2)}{2(\xi_{n_1\downarrow} + \xi_{n_2\uparrow})}. \tag{3.34}$$

This equation determines T_c for the channel with COM kinetic energy $(j + 1/2)\hbar\omega$. It was first derived by Rajagopal and Ryan [89] and by MacDonald *et al.* [67]. Again, we see the advantage of using the symmetry of the vortex lattice. By looking for a subset of order parameters with a lattice symmetry, the integral equation determining T_c has been turned into the much simpler question of examining the size of a simple sum. As an example, we have in Fig. 3.5 plotted $\alpha_j(\beta)$ for the parameters $n_F = 12, g/\hbar\omega_c l^2 = 8$ and $\omega_D = 5$. As can be seen, $\alpha_0(\beta)$ changes sign for $\beta \simeq 2/\hbar\omega_c \Leftrightarrow T_c(j=0) \simeq \hbar\omega_c/2k_B$.

Also, we see that T_c for $j = 2$ is much larger than for $j = 0$. This is not specific to the parameters chosen above but is a general property. It turns out that $T_c(j = 0)$ is larger than $T_c(j > 0)$ when more than one Landau level participates in the pairing. From Eq. (3.34), we see that for two particles to contribute to the pairing, they must be on the same side of the chemical potential. Otherwise, the factor $\tanh(\beta\xi_{n1\downarrow}/2) + \tanh(\beta\xi_{n2\uparrow}/2)$ becomes vanishingly small. A closer analysis shows that the probability of the two single particle states being on the same side of the chemical potential for a given total energy is, in general, largest for $j = 0$ [68]. This means that additional terms in Eq. (3.34) are non-vanishing. They are all greater than zero; thus, T_c is highest for $j = 0$.

Of course, Δ_0 does not increase indefinitely in size when $\alpha_0 < 0$. This is because the quartic term γ_{0000} in Eq. (3.28) is positive close to the transition point. Thus, if Δ_0 becomes too large, the quartic contribution will start to dominate and the energy increases. Also, the fact that $\alpha_{j\neq 0} > 0$ does not necessarily mean that $\Delta_{j\neq 0} = 0$. The quartic terms γ_{000j} might make it energetically favorable to have $\Delta_{j\neq 0} \neq 0$ even though $\alpha_{j\neq 0} > 0$. To fourth order in $\Delta(\mathbf{r})$, we see from Eq. (3.28) that the values of the Δ_j's follow from the minimization of a multidimensional polynomial in Δ_j. However, close to T_c, we can conclude that the Δ_j with $\alpha_j < 0$ is much larger than the other Δ_j's for which $\alpha_j > 0$. Since we have seen that the minimum COM kinetic energy becomes unstable to pairing first ($\alpha_0 < 0$ and $\alpha_{j\neq 0} > 0$), we conclude that $\Delta_0 \gg \Delta_{j\neq 0}$ close to T_c. This conclusion leads to a major simplification of the algebra as will be seen in chapter 4.

3.8 Summary

In this chapter, we restricted the formalism presented in chapter 2 to the case when the effect of an external magnetic field must be included right from the beginning. By considering the problem of two-particle scattering, we saw that the motion of the electron pairs naturally splits into the COM and the relative motion. We then introduced the lattice symmetry of the order parameter. This symmetry was shown to simplify the BdG equations drasticly. They split into a set of equations for each conserved magnetic momentum $\mathbf{k}$. We found a solution of the BdG equations in the limit of a very high magnetic field. Then, the perturbative expansion of the grand canonical potential was considered. The symmetry of the vortex lattice enabled us to develop an algebra such that the relevant integrals in the expansion could be solved exactly; the grand canonical potential was expressed in terms of a simple polynomial in a finite set of variables and the self-consistency problem reduced to the simple task of minimizing this polynomial. Finally, we calculated the transition temperature for a given magnetic field. It turned out that there is a transition temperature for Cooper pair formation in each COM channel. By considering the transition in each channel, we concluded that the lowest T_c is obtained for Cooper pair formation with minimum COM kinetic energy.

Chapter 4

de Haas-van Alphen oscillations in the mixed state

4.1 Introduction

When a system of electrons in the normal (i.e. non-superfluid) state is subjected to a varying external magnetic field, one observes oscillations in the magnetization, magnetoresistance and various other observables. The oscillations in the magnetization M are called de Haas-van Alphen (dHvA) oscillations. As is well known [6], dHvA oscillations are a powerful tool for probing the Fermi surface for electron systems. Indeed, the presence of the dHvA oscillations has in some sense been considered as one of the prime experimental evidences for the existence of the Fermi surface. Interestingly, these oscillations have also been observed in the mixed state of several type-II superconductors. The first experimental evidence that such oscillations exist in the mixed state, was provided over 20 years ago for the layered superconductor 2H-$NbSe_2$ [49]. These observations were confirmed much later by Onuki *et al.* [85] and by Janssen *et al.* [61]. Recently, dHvA oscillations have been observed in several other systems such as the organic superconductor κ-$(ET)_2Cu(NCS)_2$[110, 111], the A15 compounds V_3Si [29, 61] and Nb_3Sn [53], the borocarbide superconductor YNi_2B_2C [45], and the high temperature superconductors $YBa_2Cu_3O_6$ [43] and $BaO_6KO_4BiO_3$ [46]. The occurrence of the dHvA oscillations in such a variety of systems seems to suggest that this effect is a fundamental property of a type-II superconductor in the mixed state. This is somewhat surprising at first sight, as the development of the superconducting gap normally is associated with the breakdown of the Fermi surface. Superficially, one would therefore expect the magnetic oscillations to disappear once the superconducting order parameter is formed. For type-I superconductors, there are of course no oscillations below H_c since the Meissner effect means that the magnetic field is expelled from the bulk of the conductor. But, as we know, type-II superconductors allow a partial penetration of the magnetic field in the mixed state making the situation less straight forward. The experimental results for the materials mentioned above show that there are indeed oscillations in the magnetization close to H_{c2} and that these oscillations in the mixed state suffer an additional damping as compared to the normal state oscillations. Eventually, when the field is low enough such that the system is deep into the mixed state, the oscillations are completely washed out. These observations have motivated a lot of theoretical work and several theories for the dHvA effect in the mixed state have been proposed in recent years. However, there seems to be a general disagreement about the mechanism leading to these oscillations. As the dHvA effect is essentially the occurrence of oscillations in the appropriate thermodynamic potential, one would expect a successful theory to yield information about the magnetic field dependence of the quasiparticle spectrum and of the superfluid correlations in the ground state[1].

In this chapter, we will develop a theory for the magnetic oscillations of the grand potential and hence of the magnetization. The formalism we have

[1]Some of the theories for the dHvA oscillations in the mixed state have only focused on the quasiparticle excitations. In my opinion, this cannot provide the full picture as the dHvA effect is strongest for $T = 0$ when there are no quasiparticles present.

set up in chapter 3 is well suited to handle such a problem in the limit of extreme type-II superconductors. This is because the single-particle Landau level structure is included in the theory from the outset. It is precisely this level structure which is responsible for the magnetic oscillations in the normal state. Thus, one would expect the formalism to describe fairly well the transition to the damped oscillations in the mixed state. This was one of the reasons why we set up the theoretical formalism outlined in chapter 3. In this chapter, we will present the resultant theory for the dHvA effect for 2D systems. The reason why we restrict the theory to describe 2D systems is partly because some materials, such as the layered organic superconductors, can be regarded as quasi-2D systems. Also, the notation for 2D is somewhat simpler than the 3D case. The generalization of the theory to describe 3D systems should be fairly straightforward. This chapter is essentially a more detailed description of the theory first presented in Ref. [23].

In section 4.2, we will briefly outline the theory of the dHvA oscillations for metals in the normal state. Then in section 4.3, the theory of the dHvA oscillations in the mixed state based on the Gor'kov expansion will be developed. In order to check the validity of this theory, section 4.4 compares its predictions to an exact numerical solution of the BdG equations. It turns out that the theory works well close to H_{c2} and that it predicts the existence of the damped dHvA oscillations in the mixed state. A straightforward physical interpretation of the existence of the damped oscillations emerges quite naturally from the perturbation theory. This is discussed in section 4.5. The effect of a finite Zeeman term and the difference between a fixed chemical potential and a fixed number of particles are then discussed in sections 4.6-4.7. In section 4.8, we simplify the perturbation theory in order to be able to make some precise predictions concerning the dependence of the damping on the magnetic field, temperature and various other quantities. Using these simplified expressions, we compare our theory with experimental data in section 4.9. The agreement between theory and experiment is found to be good.

In section 4.10, we briefly describe some of the other theories developed to describe the dHvA oscillations in the mixed state. Finally, in section 4.11, we summarize the results presented in this chapter.

4.2 The normal state oscillations

Before describing the theory for the magnetic oscillations in the mixed state, we will in this section briefly develop the corresponding well-known theory for the normal state. We are interested in the magnetization M which is given by $M = -\left.\frac{\partial\Omega}{\partial H}\right|_{\mu_F,T}$. Within the approximations leading to Eq. (2.8), the normal state is just a set of non-interacting quasiparticles with effective mass m in an external magnetic field H. The quasiparticle states are simply the 2D form of the Landau levels introduced in section 3.2 with a wave function given by $\phi_{N,k}(x,y)$ and an energy ξ_N. For such a system of non-interacting quasiparticles, one can easily obtain the grand canonical potential; for a given temperature, magnetic field, and chemical potential, it is given by (ignoring the Zeeman splitting for the moment) [58]:

$$\Omega_N(\mu_F, T, H) = -2k_B T \mathcal{D} \sum_n \ln\left(1 + e^{-\beta\xi_n}\right) \tag{4.1}$$

with $\mathcal{D} = \frac{L_x L_y}{2\pi l^2}$ being the degeneracy of each Landau level, while the factor of 2 accounts for the electron spin. We are interested in extracting the oscillations of the grand canonical potential as the magnetic field is varied. The origin of these oscillations can easily be seen: they arise because the Landau level energies cross the chemical potential as the magnetic field varies. With increasing field, the energies rise and the grand canonical potential increases. Then, as a level goes through the chemical potential μ_F, it is depleted and the grand potential decreases again. Thus, when a Landau level is at the chemical potential the grand canonical potential is at a local maximum and when μ_F is in between two levels, the grand canonical potential is at a local minimum. This is the origin of the magnetic oscillations of Ω_N and the various thermodynamic quantities derived from it. To extract the oscillatory behaviour of the grand canonical potential, it is convenient to rewrite the sum in Eq. (4.1) using the Poisson summation formula:

$$\sum_{n=-\infty}^{\infty} F(n) = \sum_{l=-\infty}^{\infty} \int_{-\infty}^{\infty} dx\, F(x) e^{2\pi i l x}. \tag{4.2}$$

This formula is essentially a Fourier decomposition of the summand $F(n)$. By using it to calculate Ω_N in Eq. (4.1), we obtain after using the variable substitution $x \to x - \mu_F$, the Fourier components of the grand canonical potential as a function of H. After some integrations, we end up with the following formula for the l'th harmonic Ω_{N_l} of Ω_N:

$$\Omega_{N_l} = \mathcal{D}\frac{\hbar\omega_c}{\pi^2 l^2}\left[\frac{2k_B T\pi^2 l}{\hbar\omega_c \sinh\left(\frac{2\pi^2 k_B T l}{\hbar\omega_c}\right)}\right]\cos(2\pi l n_F) \tag{4.3}$$

with $\mu_F = (n_F + 1/2)\hbar\omega_c$ and $n_F \in \Re$ [99]. We have for clarity written the reduction factor due to a finite temperature T in square brackets. This reduction comes from the fact that for a finite T, the transition as a function of energy between occupied and un-occupied levels is smoothed out on a scale of the order k_BT. Thus, the depletion of the Landau level when it goes through the chemical potential happens less abruptly as compared to the $T = 0$ case.

4.2.1 Effect of impurities

We see from Eq. (4.3) that when $k_BT \ll \hbar\omega_c$, the grand canonical potential and thus the magnetization will contain many harmonics as a function of $1/H$ [100]. But even for $k_BT \ll \hbar\omega_c$, one normally observes only the first harmonic ($k = 1$) of the signal, i.e. the magnetization signal looks almost like a pure sine wave as a function of $1/H$. This is because the scattering of the quasiparticles on impurities tends to attenuate the higher harmonics of the grand canonical potential in much the same way as a finite T. If the effect of the impurities can be treated as a simple broadening of the quasiparticle levels, one can include them in the calculation of the grand canonical potential in much the same way as the effect of a finite temperature: The grand canonical potential with level broadening is found by convoluting the potential without any broadening with a suitable probability function for the energies, whereas the potential for finite T can be found by convoluting the $T = 0$ potential with the negative derivative of the Fermi function [100]. From the convolution theorem, we know that this procedure is equivalent to multiplying the Fourier components given in Eq. (4.3) with the Fourier transform of the relevant probability function. In this picture, the quantity in the square brackets in Eq. (4.3) is just the Fourier transform of the negative derivative of the Fermi function. Also, if several independent damping effects occur together, the appropriate convolutions can be carried out successively. The result is a multiplication of the harmonic terms in Eq. (4.3) by the various Fourier transforms of the probability functions describing the damping mechanisms. Assuming that the level broadening due to impurities can be well described by a Lorentzian distribution function, the damping factor R_D due to impurities for the k'th harmonic becomes $R_D(k) = \exp(-\pi k/\omega_c\tau)$ with τ being the (energy independent) relaxation time[2]. Thus, if $\pi/\omega_c\tau \gtrsim \mathcal{O}(1)$, the impurities cancel any higher harmonics and the oscillations are well described by the $k = 1$ term in Eq. (4.3) even for $k_B T \ll \hbar\omega$.

4.2.2 Effect of Spin

We have up till now ignored the effect of a finite Zeeman term in the quasiparticle energies. The electron spin can be taken into account simply by splitting the sum in Eq. (4.1) into two terms for the spin up and spin down part respec-

[2] R_D is often called the "Dingle reduction factor" as it was derived by Dingle in 1952[35].

tively. As the energy levels are split as $\xi_{n\sigma} = \xi_n \pm g^* \hbar\omega_c \frac{m}{4m_0}$, the corresponding harmonic of the grand canonical potential becomes the sum of two terms which differ in phase by $\pm g^* \pi l \frac{m}{2m_0}$ from the oscillations without spin. Using $\frac{1}{2}[\cos(2\pi l n_F + g^*\pi l \frac{m}{2m_0}) + \cos(2\pi l n_F - g^*\pi l \frac{m}{2m_0})] = \cos(2\pi l n_F)\cos(g^*\pi l \frac{m}{2m_0})$, we immediately see that a finite Zeeman term reduces the amplitude of the l'th harmonic by a factor $\cos(g^*\pi l \frac{m}{2m_0})$.

4.2.3 Behaviour for constant N

We have in Eq. (4.3) implicitly assumed that the chemical potential is constant such that n_F is the appropriate variable to parametrize the magnetic field. Keeping μ_F constant implies that the number of particles N in the system oscillates as a function of the magnetic field as the Landau levels pass through the chemical potential. Hence, if N is constant the chemical potential must vary with the magnetic field. From a theoretical point of view, one must calculate $N = -\partial_{\mu_F}\Omega_N$ and adjust the chemical potential such that N is constant. We will not go through the rather tedious analysis here but will just state the result: It turns out that for a 2D system, the magnetic field dependence of the chemical potential has a strong effect on the magnetic oscillations of the grand canonical potential when the system is at a low temperature and is sufficiently clean, such that many harmonics in Eq. (4.3) are important [99]. On the other hand, for higher temperatures and impurity concentrations such that only the first harmonic of the oscillations is important, the oscillations are the same when N is constant as compared to when μ_F is constant.

4.3 Perturbation Theory

As explained in section 4.1, the oscillations of the magnetization in the mixed state are observed for fields close to H_{c2}. When the field is lowered further, the superconducting correlations seem to wash out the oscillations; i.e. the dHvA effect is only observed for fields not much below the transition line $H_{c2}(T)$ such that $\Delta(\mathbf{r})$ is small. This suggests that the perturbation theory developed in section 3.7 for a superconductor in the mixed state should be well suited to describe this phenomenon. Indeed, we will see that a theory based on this perturbation expansion does predict the presence of magnetic oscillations in the mixed state. Also, it explains the additional attenuation of the amplitude of the oscillations as compared to the normal state. In this section, we will develop the main part of this perturbation theory for the dHvA oscillations.

From Eq. (3.28), we know, that the difference $\Omega_S - \Omega_N$ between the grand canonical potential in the mixed state and in the normal state state close to the transition line can be expressed as a polynomial in the parameters Δ_j, if the order parameter has a vortex lattice symmetry. The self-consistency condition $\Delta(\mathbf{r}) = g\langle\psi_\uparrow(\mathbf{r})\psi_\downarrow(\mathbf{r})\rangle$ is equivalent to minimizing this polynomial with respect to the variables Δ_j. Furthermore, in section 3.7.4, we saw that close to the transition line one can to a good approximation neglect all $\Delta_{j\neq 0}$ as the instability towards pairing occurs in the $j = 0$ channel first. Thus, one can put $\Delta_{j\neq 0} = 0$ when H is close to H_{c2}. This important fact will simplify the subsequent analysis significantly. We have checked the validity of this assumption by numerically solving the BdG equations using the formalism outlined in section 3.5. In the region of interest (i.e. close to H_{c2}), the numerical solutions show as expected that $\Delta_0 \gg \Delta_{j\neq 0}$ thereby justifying the approximation. Therefore, from Eq. (3.28), the difference $\Omega_S - \Omega_N$ now has the simple Landau form:

$$\Omega_S(T, H) - \Omega_N(T, H) = \alpha(T, H)\Delta_0^2 + \gamma(T, H)\Delta_0^4 \qquad (4.4)$$

with $\alpha(T, H) = \alpha_0(T, H)$ and $\gamma(T, H) = \gamma_{0000}(T, H)$. We have explicitly written the dependence of the expansion coefficients on the temperature and magnetic field. Because the magnetic quantization has been included in this

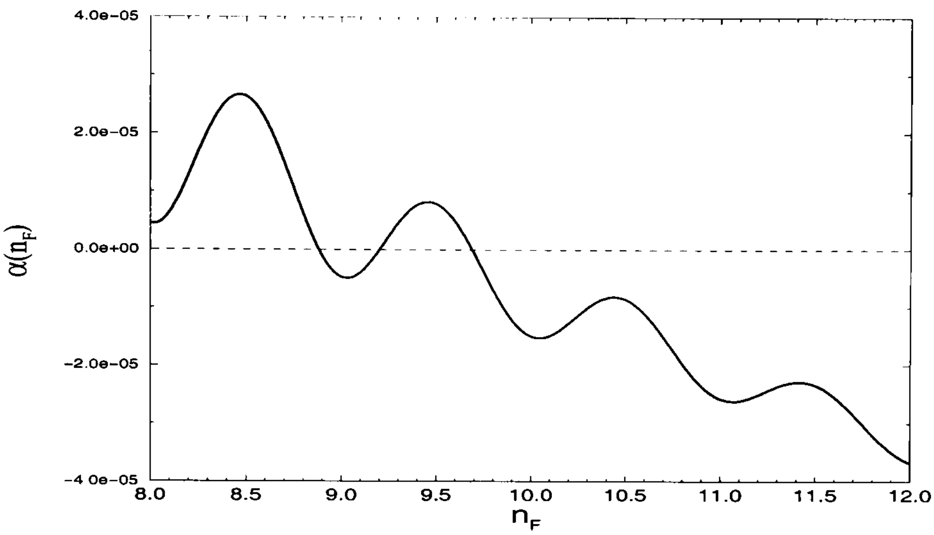


Figure 4.1: α as a function of n_F for fixed T. The transition between the normal and the mixed state is indicated by a thin dashed line.

formalism from the beginning, the coefficients will in general be oscillating functions of H. This oscillatory behaviour of the expansion coefficients forms the core of the perturbation theory of the dHvA effect.

4.3.1 The transition line

To gain some familiarity with the behaviour of the expansion coefficients, we will in this section briefly describe the behaviour of $\alpha(T, H)$ when the external field H varies. In Fig. 4.1, we plot $\alpha(T, H)$ calculated from Eq. (3.29), as a function of $n_F = \mu_F/\hbar\omega_c - 0.5$ for the parameters $\omega_D/\omega_c = 5$, $\frac{g}{\hbar\omega_c l^2} = 8.2$ and $k_B T/\hbar\omega_c = 0.28$ when $n_F = 12$. For the moment, we are ignoring the Zeeman effect and the temperature and the chemical potential are constant. We see that α in general is a decreasing function of n_F and hence with decreasing external field H. We know from section 3.7.4 that the transition from the normal state to the mixed state occurs when α becomes negative. Therefore, the decrease of α with decreasing field simply reflects the fact that the system becomes increasingly unstable towards superconducting pairing with decreasing field[3]. From Fig. 4.1, we see that for the specific set of parameters chosen in this section, the system becomes superfluid for $n_F \approx 9.7$. Importantly, we also see that α *oscillates* as the external field varies. It has a local minimum when the chemical potential is at a Landau level (n_F integer) and a local maximum when the chemical potential is in between two Landau levels (n_F half-integer). Thus, the instability towards superconductivity has an oscillatory behaviour reflecting the shell structure of the Landau level spectrum. This behaviour is exactly what we predicted above. Mathematically, this comes from the fact that when the chemical potential is at a Landau level, the sum in Eq. (3.29) is dominated by the terms with zero denominator, as an application of l'Hospital's rule confirms. If one calculates $H_{c2}(T)$, i.e. the upper phase transition line in Fig. 3.1 (b) by finding the zero of $\alpha(T, H)$, then one finds that the transition line exhibits oscillations as a function of the field. This effect was predicted already in 1966 by A. K. Rajagopal and R. Vasudevan [90, 91]. We see that this is simply a reflection of the discreteness of the Landau level quasiparticle spectrum: when n_F is an integer the density of states is high at the chemical potential and the instability towards superconductivity is enhanced. Also, from Fig. 4.1 we see that this oscillatory behaviour gives rise to the phenomenon of re-entrance: the system becomes superfluid for $8.85 \lesssim n_F \lesssim 9.2$, it is then in the normal state for $9.2 \lesssim n_F \lesssim 9.7$, and then finally becomes superfluid for $n_F \gtrsim 9.7$. This rather striking effect of the magnetic field is destroyed if we include the effect of a finite Zeeman term and a level broadening due to a realistic impurity concentration. As we will see later, inclusion of these effects will attenuate the oscillatory part of α such that the re-entrance effect is suppressed [23].

[3]We are not considering the special case of the quantum limit discussed in section 3.6 where the instability towards superconductivity actually increases with *increasing* field.

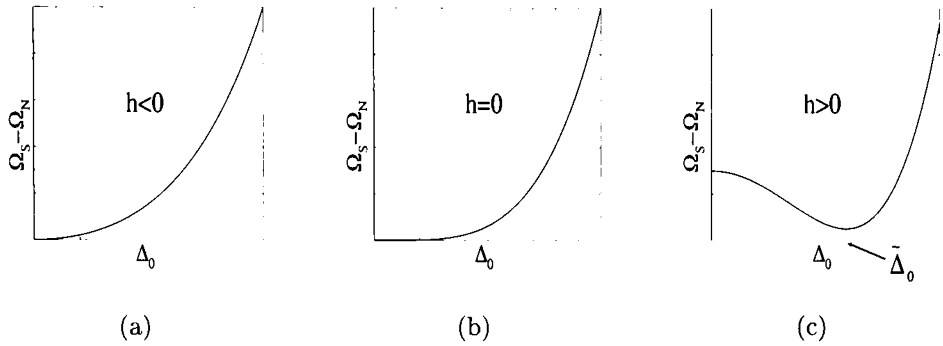


Figure 4.2: $\Omega_S - \Omega_N$ as a function of Δ_0 in arbitrary units for different values of $h \equiv \frac{H_{c2}-H}{H_{c2}} \ll 1$. For $h > 0$ the value $\tilde{\Delta}_0$ of Δ_0 for which the grand canonical potential has a minimum is indicated on the figure by the arrow.

4.3.2 Self-consistency

From the simple Landau form of $\Omega_S - \Omega_N$ given in Eq. (4.4), we see that the self-consistency problem to fourth order in $\Delta(\mathbf{r})$ is reduced to a simple minimization problem of a quadratic polynomial in the variable Δ_0^2. From this form, we can easily understand the transition from the normal state to the mixed state when the external field is varied. When $H > H_{c2}$, we have $\alpha > 0$ and the minimum of the grand canonical potential occurs at $\Delta_0 = 0$; the system is in the normal state. The transition occurs when $H = H_{c2}$. Here $\alpha = 0$ and $\Omega_S - \Omega_N$ is a very flat function of Δ_0 around the origin. The minimum is still at $\Delta_0 = 0$ making the phase transition second order. For $H < H_{c2}$, we have $\alpha < 0$ and the minimum of $\Omega_S - \Omega_N$ is now at $\Delta_0 \neq 0$; the system is in the mixed state. The behaviour of $\Omega_S - \Omega_N$ as a function of Δ_0 for different fields is depicted in Fig. 4.2. Below H_{c2}, the potential is of the so-called "Mexican hat" form. The reason for this name becomes apparent when one remembers that energy is independent of the phase of the order parameter. By rotating the plot given in Fig. 4.2(c) around the $\Omega_S - \Omega_N$ axis in order to reflect the phase degree of freedom of the order parameter, one ends up with the shape of a Mexican hat (in the case of Fig. 4.2(c) albeit a rather distorted one)[4]. The minimimum of a quadratic polynomial can readily be found. From the requirement $\partial_{\Delta_0}(\Omega_S - \Omega_N)|_{\tilde{\Delta}_0} = 0$ and Eq. (4.4), we obtain:

$$\begin{aligned} \tilde{\Delta}_0^2 &= -\frac{\alpha(T,H)}{2\gamma(T,H)} \\ \Omega_S - \Omega_N &= -\frac{\alpha^2(T,H)}{4\gamma(T,H)}. \end{aligned} \tag{4.5}$$

When $\alpha(T,H) \leq 0$, Eq. (4.5) yields $\tilde{\Delta}_0$ and therefore $\Delta(\mathbf{r})$ and $\Omega_S - \Omega_N$ as a function of H. The value $\tilde{\Delta}_0$ which minimizes $\Omega_S - \Omega_N$, will be a function of H and T through the coefficients α and γ. Note that $\Omega_S - \Omega_N \leq 0$ as it should be for $H \leq H_{c2}$. From Eq. (4.5) and section 4.2, we can calculate the grand canonical potential and thus the magnetization $M_S \equiv -\left(\partial_H \Omega_S\right)_{\mu_F} = -\left[\partial_H(\Omega_N + [\Omega_S - \Omega_N]))\right]_{\mu_F}$.

4.4 Comparison between numerical data and perturbation expansion

Before employing perturbation theory, it is important to establish its range of validity. We have set up a code to solve the BdG equations self-consistently using the formalism outlined in section 3.5. In order to estimate the accuracy of the perturbation expansion, we will in this section compare it to an exact numerical solution of the corresponding BdG equations. We have chosen the same parameters as in section 4.3.1, i.e. $\omega_D/\omega_c = 5$, $\frac{g}{\hbar\omega_c l^2} = 8.2$ and $k_B T/\hbar\omega_c = 0.28$ when $n_F = 12$. Fig. 4.3 depicts the self-consistent order-parameter $\tilde{\Delta}_0$ as a function of n_F. The chemical potential μ_F is fixed. We have plotted both the numerical result and the fourth order prediction obtained from Eq. (4.5). The eighth order perturbative solution is shown as

[4]This fact is the origin of the so-called Goldstone collective modes. These modes are not important for our purposes and we are keeping $\Delta(\mathbf{r})$ real.

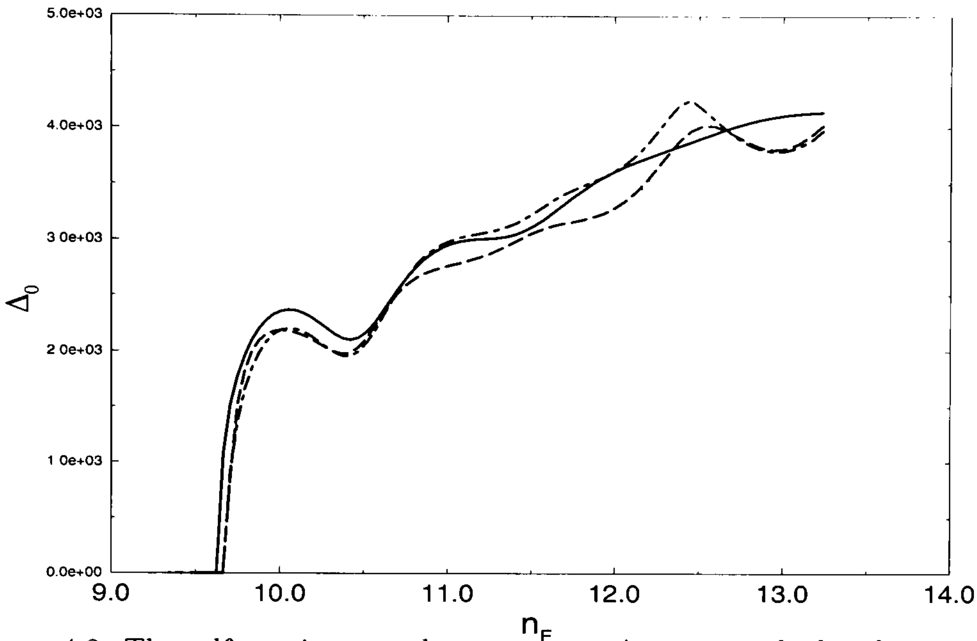


Figure 4.3: The self-consistent order parameter Δ_0 vs n_F calculated numerically (solid line), to fourth order in Δ_0 (dashed line), and to eighth order in Δ_0 (dash-dot line).

well. This solution is obtained by keeping terms up to order $\Delta(\mathbf{r})^8$ in the expansion given by Eq. (3.21). The algebra is a straightforward extension of the one developed in section 3.7.3 and one ends up with the problem of minimizing a fourth order polynomial in Δ_0^2 instead of the quadratic one in Eq. (4.4). This can be done analytically and the details are given in Ref. [23]. Not surprisingly, the notation becomes somewhat cumbersome for the sixth and the eighth order terms. Since the essential physics is contained in the quadratic and quartic term, we have for simplicity left out the formulae connected with the eighth order perturbation terms. From Fig. 4.3, we see that there is good agreement between the numerical solution and our perturbation expansion for both fourth and eighth order. The general behaviour of Δ_0 is correctly predicted by the perturbation expansion. Note that the order parameter exhibits oscillations in magnitude as the external field is varied. As expected, it has local maxima whenever the chemical potential is at a Landau level (n_F

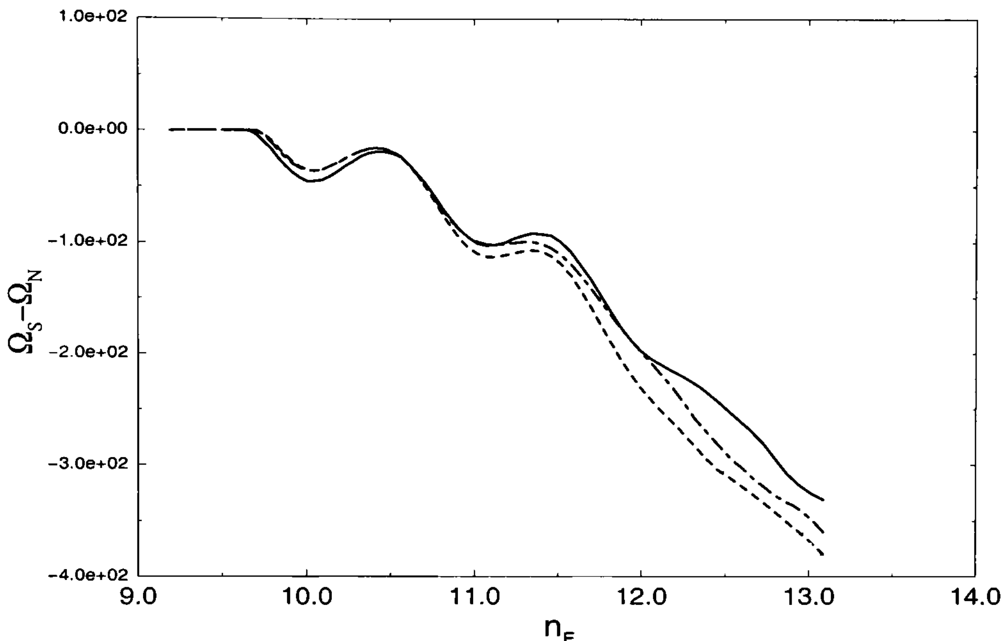


Figure 4.4: The difference $\Omega_S - \Omega_N$ in the grand canonical potential between the mixed state and the normal state. The solid line is a numerical calculation, the dashed line corresponds to fourth order perturbation theory, and the dash-dot line is eighth order perturbation theory.

integer) reflecting the enhanced instability towards superconductivity. It is important to include this oscillatory behaviour of the order parameter in any self-consistent treatment of the dHvA effect. As will be seen in section 4.10, this fact casts doubts on some of the alternative theories developed in the last few years to describe the magnetic oscillations in the mixed state.

In Fig. 4.4, we plot the corresponding condensation energy $\Omega_S - \Omega_N$. The fourth order result is obtained from Eq. (4.5) and the expression for the eighth order result is given in Ref. [23]. We are measuring energies in units of $\hbar\omega_c$. The grand canonical potential can easily obtained from the numerical solution as well. Using $\Omega = \langle \hat{H} \rangle - TS$, we obtain after some algebra

$$\Omega_S = \sum_{n\sigma} \xi_{n\sigma} N_{n\sigma} + E_{int} - TS \tag{4.6}$$

with the interaction energy given as

$$E_{int} = -g\frac{a_x}{\sqrt{2}L_xL_yl}\Delta_0^2. \tag{4.7}$$

The occupation number of the n'th Landau level with spin σ is

$$N_{n\sigma} = \sum_{\eta\mathbf{k}} \left\{ f(E^{\eta}_{\mathbf{k}\sigma})|u^{\eta}_{n\mathbf{k}}|^2 + [1 - f(E^{\eta}_{\mathbf{k}-\sigma})]|v^{\eta}_{n\mathbf{k}}|^2 \right\}, \tag{4.8}$$

and the expression for the entropy reads

$$S = -k_B \sum_{\eta\mathbf{k}\sigma} \left\{ [1 - f(E^{\eta}_{\mathbf{k}\sigma})] \ln[1 - f(E^{\eta}_{\mathbf{k}\sigma})] + f(E^{\eta}_{\mathbf{k}\sigma}) \ln[f(E^{\eta}_{\mathbf{k}\sigma})] \right\}. \tag{4.9}$$

Using these formula, we can calculate Ω_S and hence, using Eq. (4.1), $\Omega_S - \Omega_N$ from the numerically obtained solution to the BdG equations. From Fig. 4.4, we see that the agreement between the perturbative results and the numerical solution is good when the field is close to H_{c2}. Again, we see an oscillatory behaviour when the magnetic field is varied. The difference $\Omega_S - \Omega_N$ has local minima for n_F integer. This simply reflects the fact that the superconducting order has local maxima at these fields. We can now understand the damping of the magnetic oscillations of the grand canonical potential and therefore the magnetization when the system enters the mixed state. Since the normal state grand canonical potential Ω_N has local maxima for n_F integer, the condensation energy oscillates 180° out of phase with the contribution from the normal state. We therefore get partial cancellation of the normal state oscillations and a damping of the corresponding dHvA-oscillations.

This is seen in Fig. 4.5 where we plot the magnetization for both the normal and the mixed state. When the superconducting order starts to increase at $n_F \simeq 10$, we get significant damping of the dHvA oscillations. Again the agreement with the numerical data is good as long as $n_F \lesssim 12$. Eighth order theory tends to agree better with numerical data than does the fourth order

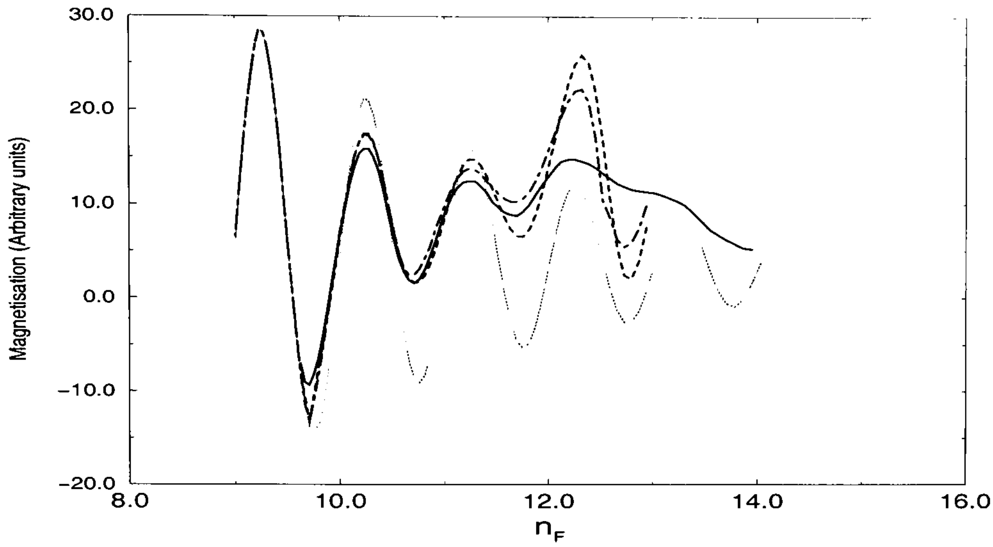


Figure 4.5: The magnetization vs n_F. The solid line is a numerical calculation, the dashed line corresponds to fourth order, the dash-dot line eighth order, and the dotted line is the magnetization in the underlying normal state.

theory, indicating that the perturbation expansion is convergent. However, once we go too far into the superconducting state, the perturbation theory starts to disagree with the numerical results, also as expected. We see from Fig. 4.3 and Fig. 4.4 that the magnitude of Δ_0 and $\Omega_S - \Omega_N$ is still fairly well described for $n_F > 12$, but the perturbative results start to pick up spurious oscillations in the order parameter and in the energy. $\Omega_S - \Omega_N$ actually starts to oscillate *in phase* with Ω_N according to the perturbation theory yielding an enhancement of the dHvA-oscillations in the mixed state as compared to the normal state, as seen from Fig. 4.5. This is an unphysical effect and is absent in the exact numerical solution. As this enhancement is neither confirmed numerically nor experimentally, we conclude that perturbation theory in the single parameter Δ_0 breaks down at this point; we are simply beyond the convergence radius for the Gor'kov series. In chapter 6, we will examine in detail when the Gor'kov expansion is convergent. It will be shown that the Gor'kov expansion is convergent if the change in the quasiparticle energies $|E_{\mathbf{k}}^{\eta} - \xi_{\eta}|$ is not larger than $\sim \mathcal{O}(k_B T)$. We have looked at the numerically calculated quasiparticle energies as a function of n_F. As expected, we observe that the quasiparticle bands go from being essentially broadened Landau levels close to the transition point to losing all their Landau level structure deeper into the mixed state. This broadening of the Landau levels with increasing superconducting order was first predicted by Norman *et al.* [84]. It gives a complementary view on the damping of the dHvA oscillations; i.e. the damping directly reflects the broadening of the Landau levels. For the above specific case, we have found that for $n_F \gtrsim 12$ the quasiparticle energies are changed so much that the above condition for the validity of the Gor'kov series does not hold in large regions of $\mathbf{k}$-space, thus explaining the breakdown of perturbation theory.

From Fig. 4.5, it can be seen that the numerical results show total suppression of the dHvA effect once we are deep enough into the mixed state ($n_F \gtrsim 12$). This effect is general and not dependent on the specific parameters chosen above. It reflects the fact that when the order parameter becomes large enough, the Landau level structure of the spectrum is completely washed out. This numerical result is in agreement with what is observed experimentally.

We have compared the numerical solution and the perturbation expansion for a number of different parameters. Our conclusion is that both fourth and eighth order perturbation theories describe well the superconducting state and the corresponding damping of the magnetic oscillations near the transition point. We have established that a theory for the mixed state based on this perturbative expansion must be expected to describe well the presence of the damped dHvA oscillations close to H_{c2}. However, the perturbation theory eventually breaks down when the quasiparticle levels are changed too much in the sense described above.

4.5 Damping of the magnetic oscillations

In section 4.4, we saw that both the numerical results and the perturbative theory predicted the experimentally observed damping of the dHvA oscillations in the mixed state. Also, we noted that the perturbation theory gives a natural explanation of this effect[5]. To get a physical understanding of the damping of the magnetic oscillations due to the superconducting order, it is helpful to consider the ground state energy which gives the dominant contribution to the grand canonical potential for low temperatures. From section 2.4 and section 3.5, we know that our theory is based on the following canonical transformation:

$$\hat{\gamma}^{\eta}_{\mathbf{k}\uparrow} = \sum_{N} \left[u^{\eta *}_{N\mathbf{k}} \hat{a}_{N\mathbf{k}\uparrow} + v^{\eta *}_{N\mathbf{k}} \hat{a}^{\dagger}_{N-\mathbf{k}\downarrow} \right]$$

$$\hat{\gamma}^{\eta}_{\mathbf{k}\downarrow} = \sum_{N} \left[u^{\eta *}_{N\mathbf{k}} \hat{a}_{N\mathbf{k}\downarrow} - v^{\eta *}_{N\mathbf{k}} \hat{a}^{\dagger}_{N-\mathbf{k}\uparrow} \right] \qquad (4.10)$$

The corresponding ground state $|\Psi_g\rangle$ of the mean field Hamiltonian is defined as having no quasiparticle excitations present, i.e. $\hat{\gamma}^{\eta}_{\mathbf{k}\sigma}|\Psi_g\rangle = 0$. It can be be shown to be given by:

$$|\Psi_g\rangle \propto \prod_{\eta\mathbf{k}} \hat{\gamma}^{\eta}_{\mathbf{k}\uparrow} \hat{\gamma}^{\eta}_{-\mathbf{k}\downarrow} |\Psi\rangle. \qquad (4.11)$$

Here $|\Psi\rangle$ is a state in which all single particle states with energy less than $\mu_F - \omega_D$ are empty and all single particle states with energy higher than $\mu_F + \omega_D$ occupied. If this were not the case, Eq. (4.11) would yield zero since

$$\hat{\gamma}^{\eta}_{\mathbf{k}\sigma} = \begin{cases} \hat{a}_{\eta\mathbf{k}\sigma} & \text{for } \xi_{\eta\sigma} > \omega_D \\ \hat{a}^{\dagger}_{\eta\mathbf{k}\sigma} & \text{for } \xi_{\eta\sigma} < -\omega_D \end{cases} .$$

[5] At least close to H_{c2}.

From Eqs. (4.10)-(4.11), we see that the ground state is a coherent superposition of states where the pairs $\hat{a}^{\dagger}_{N\mathbf{k}}\hat{a}^{\dagger}_{N',-\mathbf{k}}|0\rangle$ are either occupied or unoccupied. When we have a Landau level at the chemical potential μ_F (n_F =integer), it does not cost any kinetic energy to make a superposition of states with either occupied or unoccupied pairs formed by electrons in that level. The instability towards superconductivity is therefore at a maximum when we have $\mu_F = (n+1/2)\hbar\omega$. As we noted before, the grand canonical potential of the normal state is at a maximum [100] when $\mu_F = (n+1/2)\hbar\omega$ and we conclude that $\Omega_S - \Omega_N$ and Ω_N oscillate 180° out of phase. This analysis is true for both constant chemical potential and constant number of particles. In the latter case one works with the Helmholtz free energy but the conclusions are the same. This is the physical picture of the damping of the magnetic oscillations that naturally emerges from our formalism.

Norman *et al.* [84] interpret the damping of the magnetic oscillations as an effect of the broadening of the Landau levels due to superconducting order. An alternative explanation has been put forward P. Miller and B. L. Györffy [78] which emphasizes the role of non-diagonal pairing. There is in fact an intimate link between the two approaches that we can elucidate by the following simple calculation: we estimate $\Omega_\mathrm{S} - \Omega_\mathrm{N}$ (for simplicity we consider $T = 0$ where the grand canonical potential is simply the ground state energy) for the two cases when (I) the chemical potential is at a Landau level (n_F integer; maximum of the free energy) and (II) when it is exactly between two LL (n_F is half an odd integer; minimum of the free energy). In both cases, the lowest order effect of the pairing is to mix degenerate hole and electron levels as explained in section 3.6.2. Thus, from degenerate perturbation theory we obtain to lowest order in $\Delta(\mathbf{r})$ that the quasiparticle levels are given by $E^{\eta}_{\mathbf{k}} = |\xi_\eta| \pm |F_{\mathbf{k}\eta}|$. Here $|F_{\mathbf{k}\eta}|$ is the pairing matrix element connecting the degenerate states. However, for n_F integer only the positive solution $E^{n_F}_{\mathbf{k}} = +|F_{\mathbf{k}n_F}|$ should be taken for the Landau level at the chemical potential. Now, using the following expression for the ground state energy

E_g [6]

$$E_g \equiv \langle \Psi_g | \hat{H}_{mean} | \Psi_g \rangle = -\sum_{\eta \mathbf{k} \sigma} E^{\eta}_{\mathbf{k}\sigma} \int d^3r \, |v^{\eta}_{\mathbf{k}}(\mathbf{r})|^2 + \sum_{\eta \mathbf{k} \sigma} \int d^3r \, v^{\eta}_{\mathbf{k}}(\mathbf{r}) \mathcal{H}_{0,\sigma} v^{\eta}_{\mathbf{k}}(\mathbf{r})^*$$

it is easy to show that to lowest order in $\Delta(\mathbf{r})$:

$$\Omega_S - \Omega_N = \begin{cases} -\frac{1}{2}\sum_{\mathbf{k}} |F_{n_F \mathbf{k}}| & \text{for } n_F \text{ integer} \\ 0 & \text{for } 2n_F \text{ equal to an odd integer.} \end{cases}$$

This is essentially because the change in the quasiparticle energies cancel pairwise when n_F is half an odd integer whereas one is left with the change $|F_{n_F \mathbf{k}}|$ of the level at the chemical potential when n_F is an integer. Therefore, the minimum of the oscillation is reduced by substantially less than the maximum, which shows that the damping of the oscillations is a direct consequence of the broadening of the quasiparticle levels accompanied by the mixed orbital character of quasiparticle excitations.

4.6 Finite Zeeman splitting

We saw in section 4.2.2 that the effect of including the electron spin in the normal state was to attenuate the k'th harmonic of the oscillations of the grand canonical potential by a factor $\cos(g^* \pi k \frac{m}{2m_0})$. This reduction in amplitude was simply due to the splitting of the Landau levels into two sublevels corresponding to spin up and spin down. In the mixed state, we must also expect that the inclusion of spin reduces the magnitude of the oscillations in Δ_0 and $\Omega_S - \Omega_N$. In the language of section 4.5, we can never have the situation whereby pairing betweens electron of opposite spins occurs without a cost in kinetic energy. Thus, the increase in the instability towards superconductivity when n_F is an integer is decreased, and the oscillatory effect of

[6] This expression can easily be derived by expressing the field operators using Eq. (2.6) and the BdG equations.

$\Omega_S - \Omega_N$ is damped. The mathematical reason for the reduction in oscillations is that for finite spin, $\xi_{n_1\downarrow}$ and $\xi_{n_2\uparrow}$ can never be zero at the same time. Thus, the large factors $[\tanh(\beta\xi/2) + \tanh(-\beta\xi/2)]/(\xi - \xi) = \frac{\beta}{2}\cosh^{-2}(\beta\xi/2)$ in Eq. (3.29) coming from the terms with $\xi_{n1\downarrow} = -\xi_{n1\uparrow}$, are reduced by a factor $\cosh^{-2}(\beta\xi/2)$ as compared to the $\xi_{n1\downarrow} = \xi_{n1\uparrow} = 0$ case for no spin splitting. Hence, we expect the magnetic oscillations in the mixed state to be reduced due to spin. The question is whether this reduction is larger or smaller than the corresponding reduction in the normal state oscillations, thus giving rise to extra damping effects. Within the region of validity of the perturbation expansion of $\Omega_S - \Omega_N$, the answer is that the amplitude of the first harmonic of the dHvA oscillations in the mixed state is reduced by a factor $\cos(\pi\frac{gm}{2m_0})$. Thus, the reduction of the oscillations due to the presence of a finite Zeeman term is the same as in the normal state and the relative damping due to superconductivity is therefore insensitive to the electron spin. This result will be proved in section 4.8.2. We have confirmed this result by solving the BdG-equations numerically with and without a finite Zeeman splitting. The reduction in the amplitude in both the mixed and in the normal state, as compared to the amplitude with no spin splitting, corresponds very well to a $\cos(\pi\frac{gm}{2m_0})$-factor in the region where the mixed state is described well by the perturbation expansion. Deeper into the mixed state, beyond the convergence radius of the perturbation series, the numerical results indicate that the effect of spin is suppressed by the superconducting order. The reduction in the amplitude of the magnetic oscillations due to a finite Zeeman term is less than the $\cos(\pi\frac{gm}{2m_0})$-factor. This is due to the fact that when the superconducting order increases, the pairing interaction starts to dominate the Zeeman term and the effect of any finite g^*-factor is suppressed.

So we conclude that within the region described well by our perturbative expansion, a finite Zeeman term does not alter the rate of the damping of the magnetic oscillations due to superconductivity. When only the first harmonic is important, the effect of the Zeeman term close to H_{c2} is simply a reduction by a factor $\cos(\pi \frac{gm}{2m_0})$ of the amplitude of the oscillations in both the mixed and normal states. Deeper into the mixed state, the superconducting order starts to suppress the effect of the spin splitting and the magnetic oscillations are less affected by a finite Zeeman term. Hence in this region, the relative size of the magnetic oscillations in the mixed state as compared to the normal state is larger for finite spin-splitting and the damping is less efficient as compared to the spinless case.

4.7 Conserved number of particles

As mentioned in section 4.2.3, it is well known that for a 2D system with a fixed number of particles, the magnetic field dependence of the chemical potential $\mu_F(H)$ has a strong effect on the magnetic oscillations in a normal metal when higher harmonics are important. For low temperatures and clean samples, the shape of the oscillations look qualitatively different in the normal state when the chemical potential is fixed as compared to when the number of particles N is fixed [99]. In the theory presented in this chapter, we have until now only considered the case of a constant chemical potential. It is of interest to examine the behaviour of the oscillations in the mixed state for fixed N. When the number of particles is constant, we need to consider the Helmholtz free energy $F = \Omega + N\mu_F$ instead of the grand canonical potential. The chemical potential is determined implicitly by the equation

$$\langle \hat{N} \rangle = \sum_{\sigma N \mathbf{k} \eta} [|u^{\eta}_{N\mathbf{k}}|^2 f(E^{\eta}_{\mathbf{k}\sigma}) + |v^{\eta}_{N\mathbf{k}}|^2 (1 - f(E^{\eta}_{\mathbf{k}-\sigma})] = N \tag{4.12}$$

This is a numerically cumbersome problem since we need to solve the BdG-equations self-consistently for a given chemical potential, then calculate $\langle \hat{N} \rangle$ and repeat the calculation for a new value of μ_F until Eq. (4.12) is obeyed. It is tempting to assume that the chemical potential is unchanged in the mixed state as compared to the normal state. Thus, we could naively calculate the

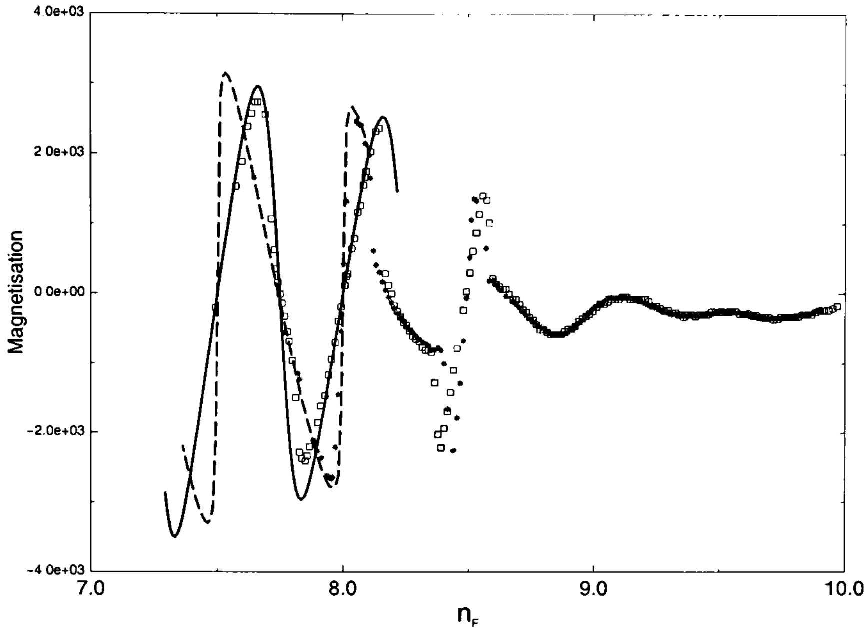


Figure 4.6: The magnetization when the chemical potential is constant (□) and when the number of particles is constant ($*$) for a very low temperature. The solid and dashed lines are the normal state magnetization for fixed chemical potential and fixed number of particles respectively.

chemical potential for the normal state and then solve the BdG equations with this μ_F. This would make the numerical problem much easier. However, it is essential that we determine the chemical potential self-consistently. The reason is that the oscillations in the normal state chemical potential as the external field is varied would generate persistent magnetic oscillations of the free energy in the mixed state even when the Landau level structure is completely destroyed by superconducting order. These oscillations would, of course, be unphysical. Hence, we must resort to the numerically demanding problem of solving the BdG equations for a varying field with a fixed number of particles.

In Fig. 4.6, we plot the magnetization when the chemical potential is constant (□) and when the number of particles is constant ($*$) for a very low temperature. We have chosen parameters such that $\omega_D/\omega_c = 5$, $\frac{g}{\hbar\omega_c l^2} = 9.0$, and $k_B T/\hbar\omega_c = 0.05$ and $g^* m/m_0 = 1$ when $n_F = 12$. For comparison, the

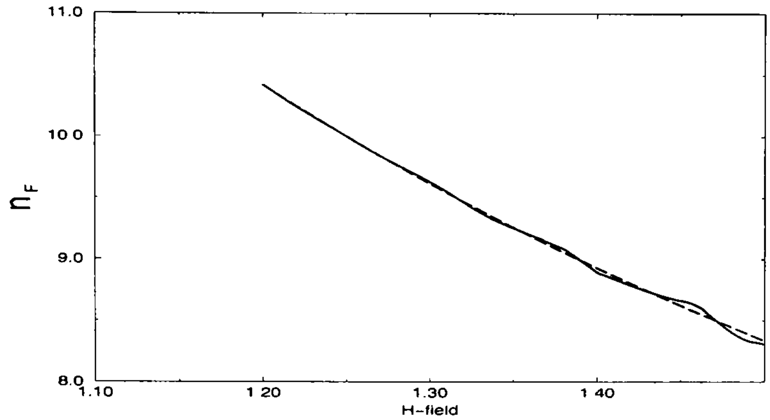


Figure 4.7: n_F as a function of the magnetic field for fixed chemical potential (dashed line) and fixed number of particles (solid line).

solid and dotted lines give the magnetization in the normal state for $n_F \gtrsim 8.2$ for conserved μ_F and N respectively. In the normal state, we note the difference between the oscillations in the two cases. The reason for the difference is that we have chosen a perfectly clean system at a very low temperature such that many harmonics in Eq. (4.3) contribute to the magnetization in the normal state. In the mixed state, we see that there is only a significant difference between the two curves close to H_{c2} ($n_F \approx 7.7$ at H_{c2}). Deeper into the mixed state, the oscillatory behaviour of the chemical potential is damped by the superconducting order and it becomes practically constant. In this regime, there is no difference between the oscillations for constant N and for constant μ_F as can be seen from Fig. 4.6 for $n_F \gtrsim 8.6$. This is illustrated in Fig. 4.7 where we have plotted $n_F = \mu_F(H)/\hbar\omega_c - 0.5$ as a function of the magnetic field ($H_{c2} \approx 1.5$) for the parameters given above, when the number of particles N is constant (solid line) and when the chemical potential is constant (dashed line). Above H_{c2}, the chemical potential oscillates with the varying external field in order to keep N constant, as explained in section 4.2.3. From Fig. 4.7, we see that the oscillations in the chemical potential when N is constant are damped in the mixed state. The reason is that the order parameter broadens the Landau levels thereby making the depletion of a level going through the chemical potential less abrupt. Once the superconducting order has damped the oscillations in the magnetization, it has also damped the oscillations in $\mu_F(H)$ and the behaviour for fixed N is essentially the same as for fixed μ_F. Thus, the conclusion is that although there is some difference in the dHvA signal close to H_{c2} when N is conserved as opposed to fixed μ_F, the overall rate of damping of the oscillations is essentially the same in the two cases. We are reminded that the difference between the two cases is only important for very pure systems and low temperatures such that many harmonics contribute in Eq. (4.3). Experimentally, one often only observes the leading harmonic ($k = 1$) in the magnetization since the systems are never perfectly clean. Assuming that the impurity scattering is unaltered by the superconducting order, we therefore expect there will be no difference between the case of fixed N and fixed μ_F in the mixed state for realistic impurity concentrations. In the rest of this chapter, we will therefore restrict ourselves to considering experimentally realistic conditions, in which case only the first harmonic is important. We can then, to a good approximation, assume that the chemical potential is constant.

4.8 Simplified form for the damping

The perturbative theory for the magnetic oscillations has yielded a natural interpretation of the damping of the magnetic oscillations in the mixed state. Also, it provides a significantly quicker way of calculating the damping close to H_{c2}, as it is much easier to calculate the $\alpha(T, H)$ and $\gamma(T, H)$ coefficients given in Eq. (3.29)-(3.30) as a function of the field, than it is to solve the BdG equations self-consistently for a varying field. In fact, for most experimentally realistic parameters, it is unfeasible to solve the BdG equations numerically as there are too many Landau levels participating in the pairing. Then, the perturbative expansion offers a way of calculating the onset of the damping close to H_{c2}. However, it would be interesting to simplify the theory such that we can make predictions concerning the dependence of the damping on the magnetic field, temperature, spin etc. Such predictions are very useful in order to compare the theory with experimental results. As they stand, Eqs. (3.29)-(3.30) are rather complicated and, in order to make the predictions stated above, they must be simplified. In this section, we will give some simple analytical expressions for the expansion coefficients. Using these, the dependence of the damping on the temperature, spin and the magnetic field can then be extracted.

4.8.1 The first harmonic of the condensation energy

To obtain a simple form for the damping, we must take a closer look at the coefficients $\alpha(H)$ and $\gamma(H)$ given in Eq. (3.29) and Eq. (3.30). As mentioned in section 4.4, the Gor'kov expansion is a high temperature expansion and it is therefore most relevant for temperatures such that only the lowest harmonics of the dHvA signal are significant. This allows us to focus only on the zeroth and first harmonics of the relevant quantities. Thus, we take $\alpha(H)$ to have the form:

$$\alpha(H) \simeq a_1(1 - H_{c2}/H) - a_2 \cos(2\pi n_F) \tag{4.13}$$

where $a_1 > 0$ and $a_2 > 0$. The coefficients a_1 and a_2 will in general depend weakly on the magnetic field but we assume they are constant. This is reasonable since for $n_F \gg 1$ the rate of change of a_1 and a_2 is very slow as compared to the frequency $\mu_F mc/\hbar e$ of the oscillations. The essential physics comes from the sign change of $\alpha(H)$ at H_{c2} and its oscillatory behaviour, combined with the features of $\gamma(H)$ described below. We have assumed that $\alpha(H)$ has a local minimum when n_F is an integer. This is in agreement with the conclusion made in section 4.3.1, that the instability towards superconductivity is greatest when a Landau level is at the chemical potential (See Fig. 4.1). Note that Eq. (4.13) does not seem to be a very good approximation to describe the functional form of $\alpha(n_F)$ as depicted in Fig. 4.1. This is because the relative variation of n_F for this plot is rather big as $n_F \sim \mathcal{O}(10)$ is small. For larger n_F ($n_F \gtrsim 100$), the relative change of n_F around H_{c2} is small such that Eq. (4.13) is an excellent description of the functional form of $\alpha(n_F)$. This has been checked by evaluating $\alpha(n_F)$ exactly from Eq. (3.29). Likewise, the fourth order coefficient $\gamma(H)$ is assumed to have the form:

$$\gamma(H) \simeq g_1 + g_2 \cos(2\pi n_F) \tag{4.14}$$

where $g_1 > 0$ and $g_2 > 0$. Again, both g_1 and g_2 depend on the magnetic field but this dependence is weak as compared to the strong oscillatory behaviour coming from the Landau level structure. Note that we have opposite signs for the first harmonics of $\alpha(H)$ and $\gamma(H)$. This is because $\gamma(H)$ has a local maximum when n_F is an integer since we then have terms in Eq. (3.31) where the denominator is zero. Again, by using l'Hospital's rule, it is easy to see that these terms will dominate the sum and that $\gamma(H)$ thus has a local maximum. In Appendix A, we outline the calculations in order to extract a_2 and g_2 from Eq. (3.29) and Eq. (3.30) whereas the calculations to obtain a_1 and g_1 are given in Appendix B. Using these approximate forms for $\alpha(H)$ and $\gamma(H)$, we obtain for the condensation energy

$$\Omega_S - \Omega_N = -\frac{\alpha^2(T,H)}{4\gamma(T,H)} \simeq -\frac{[a_1(1 - H_{c2}/H) - a_2\cos(2\pi n_F)]^2}{4[g_1 + g_2\cos(2\pi n_F)]}. \tag{4.15}$$

Assuming that $g_2 \ll g_1$, we obtain the following approximate form for the first harmonic of $\Omega_S - \Omega_N$ to first order in g_2/g_1:

$$\begin{aligned}(\Omega_S - \Omega_N)_1 \;\simeq\; & -\frac{1}{4}\left[\frac{2a_1a_2}{g_1}(H_{c2}/H - 1)\right.\\ & \left. - \frac{g_2a_1^2}{g_1^2}(H_{c2}/H - 1)^2 - \frac{3g_2a_2^2}{4g_1^2}\right]\cos(2\pi n_F)\end{aligned} \tag{4.16}$$

where $\Omega(H)_n$ is the n'th harmonic of $\Omega(H)$. It should be recalled that the above expression is, of course, only valid for $\alpha(H) < 0$. We thus obtain the following form for the first harmonic of the grand canonical potential:

$$\Omega_{S1} = \Omega_{N1} + (\Omega_S - \Omega_N)_1 \tag{4.17}$$

where the first harmonic Ω_{N1} of the normal state grand canonical potential is given by Eq. (4.3) and $(\Omega_S - \Omega_N)_1$ is given in Eq. (4.16).

4.8.2 The dependence of the damping on spin, temperature and magnetic field

As we now have approximate closed expressions for the perturbation terms, we will in this section draw some conclusions from the general form of the damping of the dHvA-oscillations due to the growth of the superconducting order as described by Eq. (4.16). The first thing we notice is that in this approximation, the superconducting damping has a simple polynomial form in $(H_{c2}/H - 1)$. The damping is maximum for $(H_{c2}/H - 1) = \frac{a_2 g_1}{a_1 g_2}$. For $(H_{c2}/H - 1) > \frac{a_2 g_1}{a_1 g_2}$, the damping decreases when we go deeper into the superconducting state and for $(H_{c2}/H - 1) > \frac{2a_2 g_1}{a_1 g_2}$ the magnetic oscillations are *enhanced* by the superconducting order; perturbation theory predicts that $\Omega_S - \Omega_N$ oscillates in phase with Ω_N. This explains the observations made in section 4.4 were we noticed that once the field got too low, the perturbative result predicted an enhancement of the dHvA oscillations. The in-phase oscillations between $\Omega_S - \Omega_N$ and Ω_N are due to the oscillatory behaviour of $\gamma(H)$. As we noted in section 4.8.1, $\gamma(H)$ oscillates in phase with Ω_N. When the smooth part of $\alpha(H)$ is sufficiently large, the oscillatory behaviour of $\Omega_S - \Omega_N = -\alpha^2/4\gamma$ will be determined by $\gamma(H)$. Then, $\Omega_S - \Omega_N$ will oscillate in phase with Ω_N and we will get an enhancement of the oscillations of Ω_S compared to Ω_N. Again, as in section 4.4, we must emphasize that this prediction is obviously an indication that our perturbative scheme has broken down. The enhancement has never been observed experimentally nor does it agree with any numerical results: it is not a real physical effect.

Using the approximate closed analytical expressions for a_i and g_i, we can now make some quantitative predictions concerning the spin and temperature dependence of the damping. From Eq. (4.16) and the temperature dependence of a_i and g_i, we conclude that the first harmonic of the condensation energy $(\Omega_S - \Omega_N)_1$ is proportional to $k_B T \exp(-2\pi^2 \frac{k_B T}{\hbar\omega_c})$. From Eq. (4.3), we have $\Omega_{N1} \propto k_B T \exp(-2\pi^2 \frac{k_B T}{\hbar\omega_c})$ when $2\pi^2 k_B T/\hbar\omega_c \gtrsim 1$. Thus, the temperature dependence of the magnetic oscillations in the mixed state is the same as in the normal state. This result has been confirmed by experimental observations [30]. Likewise, from the spin dependence of a_i and g_i, we see that the effect of a finite Zeeman term on $(\Omega_S - \Omega_N)_1$ is a reduction in the amplitude by a factor $\cos(\pi \frac{g^* m}{2m_0})$. Hence, our perturbation theory reproduces the numerical result stated in section 4.6 for fields close to H_{c2}. The reduction factor is the same as for the oscillations in the normal state (see section 4.2.2). We therefore have no extra damping effects due to spin close to the transition line where the perturbation theory is valid.

In order to compare with experimental data, it is convenient to express the damping of the oscillations through a factor $R_s \equiv \Omega_{S1}/\Omega_{N1}$. It is customary to define a field dependent "scattering rate" τ_s such that $R_s = e^{-\pi/\omega_c \tau_s}$. This brings the damping of the oscillations due to superconductivity into the same form as the damping due to impurity scattering (see section 4.2.1). We will assume that the damping of the oscillations due to impurity scattering is the same in the mixed state as in the normal state, i.e. we write for the total scattering rate $\tau_t^{-1} = \tau_s^{-1} + \tau^{-1}$ (Matthiessen rule) where τ is the scattering rate due to impurities in the normal state. Now, from Eq. (4.17) we have:

$$\tau_s^{-1} = -\frac{\omega_c}{\pi} \ln(1 + (\Omega_S - \Omega_N)_1/\Omega_{N1}) \simeq -\frac{\omega_c a_1 a_2}{2\pi g_1 \Omega_{N1}} (H_{c2}/H - 1) \tag{4.18}$$

where we have used Eq. (4.16). The approximate equality is only valid for

$\frac{a_2 g_1}{a_1 g_2} \gg H_{c2}/H - 1$ such that only the linear term in Eq. (4.16) contributes to the damping. Using the expressions for a_i, g_i, and Ω_{N1}, we obtain

$$\frac{1}{\tau_s} = \frac{\omega_c(H_{c_2}) a_x^2 5.4\sqrt{n_F}}{8l^2\sqrt{\pi}}(1 - H/H_{c2}) \tag{4.19}$$

where $\omega_c(H_{c2}) = \frac{eH_{c2}}{mc}$. We see that the magnetic field dependence of the scattering rate close to H_{c2} is determined by the factor $1 - H/H_{c2}$ apart from the weak dependence through $\sqrt{n_F}$. One of the most thorough experimental investigations of the dHvA oscillations in the mixed state has been performed by Janssen *et al.* [61] on the compounds Nb_3Sn and V_3Si. In a series of careful experiments, they measured the field dependence of the scattering rate. It was found that the scattering rate for Nb_3Sn obeys the relation $\tau_s^{-1} \propto 1 - H/H_{c2}$ very well in agreement with our theoretical prediction. However, although Nb_3Sn is a layered compound, the Fermi surface is really three dimensional since the variation of the Fermi surface area perpendicular to the applied field is much greater than the difference $2\pi eH/\hbar c$ in area of consecutive Landau orbits. Thus, a quantitative comparison between their data and our 2D theory is unfortunately not possible.

4.9 Comparison with experiments

We will in this section compare the predicted damping rate, as given in Eq. (4.19), with experimental data. In this thesis, we have concentrated on a model for 2D systems. Hence, we need to compare with an essentially 2D material. The charge transfer salts such as κ-$(ET)_2Cu(NCS)_2$ are layered systems with almost perfect 2D Fermi surfaces[7]. They are characterized by the formation of a salt as a result of the partial oxidation of an organic molecule [27]. The ET molecules stack in planes separated by layers of the

[7] ET is an abbreviation for the molecule bis(ethylenedithio)-tetrathiafulvalene or BEDT-TTF.

$Cu(NCS)_2$ anions. The transfer of electrons occurs readily within the 2D planes since the organic molecules contain unpaired electrons in π orbitals and the π orbitals on neighbouring molecules overlap within the plane. Since there is almost no electron transfer through the planes of the inorganic anions, the system behaves to a good approximation as if it consisted of conducting planes separated by insulating layers [27]. Such materials should therefore be well described by a 2D theory such as the one developed in this chapter .

The salt which is of interest to us is κ-$(ET)_2Cu(NCS)_2$ because it is superconducting with $T_c = 10.4$K at $H = 0$. The Fermi surface of this compound consists of a quasi-2D hole pocket and a quasi-1D electron section [108]. It is the quasi-2D hole pocket which contributes to the fundamental frequency of the dHvA oscillations. The quasi-1D section of the Fermi surface only plays a role when magnetic breakdown effects cause the electrons to jump from the 2D pocket to the 1D section. This magnetic breakdown only appears at very high fields $H \gtrsim 20T \gg H_{c2}$ [26] and the 1D section of the Fermi surface is thus irrelevant to the present analysis. κ-$(ET)_2Cu(NCS)_2$ is an extreme type-II superconductor with a short coherence length (between 70 and 100Å) and a penetration depth of $\approx$ 5350Å [27] giving a Ginzburg-Landau parameter $\kappa \approx 70$. It is therefore well-suited to test our theory which is only valid for materials with $\kappa \gg 1$. dHvA measurements for the system in the normal state (i.e. $H > H_{c2}$) yield magnetic oscillations with a fundamental frequency of 597 ± 5T [110, 111]. The frequency exhibits almost perfect $\cos^{-1}\theta$ behaviour as a function of the angle θ between applied field and the normal to the layers, indicating the strong two-dimensionality of the compound [114]. The effective mass m associated with this hole pocket, deduced from the temperature dependence of the dHvA oscillations, is $m \approx 3.5m_0$ when $\theta = 0°$. One also observes the dHvA oscillations in the mixed state below H_{c2} [110, 111]. The frequency of the oscillations is unaltered as compared to the normal state but the amplitude is reduced. As explained in section 4.8.2, this attenuation of the oscillations can be parametrized by a

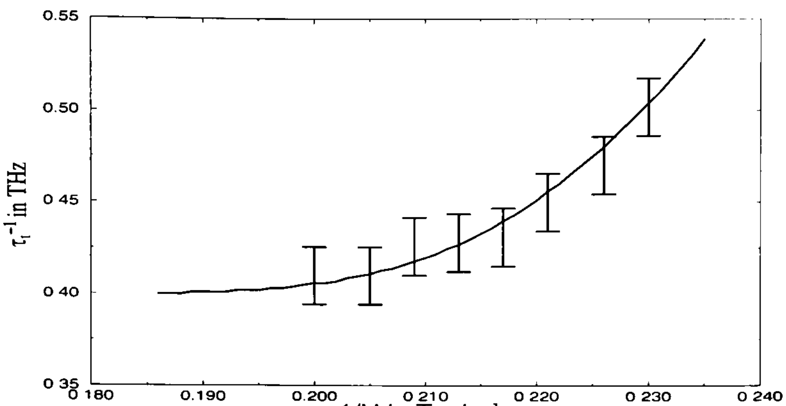


Figure 4.8: τ^{-1} as a function of $1/H$. The solid line is the theoretical prediction based on Eq. (4.19) and the bars are the experimental data.

field dependent scattering rate τ_s such that the total damping due to superconductivity and impurities is $e^{-\pi/\omega_c\tau}$ with $\tau_t^{-1} = \tau_s^{-1} + \tau^{-1}$, τ being the scattering rate from impurities. By assuming that the impurity scattering rate τ is unaltered by the presence of superconductivity, one can deduce τ_s from the extra attenuation of the dHvA oscillations in the mixed state. In Fig. 4.8, we plot the experimental data for τ_t^{-1} (bars) measured in (THz) as a function of $1/H$ measured in Tesla^{-1}. The data are obtained from the experiments by van der Wel *et al.* [110, 111]. We see that there is a constant scattering rate due to impurities of $\tau \simeq 0.4 \times 10^{12} s^{-1}$ when the system is in the normal state. More importantly, we note that the onset of the additional attenuation on passing from the normal to the mixed state. From Fig. 4.8, we see that $H_{c2} \approx 4.6$T giving $n_F \approx 150$ at H_{c2}. Unfortunately, it is experimentally impossible to determine H_{c2} precisely. Due to impurities and sample inhomogeneities, the transition from the normal state to the superconducting state occurs over a field range of approximately 2T [27].

To compare our theory with this set of experimental data, we have calculated the damping rate due to superconductivity from Eq. (4.19). We note that for this many Landau levels participating in the pairing, a numerical solution of the BdG equations is not feasible and we have to rely on the perturbation theory in order to come with any theoretical predictions. From Eq. (4.19), we immediately see that the theory predicts a sharp onset of an additional damping due to superconductivity when $H < H_{c2}$. This does not correspond to the observed smooth increase of τ_t^{-1} as seen in Fig. 4.8. To reproduce this effect, we assume a Gaussian spread in H_{c2}. This method was introduced by van der Wel *et al.* [110, 111] in order to model the experimental uncertainty in H_{c2} and thus to obtain a better fit with theoretical predictions[8]. The solid curve in Fig. 4.8 is our theoretical prediction obtained from Eq. (4.19) using $n_F = 150$. We have used the Gaussian distribution of H_{c2} around $H_{c2} = 4.6$T explained in Ref. [110, 111]. The agreement between the theory and the experimental data is good. Importantly, the theory based on Eq. (4.19) predicts the right order of magnitude of the additional damping due to superconductivity. Note, that the only free parameter in our theory is H_{c2} (see Eq. (4.19)). Contrary to the theories described in section 4.10, we do not have free parameters such as the size of the order parameter. This fact makes the agreement between theory and experiment somewhat more satisfactory. Unfortunately, due to the uncertainty in H_{c2} and the rather few experimental data points for $H < H_{c2}$, a more precise and rigorous comparison between our theory and the experiment cannot be made.

Much better experimental data for the 3D systems V_3Si and 2H-$NbSe_2$ has recently been published [61]. Therefore, in order to check the validity of the theory presented, it would be desirable to extend our theory to 3D systems and then compare its predictions with the data published in Ref. [61]. This extension should be rather straightforward, as we know from section 3.2 that the motion along the field is unaltered by a non-zero H. This line of research may possibly be taken up in the future.

[8]These authors compared their experimental results with the theory of Maki [71] which will be described in section 4.10.1.

4.10 Other theories

A number of competing theoretical models have been proposed for the dHvA effect below H_{c2}. We will finish this chapter by briefly describing some of these theories and compare their predictions with the ones stated in this chapter.

4.10.1 The theories of Stephen, Maki and Wasserman and Springford

The approach of Stephen [102] is based on solving the Gor'kov equations given in Eq. (2.19). They are solved by regarding the order parameter $\Delta(\mathbf{r})$ as a random potential in which the electrons scatter. In the limit of strong fields, the author obtain a damping of the oscillations $\exp(-\pi/\omega_c\tau_s)$ with the scattering rate τ_s given by:

$$\frac{1}{\tau_s} = \frac{\Delta^2}{\hbar^2\omega_c}\sqrt{\frac{\pi}{n_F}} \tag{4.20}$$

Here Δ is the spatial average of the order parameter. Maki [71] obtained the same result by quantizing a semiclassical Green's function introduced by Brandt et al. [18]. By using this Green's function in a more general field theoretical scheme, Wasserman and Springford [112, 113] also obtained the result given in Eq. (4.20). They considered corrections to this result coming from the spatial dependence of $\Delta(\mathbf{r})$, but they found that such corrections were insignificant.

Note that a common feature of these theories is that the order parameter is *not* determined self-consistently; it is simply a free parameter which can be determined, for instance, by the semiclassical equation $\Delta(H) = \Delta(0)\sqrt{1 - H/H_{c2}}$. Thus in order to compare our theory with this result, we must ignore for the moment the oscillations in Δ_0 and treat it formally as a free parameter (i.e. $(\Omega_S - \Omega_N)_1 = -a_2\Delta_0^2 + g_2\Delta_0^4 + \dots$). We will focus on the Δ^4-term since there are discrepancies between the predictions of different authors for this term. From Eq. (3.10), we have:

$$\Delta^2 \equiv (L_x L_y)^{-1} \int d^2r |\Delta(\mathbf{r})|^2 = \frac{g^2 a_x}{\sqrt{2} L_x^2 L_y^2 l} \Delta_0^2. \tag{4.21}$$

Using Eq. (A.10) and Eq. (4.3), we obtain the formal result for the fourth order term:

$$(\Omega_S - \Omega_N)_1|_{\Delta^4-term} = g_2 \Delta_0^4 \approx \Omega_{N1} \frac{10}{n_F} \left(\frac{\Delta}{\hbar\omega_c}\right)^4 \tag{4.22}$$

By expanding $\exp(-\pi/\omega_c \tau_s)$ using Eq. (4.20), we obtain $\sim 16\Omega_{N_1}/n_F(\Delta/\hbar\omega_c)^4$ for the same quantity, according to the theory presented by Stephen. Note that the n_F dependence of the two results agree. As we will see in section 4.10.2, this n_F dependence does not agree with some other theories. The numerical prefactors have the same order of magnitude but differ by about 50%. Considering the difference in the approaches of the two theories, such a difference is not surprising. The arguments stated in appendix A can easily be generalized to the first harmonic of the Δ^{2n} expansion coefficient taking Δ as a free parameter. Since this dependence comes from the coefficients $B_0^{n_1,n_2}$, we immediately get from Eq. (A.1) that the n_F dependence of the first harmonic of the Δ^{2n}-term is ${n_F}^{-n/2}$. This n_F dependence agrees with the result obtained by Stephen. However, one must remember that the order parameter itself is an oscillatory function of the field as can be seen numerically from Fig. 4.3 or analytically from Eq. (4.5). This oscillatory behaviour is important to include in a self-consistent theory for the dHvA oscillations. In my opinion, theories, such as the one by Stephen *et al.* described in this section, which present the damping of the oscillations as a function of a free but smoothly varying order parameter Δ, have limited validity.

4.10.2 The theory of Maniv, Rom, Vagner and Wyder

The theory of Maniv *et al.* is based on the same idea as the one presented in this chapter. It uses the Gor'kov expansion Eq. (3.22)-(3.25) of the grand canonical potential up to fourth order in $\Delta(\mathbf{r})$ as a starting point. Also, the theory is for simplicity only considered for 2D systems and the approximation $\Delta_{j\neq 0} = 0$ is made. However, since the symmetry of the order parameter is not used to simplify the calculations, the algebra is complicated and they have to use various semiclassical and other approximations in order to solve the integrals given in Eqs. (3.23)-(3.24) [72, 116]. Note that the use of the symmetry of $\Delta(\mathbf{r})$ was crucial in enabling us to solve these integrals exactly as explained in section 3.7.3. Perhaps owing to the complexity of the algebra, the authors draw some rather surprising and contradictory conclusions from their calculations:

They predict that the amplitude of the dHvA oscillations *increases* in the mixed state below H_{c2} [73, 76]. This prediction is in contradiction to the analytical results for the perturbation terms presented in this thesis. In particular, it cannot be reconciled with the simple physical picture of $\Omega_S - \Omega_N$ oscillating in anti-phase with Ω_N due to the enhanced instability towards superconductivity when there is a Landau level at the chemical potential. Also, it is not confirmed by numerical solutions to the BdG equations as presented in this thesis and by other authors [83, 84]. Furthermore, this increase has never been observed experimentally. These facts indicate, in my opinion, that their prediction must be based on a flawed evaluation of the expansion terms.

Indeed, this assumption is confirmed by some later publications, where, in contradiction to their predictions stated above, they state that $\Omega_S - \Omega_N$ oscillates in antiphase with Ω_N thus giving rise to the damping [74]. This result is in agreement with the conclusions reached in this chapter. However, as in the theories outlined in section 4.10.1, they take the order parameter as a free parameter thereby neglecting its oscillatory behaviour. Also, they predict that the Δ^4-term is $\propto n_F^{-3/2}$ in contradiction with the n_F^{-1} dependence obtained by the theory presented in this chapter and the theories described in section 4.10.1.

The question of the sign inversion

The anti-phase oscillation of $\Omega_S - \Omega_N$ leads Maniv *et al.* to an exiting prediction: one should be able to observe a *sign change* of the first harmonic of the magnetization for fields below $H_{inv} < H_{c2}$ [75, 116]. The oscillations are claimed not to be damped below H_{inv}. Instead, they should persist virtually undamped with a reversed sign in the amplitude. This surprising effect is postulated to occur because the superconducting contribution to the oscillations overwhelms the contribution from the normal grand canonical potential deep enough into the superconducting state. Based on an approximate evaluation of the Gor'kov expansion parameters and assuming that $\Delta(H) = \Delta(0)\sqrt{1 - H/H_{c2}}$, they calculate an expression for H_{inv} [116, 75]. However, they fail to take into account that the order parameter has to be determined self-consistently. Using Eq. (4.16), we easily obtain the result that the maximum amplitude of the antiphase oscillations of $\Omega_S - \Omega_N$ is given by $\frac{a_2^2}{4g_2}$. From our approximate expressions for a_2 and g_2, we have

$$\frac{a_2^2}{4g_2} \simeq \frac{L_x L_y a_x^2 \pi}{l^4 27} k_B T e^{-2\pi^2 \frac{k_B T}{\hbar\omega_c}} \tag{4.23}$$

By comparing this amplitude with the contribution from the normal state oscillations given in Eq. (4.3), one can easily show that the antiphase oscillations of $\Omega_S - \Omega_N$ will never exceed the oscillations in Ω_N [23]. Hence, we can conclude that the argument for the inversion of the oscillations based on the Gor'kov expansion is flawed.

These authors also base their prediction of the sign change on another line of argument: they assume that the quasiparticle spectrum in the mixed state can be described by a simple splitting of the Landau levels into two levels symmetrically placed around each Landau level. This splitting should generate a beating frequency in the oscillatory behaviour of the magnetization M. Once the splitting of the Landau levels due to the superconducting order is of the order $|E_{\mathbf{k}}^{\eta} - \xi_{\eta}|/\hbar\omega_c \approx \pm 0.23$, one should observe a sign change of the dHvA oscillations [75]. However, by solving the BdG equations numerically for various sets of parameters, we have found that the low lying quasiparticle levels lose their Landau level structure and describe essentially localized bound states when the change in energies is of the above magnitude. The crossover to localized states makes the argument leading to the sign change of the first harmonic based on the quasiparticle spectrum invalid. This conclusion is in agreement with the numerical analysis presented by Norman and MacDonald [83]. It therefore seems that there is no theoretical grounding, neither within perturbation theory nor within a numerical solution of the BdG equations, to support the prediction that the dHvA oscillations would persist virtually undamped below H_{c2} and that they would have opposite sign compared to the oscillations in the normal state. Also, there has been no experimental observation of this striking effect, thereby supporting our rejection of its existence.

4.10.3 The theory of Dukan and Tešanović

Dukan and Tešanović focus on the quasiparticle contribution to the grand canonical potential [39]. Inspired by the results for a very high magnetic field as given in section 3.6, they assume that the quasiparticle energies are given by $E_{\mathbf{k}}^{N} = \sqrt{\xi_N^2 + |F_{\mathbf{k}NN}|^2}$. As mentioned in section 3.6, there will be points in the MBZ where $F_{\mathbf{k}NN} = 0$. According to their theory, it is exactly the gapless excitations connected to these zeros that contribute to the magnetic oscillations in the mixed state. To simplify the theory, they assume a simple field-independent form for the order parameter in $\mathbf{k}$-space with gapless and gapped regions. This simplification of the quasiparticle spectrum is not applicable in 2D where the number of gapless points and their dispersion relation vary strongly with the magnetic field. However, the approximation should be somewhat better in 3D as described in chapter 5. These approximations lead to the amplitude of the dHvA oscillations containing an additional damping factor R_s as compared to the normal state, in particular

$$R_s = 2\left[C\max\left(\frac{T}{\Delta},\frac{\Gamma}{\Delta}\right)\right]^2 e^{-2\pi\Gamma/\hbar\omega_c}. \tag{4.24}$$

Here the scattering rate is given by $\Gamma(H) = \sqrt{\Gamma_0\Delta(H)/2}$ with $\Delta(H) = \Delta(0)\sqrt{1-H/H_{c2}}$. The parameter C is a constant of order unity describing the radius of the gapless region in $\mathbf{k}$-space. Again, we note that this theory does not use a self-consistent order parameter but assumes that it has the simple semiclassical form $\Delta(H) = \Delta(0)\sqrt{1-H/H_{c2}}$ thereby ignoring its oscillatory behaviour. Also, the theory completely ignores the contribution from the ground state to the grand canonical potential by focusing only on the quasiparticle excitations. This is rather questionable as the grand canonical potential is *identical* to the ground state energy for $T=0$. One would therefore expect the ground state energy to make a major contribution to the grand canonical potential for the low temperatures relevant for dHvA measurements.

4.10.4 The theory of Miller and Györffy, and Miyake

Miller and Györffy solve numerically the BdG equations corresponding to a tight binding model [78]. Contrary to the theory of Dukan and Tešanović, they focus on the oscillations in the ground state energy by restricting their calculations to $T=0$. They obtain the interesting result that the damping of the oscillations in the mixed state can essentially be ascribed to the fact that the Landau level occupation number $N_{n\sigma}$ changes less abruptly with the magnetic field, since it contains the factors $|u^{\eta}_{n\mathbf{k}}|^2$ and $|v^{\eta}_{n\mathbf{k}}|^2$ which vary on an energy scale Δ (See Eq. (4.8)). In the large gap limit $\Delta \gg k_BT$ they conclude that the damping can be described by a factor

$$R_s = zK_1(z) \tag{4.25}$$

where $z = 2\pi\Delta/\hbar\omega_c$ and K_1 is the Bessel function of imaginary argument. The same result was obtained by Miyake by using various semiclassical approximations [79].

4.10.5 Comparison of the theories with experimental results

As mentioned in section 4.9, Janssen *et el.* [61] have performed a series of dHvA experiments on the 3D materials V_3Si and 2H-$NbSe_2$. They compare their results for the damping of the dHvA oscillations in the mixed state with the theoretical predictions described in sections 4.10.1-4.10.4. Their conclusion is that *none* of the theories presented in this section can explain their experimental data for both V_3Si and 2H-$NbSe_2$. Thus, it seems that more theoretical work is required in order to clarify the mechanism behind the damped dHvA oscillations in the mixed state. As it stands, we cannot compare our theory, which is developed for 2D systems, directly to these measurements, although the $1 - H/H_{c2}$ dependence of $1/\tau_s$ agrees well with their measurements on 2H-$NbSe_2$. It would therefore be very interesting to extend the theory presented in this chapter, which seems to be the only one taking into account the oscillatory behaviour of the order parameter, to 3D systems in order to compare it with their data. Alternatively, more precise measurements of the dHvA oscillations in 2D systems such as κ-$(ET)_2Cu(NCS)_2$ would enable a more rigorous test of our theory.

4.11 Summary

In this chapter, we have presented a theory for the experimentally observed dHvA oscillations in the mixed state of a type II superconductor in the 2D limit. The basis for the theory is a self-consistent Gor'kov expansion of the grand canonical potential. The use of translational and rotational symmetry has simplified the analysis to such an extent that we have been able to calculate the expansion coefficients exactly to any order without using semiclassical or other approximations. Contrary to many other theories for the dHvA effect, an inherent feature of our analysis is the self-consistent determination of the order parameter. This seems to be important as $\Delta(\mathbf{r})$ is an oscillatory function of the external field. The theory has been carefully checked against an exact numerical solution of the BdG equations; we concluded that the perturbation theory works well close to H_{c2}. A physical interpretation of the damping emerged naturally from the perturbative theory: the condensation energy oscillates in antiphase with the normal state grand canonical potential thus producing damping of the dHvA oscillations. The damping is directly connected with the enhancement of superconductivity when we have a Landau level at the chemical potential. Superficially, these antiphase oscillations open up the possibility of a sign change of the first harmonic of the dHvA oscillations in the mixed state. However, a more careful analysis shows that there is no theoretical grounding for this claim.

The effect of spin and a conserved number of particles, as opposed to a conserved chemical potential, was examined. Also, we derived a simple form of our theory which is valid when many Landau levels participate in pairing. As it gives the damping in terms of closed analytical expressions, we have been able to make precise predictions concerning the dependence of the damping on the magnetic field, the temperature and various other parameters. These predictions were compared with experimental data for the quasi 2D organic superconductor κ-$(ET)_2Cu(NCS)_2$. We found good agreement between our theory and the experiment. However, due to experimental uncertainty about H_{c2}, any quantitative comparison is impossible. We concluded that in order to perform such a comparison, we would need to extend our theory to 3D systems where higher quality measurements have been performed- alternatively, it would be interesting to compare it with future experimental results for a 2D system.

Chapter 5

Acoustic attenuation

5.1 Introduction

As we saw in chapter 4, the Landau level quantization of the electron levels has important consequences on various thermodynamic quantities derived from the appropriate thermodynamic potential. We chose to focus on the experimentally observed dHvA oscillations in the mixed state. Unfortunately, as explained in section 4.10, there is a lot of confusion about the interpretation of these oscillations and the agreement between some theories and experimental data is less than convincing. Certain theories attribute the oscillations to the existence of the gapless points in the quasiparticle spectrum whereas others focus on the ground state energy. As the theory presented in chapter 4 indicates, it seems to be necessary, at least for finite T, to include both the gapless excitations and the ground state energy in a complete self-consistent treatment of the dHvA oscillations. This makes an interpretation solely in terms of gapless points dubious. However, the existence of these gapless excitations close to H_{c2} is a fundamental property of the theory for a type-II superconductor in a strong magnetic field. This fact was explained in section 3.6.1 where we solved the BdG equations in the limit of a very high magnetic field such that only one Landau level participates in the pairing.

Also, in section 3.6.2, the gapless points were shown to emerge naturally if one ignores the off-diagonal pairing in the BdG equations (i.e. the diagonal approximation). We noted that this approximation only works well for quasiparticle levels close (on the scale of $\hbar\omega_c$) to the chemical potential. For levels with higher energy, the possible degeneracy between a hole level and an electron level will invalidate the diagonal approximation. The fact that the existence of the gapless excitations close to H_{c2} follows naturally from the microscopic theory makes it desirable to propose an observable which would determine the possible existence of these quasiparticle states. Such an observable would enable a test of our theoretical understanding of superconductors on a fundamental level. Theoretical investigations have suggested that the existence of the gapless points leads to an algebraic temperature dependence of various thermodynamic functions and an algebraic voltage dependence in the tunneling conductance [38].

In this chapter, we consider the attenuation of longitudinal acoustic waves in the mixed state in the clean limit. Since the absorption of the phonons is due to quasiparticle excitations, the experiment directly probes the quasiparticle density of states. Hence, for low frequencies of the sound wave, the attenuation should in principle give information on the character of the low-lying quasiparticle spectrum and, in particular, on the predicted existence of the gapless modes. There have been several calculations of the attenuation in the mixed state. However, for clean systems, theoretical results have proved rather difficult to obtain. Theories based on a simple expansion of the attenuation in powers of the order parameter have been shown to produce unphysical results [32]. It was proposed that this difficulty could be circumvented using a conjectured equivalence between a current-carrying superconductor and a type-II superconductor in high magnetic fields [70]. A more rigorous theory based on a solution to the Gor'kov equations was provided by Brandt *et al.* [18]. Unfortunately, their solution gives completely unphysical results for the acoustic attenuation in the clean limit. Scharnberg showed that this was due to their theory being based on a semiclassical approximation for the Green's function [96]. He therefore suggested that it is crucial to take into account exactly the Landau level quantization of the quasiparticle levels due to the magnetic field when one calculates the attenuation [96]. Using the formalism in chapter 3, we are very well equipped to calculate the attenuation including the Landau levels right from the beginning. In this chapter, we will present such a calculation based on the microscopic Green's function approach. Contrary to earlier calculations, we obtain physically reasonable results for the attenuation in the clean limit. We avoid the difficulties encountered in the semiclassical treatment by Brandt *et al.*, thereby confirming the prediction of Scharnberg. Due to the presence of the Landau levels, we furthermore predict that the attenuation will be an oscillatory function of the magnetic field in analogy with the dHvA oscillations described in chapter 4. In order to obtain simple analytical results, we calculate the attenuation in two limits: $k_BT \ll \hbar\omega$ and $k_BT \gg \hbar\omega$ where $\nu = \omega/2\pi$ is the frequency of the sound wave. We will show that the frequency and temperature dependence of the attenuation is strongly influenced by the existence and the nature of the gapless points in the quasiparticle spectrum for $k_BT \ll \hbar\omega$ and $k_BT \gg \hbar\omega$ respectively. This, in principle, gives an experimental tool for probing the nature of the low-lying quasiparticle energies in the mixed state. By measuring the attenutation of a longitudinal sound wave, one should be able to probe the existence of the gapless points and their dispersion law. We therefore propose a fundamental test of the theoretical models for a type-II superconductor in a strong external magnetic field. The results described in this chapter have been presented on abridged form in Ref. [24].

The chapter is structured as follows: In section 5.2, we develop the formalism necessary to calculate the sound attenuation for a longitudinal wave in the clean limit. Then in section 5.3, we use the diagonal approximation to simplify the algebra such that some analytical results can be derived. The diagonal approximation is then checked against an exact numerical solution.

Analytical results for the attenuation are presented in section 5.4 for the low frequency case and in section 5.5 for the low temperature case. Finally, our results are summarized in section 5.6.

5.2 Formalism

We consider the problem of calculating the attenuation of a longitudinal sound wave propagating in a type-II superconductor in the mixed state. From a microscopic point of view, there is a fundamental difference between the attenuation of a longitudinal sound wave as compared to a transverse wave. The reason is that the mechanisms behind the electron-phonon coupling are quite distinct in the two cases. In the longitudinal case, the sound wave comprises density fluctuations for the ions/molecules forming the crystal. The corresponding fluctuations in the crystal potential set up fluctuations in the electron density as the quasiparticles are excited out of their equilibrium distribution. The response of the quasiparticles to a longitudinal variation of the crystal field is essentially the same in the superconducting state as compared to the normal state [88, 98]. Thus, we can, to a good approximation, assume that the electron-phonon coupling strength is the same in the two states for longitudinal phonons. This will simplify significantly a comparison between the attenuation in mixed state and in the normal state. In the transverse case however, the sound wave corresponds to varying transverse currents set up by the vibrating lattice. These currents will produce a transverse electromagnetic (EM) field which couples to the quasiparticles. From the Meissner effect, we know that a superconductor responds very differently to a transverse EM-field as compared to a normal metal; the supercurrents screen the EM-field almost perfectly. The electron-phonon coupling for transverse phonons will thus be very different in the superconducting state as compared to the normal state. This complicates the comparison between the damping of a transverse wave in the two states, as we would have to take into account the completely different screening properties. Therefore, for simplicity, we restrict ourselves to the calculation of the attenuation of a longitudinal sound wave. Also, the sound wave will be assumed to propagate parallel to the magnetic field H which defines the z-axis. For this particular geometry, there is no displacement of the lattice in the xy-plane. As the vortices formed by the order parameter move in this plane, there is no coupling between the sound wave and the collective degrees of freedom associated with the order parameter [25, 36].

The problem of calculating sound attenuation for a superconductor is an old one and various theoretical approaches have been used. In a series of papers, Pippard and Kadanoff developed an elegant model, based on the semiclassical Boltzman transport equation, to calculate the acoustic attenuation in normal metals as well as superconductors [63, 86, 87]. The approach is essentially to calculate the rate at which the quasiparticles absorb phonons. It is then implicitly assumed that the quasiparticles return their excess energy to a thermal bath such that the energy is lost for the sound wave. As the method uses semiclassical dynamics for the quasiparticles and only takes the zero field quasiparticle energy relation $E = \sqrt{\frac{1}{2}m(v - v_F)^2 + \Delta^2}$ as a microscopic input, one is able to obtain rather general results for both transverse and longitudinal waves for arbitrary impurity concentrations[1].

In this chapter, we are interested in microscopic effects such as the influence of the Landau levels and the gapless excitations on the attenuation. To consider this, it is necessary to return to a more fundamental level. From a microscopic point of view, the attenuation is due to the finite lifetime of a longitudinal phonon. This lifetime can be calculated within the language of many-body perturbation theory. We start by defining the longitudinal phonon propagator (finite temperature Green's function) as

[1]Ref. [66] provides a short and precise review of the results based on the Boltzmann transport equation.

$\mathcal{A}(\mathbf{r}\tau, \mathbf{r}'\tau') \equiv -\langle T_\tau \hat{\phi}(\mathbf{r}\tau), \hat{\phi}(\mathbf{r}'\tau')\rangle$ where the phonon field is [42]

$$\hat{\phi}(\mathbf{r}) = \sum_{\mathbf{k}} \left(\frac{\hbar\omega_{\mathbf{k}}}{2L^3}\right)^{1/2} [\hat{c}_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}} + \hat{c}^\dagger_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{r}}]. \tag{5.1}$$

Here $\omega_{\mathbf{k}} = ck$ is the phonon frequency with c being the sound velocity, L^3 is the volume of the system, $\hat{\phi}(\tau) = \exp(\hat{H}\tau)\hat{\phi}\exp(-\hat{H}\tau)$, and $\hat{c}_{\mathbf{k}}$ removes an acoustic phonon with wave number $\mathbf{k}$. The interaction between the phonon and the electrons is described by the term [42]:

$$\hat{H}_{e-ph} = \kappa \sum_\sigma \int d^3r\, \hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r})\hat{\phi}(\mathbf{r}) \tag{5.2}$$

with κ being the strength of the electron-phonon interaction. The Dyson equation for the phonon propagator is:

$$\mathcal{A}(x,x') = \mathcal{A}^0(x,x') + \kappa^2 \iint d^4y d^4y'\, \mathcal{A}^0(x,y)\Pi^*(y,y')\mathcal{A}(y',x') \tag{5.3}$$

where $\mathcal{A}^0(x,x')$ is the free phonon propagator in the absence of the electron-phonon interaction, $x = (\mathbf{r},\tau)$ and $\int d^4x = \int d^3r \int_0^\beta d\tau$. We have denoted the proper phonon self-energy as $\Pi^*(y,y')$. Using perturbation theory, we can easily calculate the self-energy to lowest order in the electron-phonon interaction given in Eq. (5.2). The result is that $\Pi^*(x,x') = \kappa^2\mathcal{D}(x,x')$ where $\mathcal{D}(x,x')$ is the density-density correlation function

$$\mathcal{D}(x,x') = -\langle T_\tau \tilde{n}(\mathbf{r},\tau), \tilde{n}(\mathbf{r}',\tau')\rangle \tag{5.4}$$

and the operator $\tilde{n}(\mathbf{r}) = \hat{n}(\mathbf{r}) - \langle\hat{n}(\mathbf{r})\rangle$ describes density fluctuations. As explained above, we consider phonons propagating with wavenumber q along the z-axis parallel to the external magnetic field. This simplifies our analysis significantly as from section 3.2, we know that the electron motion along this axis is unaltered by the magnetic field. Therefore, the momentum is a conserved quantity along this axis (in the clean limit) and we can simplify Eq. (5.3) by performing a Fourier transform. We also go to frequency space; the Dyson equation then reads:

$$\mathcal{A}(q,\omega_\gamma) = \mathcal{A}^0(q,\omega_\gamma) + \kappa^2 \mathcal{A}^0(q,\omega_\gamma)\mathcal{D}(q,\omega_\gamma)\mathcal{A}(q,\omega_\gamma). \tag{5.5}$$

We have defined

$$\mathcal{A}(q,\omega_\gamma) = \int_0^\beta e^{i\omega_\gamma\tau} \frac{1}{V_{\text{cell}}} \int_{\text{cell}} d^2r \int d^3r' e^{iqz'} \mathcal{A}(\mathbf{r}\tau, \mathbf{r}'\tau') \tag{5.6}$$

with $\omega_\gamma = 2\gamma\pi k_B T/\hbar$ (γ integer) being the bosonic Matsubara frequencies. As the phonon wave length is much larger than the inter-vortex distance, we should average over one vortex cell. This averaging is indicated by the symbol $\frac{1}{V_{\text{cell}}}\int_{\text{cell}} d^2r$ which denotes integration over one vortex lattice cell in the xy plane and division by the lattice cell area $V_{\text{cell}} = \pi l^2$. The integration $\int d^3\mathbf{r}'$ is over the whole crystal. Eq. (5.5) is now readily solved and we obtain

$$\mathcal{A}(\mathbf{k},\omega_\gamma) = \frac{\mathcal{A}^0(\mathbf{k},\omega_\gamma)}{1 - \kappa^2 \mathcal{A}^0(\mathbf{k},\omega_\gamma)\mathcal{D}(\mathbf{k},\omega_\gamma)}. \tag{5.7}$$

The phonon will in general have a finite lifetime due to its scattering with the electrons described by the interaction term in Eq. (5.2). It is this scattering which gives rise to the damping of the sound waves since, as mentioned above, we implicitly assume that the energy given to the electrons by the scattering is not returned to the sound wave but is lost to a heat bath. To calculate the lifetime of the phonon, we as usual need the real-time retarded phonon Green's function $A^R(q,\omega)$. It is a standard result that the energy of the phonon with wave vector q is given by the real part of the pole of $A^R(q,\omega)$ in the lower half of the complex ω-plane, whereas the lifetime is inversely proportional to the imaginary part of the pole [42]. The acoustic attenuation is inversely proportional to the lifetime of the phonon and hence proportional to the imaginary part of the pole. The retarded Green's function is most easily obtained by first calculating the temperature Green's function $\mathcal{A}(q,\omega_\gamma)$ as outlined above. The retarded Green's function is then given by the analytical continuation [42]:

$$A^R(q,\omega) = \mathcal{A}(q,\omega_\gamma)|_{i\omega_\gamma\to\omega+i\delta} \tag{5.8}$$

with $\delta > 0$ being an infinitesimal positive number. From Eq. (5.7), we see that the acoustic attenuation $\alpha(q,w)$ for a longitudinal sound wave with frequency ω and wavenumber q along the z-axis, is given by:

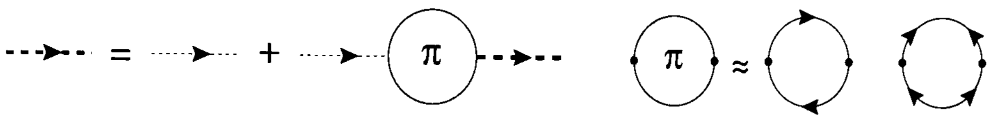
$$\alpha(q,\omega) \propto -\omega \mathrm{Im}\left\{D^R(q,\omega)\right\} \tag{5.9}$$

where $D^R(\mathbf{q},\omega)$ is the Fourier transform of the retarded density-density correlation function

$$D^R(\mathbf{x},\mathbf{x}',t-t') = -i\langle[\tilde{n}(\mathbf{x},t),\tilde{n}(\mathbf{x}',t')]\rangle\theta(t-t') \tag{5.10}$$

and $D^R(q,\omega) = \mathcal{D}(q,\omega_\gamma)|_{i\omega_\gamma\to\omega+i\delta}$. The symbol Im in Eq. (5.9) denotes the imaginary part. Note that we have omitted the strength of the electron-phonon interaction in Eq. (5.9). We simply treat the electron-phonon matrix element as an overall factor in our formalism (i.e. its frequency dependence ω is included as a prefactor in Eq.(5.9)) making use of the fact that the screening for longitudinal modes is essentially the same as in the normal phase.

We have obtained Eq. (5.9) by looking at the lifetime of a phonon within the framework of standard many-body perturbation theory. The same formula can also be derived by treating the displacement of the ions/molecules forming the sound wave as a classical field and then looking at the interaction of this displacement field with the electrons. The resultant wave equation for the field then yields Eq. (5.9) in the limit of a pure system with $ql_{mf} \gg 1$ where l_{mf} is the mean free path of the electrons [62].



(a) The Dyson equation

(b) The self-energy to lowest order.

Figure 5.1: The Dyson equation for the phonon propagator. The proper self-energy Π is drawn as a filled blob. The electron propagators are drawn as solid lines. The second term in (b) is absent in the normal state.

The density-density correlation function can be expressed in terms of single-particle Green's functions using Wicks theorem. In this chapter, we will for simplicity ignore the electronic Zeeman effect. We hence obtain

$$\begin{aligned} D^R(\mathbf{q}, \omega) &= \frac{2k_BT}{V_{\text{cell}}} \sum_{\omega_\nu} \int_{\text{cell}} d^2r \int d^3r' e^{\mathbf{q}\mathbf{r}'} \left[\mathcal{G}(\mathbf{r}, \mathbf{r}', \omega_\nu) \mathcal{G}(\mathbf{r}', \mathbf{r}, \omega_\nu - \omega_\gamma) \right. \\ &- \left. \mathcal{F}^\dagger(\mathbf{r}, \mathbf{r}', \omega_\nu) \mathcal{F}(\mathbf{r}', \mathbf{r}, \omega_\nu - \omega_\gamma) \right] \Big|_{i\omega_\gamma \to \omega + i\delta} \end{aligned} \tag{5.11}$$

where $G(\mathbf{r}, \mathbf{r}', \omega_\nu)$ and $F(\mathbf{r}', \mathbf{r}, \omega_\nu)$ are the one-particle Green's functions for the superconductor defined in section 2.5. In Fig. 5.1(a), we illustrate the Dyson equation in terms of Feynman diagrams. The thick dashed line denotes the full phonon propagator whereas the thin dashed line is the free phonon propagator. The lowest order contributions to the self-energy as given by Eq. (5.11) are illustrated in Fig. 5.1 (b). Note that the second term in Eq. (5.11) is absent in the normal state where the anomalous Green's function $\mathcal{F}$ is zero. Also, we are only considering the clean limit such that there is no impurity scattering.

In order to make any progress, we must have some expressions for the Green's functions appearing in Eq. (5.11). These functions can be obtained from the solution to the BdG equations. We need to solve these equations for a 3D system as the problem is intrinsically 3D with a sound wave traveling parallel to the magnetic field. To simplify the analysis, it is again assumed that the order parameter forms a vortex lattice in the xy-plane as explained in section 3.4. The order parameter is constant along the direction parallel to the magnetic field, such that the vortex lines run in the direction of the sound wave. It is then straightforward to extend the formalism outlined in section 3.5 to 3D. The motion along the z-direction is unaffected by the magnetic field and there is only pairing between electrons with momentum k_z and $-k_z$. We write the Bogoliubov functions as

$$
\begin{aligned}
u^{\eta}_{\mathbf{k}k_z}(\mathbf{r}) &= L_z^{-1/2} \sum_N u^{\eta}_{N\mathbf{k}k_z} \phi_{N\mathbf{k}}(x,y) e^{ik_z z} \\
v^{\eta}_{\mathbf{k}k_z}(\mathbf{r}) &= L_z^{-1/2} \sum_N v^{\eta}_{N\mathbf{k}k_z} \phi^{*}_{N-\mathbf{k}}(x,y) e^{ik_z z}
\end{aligned}
\tag{5.12}
$$

where $\phi_{N\mathbf{k}}(x,y)$ is defined in Eq. (3.4) and L_z is the extent of the system in the z-direction. The resultant BdG equations then split into a set of equations for each $\mathbf{k}, k_z$ with $\mathbf{k}$ $\in$MBZ; the quasiparticle energy associated with the Bogoliubov functions $u^{\eta}_{\mathbf{k}k_z}(\mathbf{r})$ and $v^{\eta}_{\mathbf{k}k_z}(\mathbf{r})$ is denoted $E^{\eta}_{k_z}(\mathbf{k})$. We choose the normal state dispersion law along the z-direction to be either the plane wave form $\epsilon(k_z) = k_z^2/2m$ or, more suitably for layered structures, the tight-binding form $\epsilon(k_z) = t\cos(k_z a_z)$ where a_z is the distance between the planes. The formulae for solving the BdG equations are straightforward extensions of the ones given in section 3.5. The only difference is a summation over the quantum number k_z when calculating the parameters Δ_j. For reasons of space, I will not give the precise formula here. From the solution of the BdG equations, we can calculate the appropriate Green's functions as:

$$
\begin{aligned}
\mathcal{G}(\mathbf{r},\mathbf{r}',\omega_\nu) &= \sum_{\eta\,\mathbf{k}\,k_z} \left[\frac{u^{\eta}_{\mathbf{k}k_z}(\mathbf{r}) u^{\eta}_{\mathbf{k}k_z}(\mathbf{r}')^{*}}{i\omega_\nu - E^{\eta}_{\mathbf{k}k_z}/\hbar} + \frac{v^{\eta}_{\mathbf{k}k_z}(\mathbf{r})^{*} v^{\eta}_{\mathbf{k}k_z}(\mathbf{r}')}{i\omega_\nu + E^{\eta}_{\mathbf{k}k_z}/\hbar} \right] \\
\mathcal{F}(\mathbf{r}',\mathbf{r},\omega_\nu) &= \sum_{\eta\,\mathbf{k}\,k_z} \left[\frac{u^{\eta}_{\mathbf{k}k_z}(\mathbf{r}') v^{\eta}_{\mathbf{k}k_z}(\mathbf{r})^{*}}{i\omega_\nu - E^{\eta}_{\mathbf{k}k_z}/\hbar} - \frac{v^{\eta}_{\mathbf{k}k_z}(\mathbf{r}')^{*} u^{\eta}_{\mathbf{k}k_z}(\mathbf{r})}{i\omega_\nu + E^{\eta}_{\mathbf{k}k_z}/\hbar} \right] \\
\mathcal{F}^{\dagger}(\mathbf{r},\mathbf{r}',\omega_\nu) &= \sum_{\eta\,\mathbf{k}\,k_z} \left[\frac{v^{\eta}_{\mathbf{k}k_z}(\mathbf{r}) u^{\eta}_{\mathbf{k}k_z}(\mathbf{r}')^{*}}{i\omega_\nu - E^{\eta}_{\mathbf{k}k_z}/\hbar} - \frac{u^{\eta}_{\mathbf{k}k_z}(\mathbf{r})^{*} v^{\eta}_{\mathbf{k}k_z}(\mathbf{r}')}{i\omega_\nu + E^{\eta}_{\mathbf{k}k_z}/\hbar} \right]
\end{aligned}
\tag{5.13}
$$

Using the orthogonality of the Bogoliubov functions, and the identity

$$\sum_{\omega_\nu} \frac{1}{i\omega_\nu - x_1} \frac{1}{i\omega_\nu - i\omega_\gamma - x_2} = \frac{\beta}{x_1 - x_2 - i\omega_\gamma}[f(x_1) - f(x_2)],$$

we finally obtain from Eqs. (5.9) and (5.11):

$$\begin{aligned}\alpha(q,\omega) \propto \frac{\omega}{L_x L_y} \sum_{\eta\eta'} \sum_{\mathbf{k}} \int dk_z \, \{[f(E) - f(E')][\delta(E' - E - \hbar\omega)(|U' \wedge U|^2 \\ - V' \wedge V^* U'^* \wedge U) - \delta(E - E' - \hbar\omega)(|V'^* \wedge V|^2 - U'^* \wedge U \, V' \wedge V^*)] \\ +[1 - f(E') - f(E)]\delta(E' + E - \hbar\omega)(|U' \wedge V|^2 + V' \wedge U \, U'^* \wedge V^*)\} \,.\end{aligned} \tag{5.14}$$

Here $U \equiv U^{\eta}_{\mathbf{k}k_z}(\mathbf{r})$, $V \equiv V^{\eta}_{\mathbf{k}k_z}(\mathbf{r})$, $U' \equiv U^{\eta'}_{\mathbf{k}k_z+q}(\mathbf{r})$ and $V' \equiv V^{\eta'}_{\mathbf{k}k_z+q}(\mathbf{r})$ are the Bogoliubov functions. The quasiparticle energies are given by $E \equiv E^{\eta}_{k_z}(\mathbf{k})$ and $E' \equiv E^{\eta'}_{k_z+q}(\mathbf{k})$, and the $\wedge$-product means integration over the xy-plane. The physical interpretation of the three terms in Eq. (5.14) is straightforward: the first two delta functions $\delta(E' - E - \hbar\omega)$ and $\delta(E - E' - \hbar\omega)$ describe the scattering of a quasiparticle with a phonon whereas the last delta function $\delta(E' + E - \hbar\omega)$ describes the decay of a phonon into two quasiparticles with energies E and E'. The first two terms will dominate when the frequency of the phonon is small such that there is not enough energy to create two quasiparticles, whereas the third term will dominate when the temperature is low such that there are no quasiparticles present in the medium to scatter.

5.3 The diagonal approximation

Although it is straightforward to extend the formulae for the BdG equations from 2D to 3D, finding the actual solution is significantly more demanding computationally for 3D systems as compared to 2D systems. This is, of course, because we in 3D need to find a solution for the each set of quantum numbers $(\mathbf{k}, k_z)$, $\mathbf{k}$ $\in$MBZ, whereas we only need to solve the BdG equations for the set $\mathbf{k}$ $\in$MBZ in 2D. This makes the necessity for analytical results, in order to compare with experiments, even more apparent in 3D than it was for the dHvA results for the 2D systems in chapter 4. In order to develop such an analytical theory for the attenuation, we need to make some approximations such that we can simplify Eq. (5.14). Near the upper critical field H_{c2}, we saw from section 3.6 that one can, as a first approximation, ignore the off-diagonal pairing (diagonal approximation) for quasiparticle levels close to the Fermi energy. The quasiparticle energies are then given by

$$E^n_{k_z}(\mathbf{k}) = \sqrt{\xi_n(k_z)^2 + |\Delta(\mathbf{k})|^2} \tag{5.15}$$

and the corresponding Bogoliubov functions read

$$\left.\begin{array}{l} |U^n_{\mathbf{k}k_z}(\mathbf{r})|^2 \\ |V^n_{\mathbf{k}k_z}(\mathbf{r})|^2 \end{array}\right\} = \frac{1}{2}(1 \pm \frac{\xi_n(k_z)}{E^n_{k_z}(\mathbf{k})})|\phi_{n\mathbf{k}k_z}(\mathbf{r})|^2. \tag{5.16}$$

Here $\xi_n(k_z) = (n + 1/2)\hbar\omega_c + \epsilon(k_z) - \mu_F$ and $\Delta(\mathbf{k}) = |F_{\mathbf{k}nn}|$. Again, we must remember that this approximation is only valid for energy levels close to μ_F. Further away from the chemical potential, there are degeneracies between electron and hole states belonging to different Landau levels. There is a strong mixing between the degenerate states caused by the off-diagonal matrix elements ignored by the diagonal approximation. Hence, the approximation breaks down for these states. Fortunately, for low frequencies and temperatures, only low energy levels for which Eqs. (5.15) and (5.16) hold will contribute to the damping. A closer examination yields the requirement for the diagonal approximation to hold to be $\max(k_BT, \hbar\omega) \lesssim \hbar\omega_c/4$. This follows because the mixing between hole and electron levels becomes important for levels with $E \gtrsim \hbar\omega_c/4$. Since we have $\hbar\omega \sim 10^{-7}$eV for $\omega \sim 100$ MHz, $\hbar\omega_c \sim 10^{-4}$eV for $H = 1$Tesla, and $k_BT \sim 10^{-5}$eV for $T = 1$K, the limit $\max(k_BT, \hbar\omega) \lesssim \hbar\omega_c/4$ is not unrealistic experimentally. Contrary to 2D, for 3D systems there are always normal state energies for which $\xi_n(k_z) \sim 0$

due to the dispersion law along the z-direction. This means that for small $\Delta(\mathbf{r})$ and close to H_{c2}, there are low-lying quasiparticle states for which the diagonal approximation is good for any external magnetic field. In 2D, this is only the case when the external field is such that there is a Landau level close to the chemical potential ($|\xi_n| \lesssim \hbar\omega_c/4$). Thus, the diagonal approximation is reasonable for 3D systems when calculating quantities depending only on the low-lying quasiparticle excitations, whereas it is harder to justify for 2D systems. As was shown in section 3.6, it follows directly from the diagonal approximation that there are gapless points in the MBZ [i.e $\Delta(\mathbf{k}) = 0$]. These gapless excitations will play a crucial role in the calculation of the attenuation. We are in some sense lucky, since the diagonal approximation must be expected to work best for the low-lying levels which contribute the most to the damping. The diagonal approximation breaks down when the off-diagonal matrix elements become too large. However, Dukan *et al.* [38] argued that the off-diagonal pairing does not change the qualitative behavior of the superconductor as long as one is close to H_{c2}; the quasiparticle spectrum remains essentially the same when the off-diagonal terms are included. Even when the diagonal approximation breaks down, there will still be points in the MBZ where the gap vanishes. They claimed that the role of the off-diagonal terms is to shift the value of the Fermi momentum k_{zf} where the gapless behaviour occurs, away from its diagonal approximation value $\epsilon(k_{zf}) = 0$. Eventually, true gapped behaviour sets in when the superconducting order is strong enough to increase the energies of the quasi-bound states in the vortices above $\hbar\omega_c$. Using Eq. (5.16), we can easily calculate the xy-integral in Eq. (5.14); for example $|U' \wedge U| = \frac{1}{2}\sqrt{(1+\xi/E)(1+\xi'/E')}$.

Equation (5.14) then becomes:

$$\alpha(q,\omega) \propto \frac{\omega}{4L_xL_y}\sum_{\eta}\sum_{\mathbf{k}}\int dk_z \frac{1}{EE'}\{[f(E)-f(E')]\times$$
$$\left[\delta(E'-E-\hbar\omega)[(E+\xi)(E'+\xi')-|\Delta(\mathbf{k})|^2]\right.$$
$$\left.-\,\delta(E-E'-\hbar\omega)\left[(E-\xi)(E'-\xi')-|\Delta(\mathbf{k})|^2\right]\right]$$
$$+[1-f(E')-f(E)]\delta(E'+E-\hbar\omega)[(E-\xi)(E'+\xi')+|\Delta(\mathbf{k})|^2]\} \quad (5.17)$$

where $\xi = \xi_\eta(k_z)$ and $\xi' = \xi_\eta(k_z+q)$. We have here neglected transitions between different Landau levels since we have assumed $\omega \ll \omega_c$.

In order to check the validity of the diagonal approximation, we have calculated the quasiparticle spectrum exactly by solving the BdG equations numerically for a 3D system. Then, we compare the results for the low lying energies with the analytical approximation as given in Eq. (5.15). In Fig. 5.2, we plot the lowest quasiparticle energy calculated numerically, along the $\Gamma - M$ direction in $\mathbf{k}$-space for two different values of the order parameter $\Delta(\mathbf{r})$ at a low temperature. The two points Γ and M in the MBZ are defined in section 3.5 as two of the corners in an irreducible triangle reflecting the symmetry of the BdG-equations in $\mathbf{k}$-space. We have chosen the size of the system such that $\pi/(2a_x\Delta k_x) = 50$ where $\Delta k_x = 2\pi/L_x$. The dashed lines give the diagonal approximation to the energies while the solid lines depicts the exact numerical result. The two highest-lying curves are calculated with $\langle\Delta(\mathbf{k})\rangle_{\mathbf{k}} \simeq 0.3\hbar\omega_c$ and the two lowest lying curves are with $\langle\Delta(\mathbf{k})\rangle_{\mathbf{k}} \simeq 0.05\hbar\omega_c$. Here $\langle\Delta(\mathbf{k})\rangle_{\mathbf{k}}$ means the $\mathbf{k}$-space average of the diagonal matrix element in the BdG equations. There are 10 Landau levels within the pairing width and the dispersion law along the z-direction is $\epsilon(k_z) = t\cos(k_za_z)$. The value of k_z is chosen such that $\epsilon(k_z) = 0$. As can be seen, the diagonal approximation predicts two gapless points along this $\mathbf{k}$-space direction, both with a linear dispersion law. For a small pairing parameter, there is good agreement between the diagonal approximation and

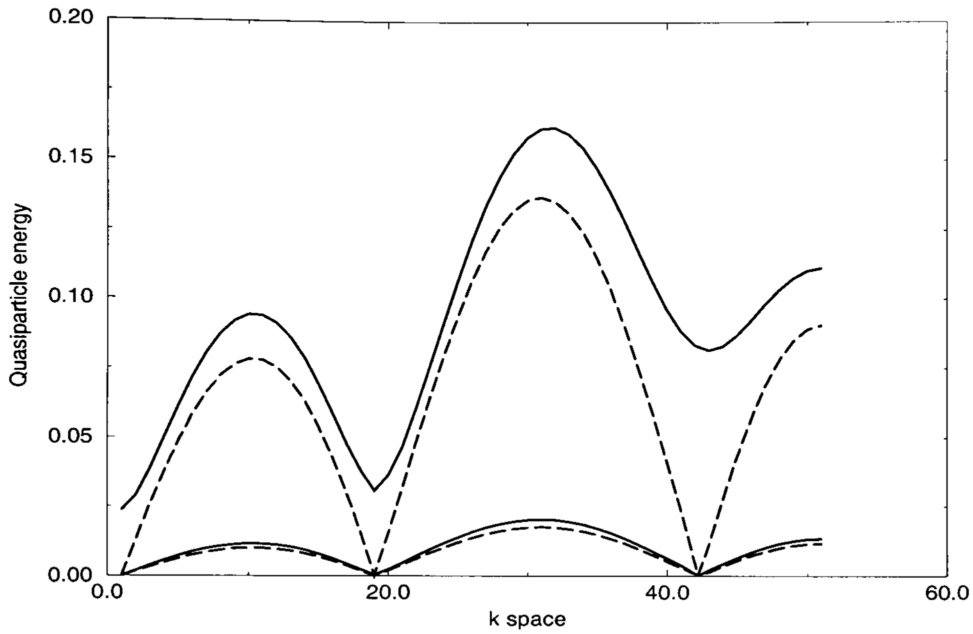


Figure 5.2: The lowest quasiparticle energy bands in units of $\hbar\omega_c$ for two different values of the order parameter. The solid lines show the exact numerical result while the dashed lines correspond to the diagonal approximation.

the full calculation. For a larger pairing parameter, i.e. $\langle\Delta(\mathbf{k})\rangle \simeq 0.3\hbar\omega_c$, the approximation is less precise; indeed the gapless points predicted by the diagonal approximation disappear in the full self-consistent calculation. This is due to the off-diagonal pairing which become increasingly important as the pairing interaction increases deeper into the mixed state. Thus, we expect our theory to be valid reasonably close to the transition line such that we can ignore the off-diagonal pairing. As mentioned above, the major contribution to the damping actually comes from the gapless points where the diagonal approximation is most valid. We will now calculate the attenuation in two limits using this approximation.

5.4 Low frequency

We will first treat the low frequency case $\hbar\omega \ll k_BT$. In this limit, we can focus on the first two delta functions in Eq. (5.14) which describe the scattering of a quasiparticle with a phonon. This is because quasiparticles with energies of the order k_BT will contribute to the damping from the first two terms whereas only quasiparticles with energies $\hbar\omega$ will contribute to the damping from the third term. We will outline the calculation for the dispersion law $\epsilon(k_z) = k_z^2/2m$. Making the approximation $\xi'/E' \simeq \xi/E$ which is valid for $\hbar\omega \ll k_BT$, the first two terms of Eq.(5.17) become:

$$\alpha(q,\omega) = \\ -\frac{\omega^2 m}{\hbar L_x L_y q}\sum_n\sum_{\mathbf{k}}\int dk_z \delta(k_z - k_z^*(n,\mathbf{k}))\partial_E f(E^n_{k_z}(\mathbf{k}))\frac{|\xi_n(k_z)|}{E^n_{k_z}(\mathbf{k})} \quad (5.18)$$

Here $k_z^*(n,\mathbf{k})$ is the solution to the equation $E^n_{k_z+q}(\mathbf{k}) - E^n_{k_z}(\mathbf{k}) = \hbar\omega$. As in chapter 4, we express the sum over Landau levels in terms of harmonics such that we can isolate the oscillatory and smooth parts. From the Poisson formula, we have the identity

$$\sum_{n=-\infty}^{\infty}\partial_E f(E^n_{k_z^*}(\mathbf{k}))\frac{|\xi_n(k_z^*)|}{E^n_{k_z^*}(\mathbf{k})} = \sum_{j=-\infty}^{\infty}\int dx^{2j\pi i x}\partial_E f(E^x_{k_z^*}(\mathbf{k}))\frac{|\xi_x(k_z^*)|}{E^x_{k_z^*}(\mathbf{k})} \quad (5.19)$$

where $\xi_x(k_z^*) = (x+1/2)\hbar\omega_c + \epsilon(k_z^*) - \mu_F = (x - n_F)\hbar\omega_c + \epsilon(k_z^*)$. We have extended the Landau level sum to go from $-\infty$ since the lowest levels do not contribute. Making the variable substitution $\xi_x(k_z^*) = z\hbar\omega_c$, we end up with

$$\alpha(\mathbf{q},\omega) = \\ -\frac{\omega^2 m}{\hbar L_x L_y q}\sum_{\mathbf{k}}\sum_{j=-\infty}^{\infty} e^{2\pi i j(n_F - \epsilon(k_z^*)/\hbar\omega_c)}\int_{-\infty}^{\infty} dz e^{2\pi i j z}\partial_E f(E_z(\mathbf{k}))\frac{|\xi_z|}{E_z(\mathbf{k})} \quad (5.20)$$

where $E_z(\mathbf{k}) = [\xi_z^2 + \Delta(\mathbf{k})^2]^{1/2}$. We have approximated k_z^* as the corresponding normal state solution (i.e. it is independent of n). This approximation which is only necessary when we calculate the oscillations of the attenuation (i.e. the terms in Eq.(5.20) with $j \neq 0$), should be good close to the gapless points and is equivalent to ignoring any phase shift in the oscillations due to the superconducting order. The zeroth harmonic is given by the $j = 0$ term. We obtain

$$\alpha(\mathbf{q}, \omega)_0 = \frac{2\omega^2 m}{\hbar^2 \omega_c L_x L_y q} \sum_{\mathbf{k}} \frac{1}{e^{\Delta(\mathbf{k})/k_B T} + 1} \tag{5.21}$$

We are now able to compare this simple and rigorous (apart from the use of the diagonal approximation) result for the zeroth harmonic of the attenuation in the clean limit, with the conjecture presented by Maki [32, 70]. Using an ansatz of a formal similarity between a pure type-II superconductor in high magnetic fields and a current-carrying superconductor, Maki arrived at the following expression for the ratio α_S/α_N between longitudinal attenuation in the mixed state and in the normal state:

$$\frac{\alpha_S}{\alpha_N} \simeq 1 - \frac{\Delta}{2k_B T} \tag{5.22}$$

where $\Delta^2 \equiv \langle |\Delta(\mathbf{r})|^2 \rangle$ is the real space average of the gap. As Maki used a semiclassical approximation, he was unable to calculate the oscillatory parts of the attenuation. To compare with this result, we expand Eq. (5.21) to first order in $\Delta(\mathbf{k})$. We obtain:

$$\frac{\alpha_S}{\alpha_N} = 1 - \frac{\langle |\Delta(\mathbf{k})| \rangle_{\mathbf{k}}}{2k_B T} \tag{5.23}$$

where $\langle |\Delta(\mathbf{k})| \rangle_{\mathbf{k}}$ is the $\mathbf{k}$-space average of $|\Delta(\mathbf{k})|$. The result for the normal state is simply obtained by putting $\Delta(\mathbf{k}) = 0$ in Eq. (5.21). We see that our theory for the zeroth harmonic, which is exact within the diagonal approximation, produces a term linear in Δ for the ratio α_S/α_N as does Maki's conjecture. This linear term is somewhat surprising as the Gor'kov expansion of the Green's functions would seem to imply that the first correction term is quadratic in Δ. However, even in the zero field BCS-state one obtains [98] $\alpha_S/\alpha_N = 2/[\exp(\Delta/k_BT)+1]$ which cannot be expanded in Δ^2. So our theory confirms Maki's ansatz of a linear correction term for the damping. Our result substitutes Maki's real space average $\Delta = (\langle|\Delta(\mathbf{r})|^2\rangle)^{1/2}$ with the $\mathbf{k}$-space average of $|\Delta(\mathbf{k})|$.

5.4.1 Zeroth harmonic

For conventional superconductors in the Meissner state, it is a well-known result [98] that a finite gap for all $\mathbf{k}$ suppresses the attenuation by a factor $2/[\exp(\Delta/k_BT+1]$. A qualitative difference between the Meissner state and the mixed state in a high magnetic field is the existence of the gapless points. We expect these gapless points to change the result for the attenuation significantly. To simplify the analysis and to highlight the importance of the gapless parts of the spectrum, we therefore split the MBZ into two qualitatively different regions: the "gapped" region where we assume $\Delta(\mathbf{k}) = \langle\Delta(\mathbf{k})\rangle_{\mathbf{k}}$ where we still define $\langle\Delta(\mathbf{k})\rangle_{\mathbf{k}}$ as the $\mathbf{k}$-space average of $\Delta(\mathbf{k})$, and the "gapless" region where we assume $\Delta(\mathbf{k}) = \gamma k^{\eta}$, with γ and η being positive constants. We furthermore take this dispersion law to hold for $\Delta(\mathbf{k})$ up to $\Delta(\mathbf{k}) \gtrsim k_BT$. This simplified form for $\Delta(\mathbf{k})$ is a slight generalization of the model used by Dukan and Tešanović [39] in their theory for the dHvA oscillations. We assume that the gapped region takes up a fraction $\mathcal{F}$ of the MBZ. The contribution $\alpha(q,\omega)_{0,gap}$ to the attenuation from the gapped region is then readily obtained from Eq. (5.21) to be:

$$\alpha(q,\omega)_{0,gap} = \frac{\omega^2 m^2}{\hbar^2 qh}\mathcal{F}\frac{2}{e^{\langle\Delta(\mathbf{k})\rangle_{\mathbf{k}}/k_BT}+1} \tag{5.24}$$

where $h = \hbar 2\pi$. As expected, the attenuation from the gapped part of the spectrum is strongly suppressed due to the $2/[\exp(\langle\Delta(\mathbf{k})_{\mathbf{k}}\rangle/k_BT)+1]$ factor.

This result for the zeroth harmonic of the attenuation from the gapped part of the spectrum in the mixed state is the same as for the total attenuation in the Meissner state of a conventional superconductor. The qualitatively new feature comes from the presence of the gapless points. We are interested in the temperature dependence of the attenuation which can be extracted directly from Eq. (5.21) by using the variable substitution $x^\eta = \beta\gamma k^\eta$. However, we can actually solve the 2D $\mathbf{k}$-space integral given in Eq. (5.21) exactly using the assumed dispersion law. After some variable substitutions, we end up with the contribution $\alpha(q,\omega)_{gl}$ from the gapless part to be:

$$\alpha(q,\omega)_{0,gl} = Q_{gl}\frac{m\omega^2}{\hbar^2\omega_c q\pi}\left(\frac{k_BT}{\gamma}\right)^{2/\eta}\frac{1-2^{1-2/\eta}}{\eta}\Gamma\left(\frac{2}{\eta}\right)\zeta\left(\frac{2}{\eta}\right) \tag{5.25}$$

where Q_{gl} is the number of gapless points in the MBZ. Here $\zeta(x) \equiv \sum_{n=1}^{\infty} n^{-x}$ is Riemann's zeta function and $\Gamma(x) \equiv \int_0^\infty \exp(-t)t^{x-1}dt$ is the gamma function. For a linear dispersion around the gapless points, we obtain

$$\alpha(q,\omega)_{0,gl} = Q_{gl}\frac{m\omega^2\pi(k_BT)^2}{12\hbar^2\omega_c q\gamma^2}. \tag{5.26}$$

The relative size of the contributions from the gapped and gapless parts of the spectrum is determined by $\langle\Delta(\mathbf{k})\rangle_{\mathbf{k}}/k_BT$, $\mathcal{F}$ and γ. For $\langle\Delta(\mathbf{k})\rangle_{\mathbf{k}} \gtrsim 3k_BT$, the contribution from the gapped part can be ignored and the attenuation is given by Eq. (5.25). Since the normal state attenuation is given by $\alpha(\mathbf{q},\omega)_{0,N} = m^2\omega^2/\hbar^2 qh$ we obtain

$$\frac{\alpha(\mathbf{q},\omega)_{0,gl}}{\alpha(\mathbf{q},\omega)_{0,N}} = Q_{gl}\frac{2\hbar}{m\omega_c}\left(\frac{k_BT}{\gamma}\right)^{2/\eta}\frac{1-2^{1-2/\eta}}{\eta}\Gamma\left(\frac{2}{\eta}\right)\zeta\left(\frac{2}{\eta}\right). \tag{5.27}$$

The calculation outlined above is valid in the clean case where the momentum is conserved during the scattering process. As a typical mean free path l_{mf} for the electrons is $\sim 10^3$Å and the wave length γ_s of the sound wave is between $\sim 10^{-5}$ m for $\nu = 100$ MHz and $\sim 10^{-7}$m for $\nu = 10$ GHz, the dirty limit is experimentally relevant. As a first approximation to the dirty limit, we can assume that there is no momentum conservation in the scattering process and take k_z and k'_z as free variables [69] (i.e $k'_z \neq k_z + q$). As in the Meissner state, this relaxation, somewhat surprisingly, does not alter the result stated in Eq. (5.27). This is due to the fact that we are looking at energies close to the Fermi level such that we can assume that the normal state density-of-states is constant. It has been shown [40] that for small impurity concentrations and weak scattering potentials, the density of states behaves essentially in the same way as for the pure case. We therefore believe that the results presented in this section are somewhat insensitive to the presence of impurities.

5.4.2 First harmonic

As in the case of the dHvA oscillations considered in chapter 4, the Landau level structure of the normal state electron energies implies that there will be oscillations in the attenuation as the external field varies. The oscillatory terms are given by the $j \neq 0$ terms in Eq. (5.20). We end up with the following expression for the first harmonic $\alpha(q,\omega)_{gl,1}$ of the attenuation from the gapless part of the spectrum:

$$\alpha(q,\omega)_{gl,1} = Q_{gl}\frac{2m\omega^2}{\hbar k_B T q\pi}\cos(2\pi(n_F - \epsilon(k_z^*)/\hbar\omega_c))\int_0^\infty kdk\int_0^\infty dx \times \\ (e^{-\sqrt{x^2\hbar^2\omega_c^2+\gamma^2k^{2\eta}}/k_BT}+1)^{-1}(e^{\sqrt{x^2\hbar^2\omega_c^2+\gamma^2k^{2\eta}}/k_BT}+1)^{-1}\times \\ \frac{\cos(2\pi x)x\omega_c}{\sqrt{x^2\hbar^2\omega_c^2+\gamma^2k^{2\eta}}}. \quad (5.28)$$

This integral can be solved in the case of a linear spectrum around the gapless points (i.e $\eta = 1$). In this case, we obtain for the first harmonic of the attenuation

$$\alpha(q,\omega)_{gl,1} = Q_{gl}\frac{m\omega^2}{q\hbar^2\omega_c\pi}\left(\frac{k_BT}{\gamma}\right)^2\cos(2\pi(n_F-\epsilon(k_z^*)/\hbar\omega_c))$$
$$\times\left[\frac{\pi^2\cosh(2\pi^2k_BT/\hbar\omega_c)}{\sinh^2(2\pi^2k_BT/\hbar\omega_c)}-\frac{1}{(2\pi k_BT/\hbar\omega_c)^2}\right]. \qquad (5.29)$$

For low temperatures, this expression varies as T^2. In the case of a general dispersion law around the gapless point given by $\Delta(\mathbf{k}) = \gamma k^\eta$, the leading term for the first harmonic varies as $(T/\gamma)^{2/\eta}$. This result is easily obtained using the variable substitutions $z^\eta = \beta\gamma k^\eta$ and $t = x\beta\hbar\omega_c$ in Eq. (5.28). This should be contrasted to the Meissner state, or the contribution from the gapped part of the spectrum, where the oscillatory terms will again be damped by a factor $2/[\exp(\langle\Delta(\mathbf{k})\rangle_{\mathbf{k}}/k_BT)+1]$. In the case of the normal state, the first harmonic can be found relatively easily from Eq. (5.20) to be [19]:

$$\alpha(q,\omega)_{N,1} = \frac{m^2\omega^2}{hq\hbar^3\omega_c}\frac{4k_BT\pi^2}{\sinh(2\pi^2k_BT/\hbar\omega_c)}\cos[2\pi(n_F-\epsilon(k_z^*)/\hbar\omega_c)] \qquad (5.30)$$

which is independent of T for low temperatures. In the case of a dispersion law along the z-direction given by $\epsilon(k_z) = t\cos(k_za_z)$, we have to substitute m/q by $2/ta_z|\sin(k_z^*a_z)-\sin((k_z^*+q)a_z)|$ in Eq. (5.25) and $m\cos(2\pi(n_F-\epsilon(k_z^*)/\hbar\omega_c))/q$ by $\sum_{i=1,2}\cos(2\pi(n_F-\epsilon(k_{z,i}^*)/\hbar\omega_c))/ta_z|\sin(k_z^*a_z)-\sin((k_z^*+q)a_z)|$ in Eq. (5.29)-(5.30) where $k_{z,i}$ are the two solutions of the equation $t\cos[(k_z+q)a_z]-t\cos(k_za_z)=\hbar\omega$.

In Fig. 5.3, we show an example of the acoustic attenuation calculated numerically from Eq. (5.14) for two different coupling strengths as a function of n_F. We have solved the BdG equations self-consistently in 3D as a function of the external magnetic field at constant chemical potential. In this chapter, we have chosen to work with a constant chemical potential. The difference between holding the chemical potential constant and holding the number of particles constant is negligible in 3D, even for the normal

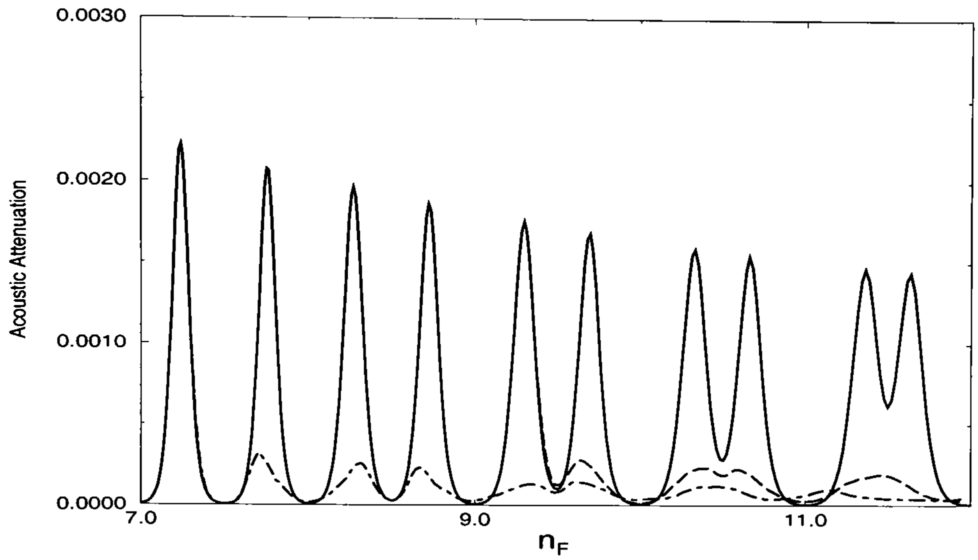


Figure 5.3: The attenuation as a function of n_F. The solid line is the normal state attenuation. The dashed line is for the coupling $g/\hbar\omega_c l^3 = 7.85$. The dash-dot line is for $g/\hbar\omega_c l^3 = 8.7$.

state [100]. From section 4.6, we know that the superconducting order tends to suppress any difference between the two cases even further. Thus, we expect the approximation of a constant μ_F instead of a fixed number of particles to introduce no serious error in the conclusions reached in this chapter. We have chosen parameters such that $\omega_D/\omega_c = 5$, $k_B T/\hbar\omega_c = 0.05$ and $\omega/\omega_c = 0.01$ when $n_F = 12$. The solid curve is the normal state attenuation which is continued into the mixed state to facilitate comparison with the mixed state attenuation; the dashed curve corresponds to the coupling strength $g/\hbar\omega_c l^3 = 7.85$ while the dash-dot curve corresponds to $g/\hbar\omega_c l^3 = 8.7$, both when $n_F = 12$. The dispersion law along the z-direction is $\epsilon(k_z) = t\cos(k_z a_z)$ where $t/\hbar\omega_c = 0.4$. The double-peak structure of the attenuation signal seen in Fig. 5.3 comes from the fact, that the condition $t\cos((k_z + q)a_z) - t\cos(k_z a_z) = \hbar\omega$ has two solutions for $k_z \in [0, 2\pi/a_z[$. It follows that the attenuation will be a superposition of two sets of harmonics. In Fig. 5.4, we plot the corresponding order parameter characterized by the dimensionless number $\Delta_0 \propto \Delta(\mathbf{k})$. The connection between Δ_0 and

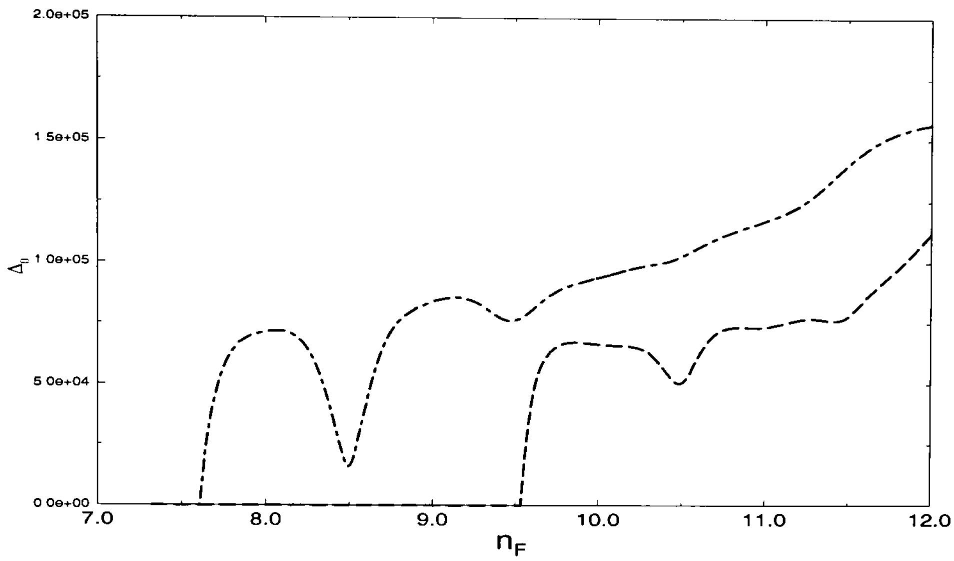


Figure 5.4: The order-parameter as a function of n_F. The dashed line is for the coupling $g/\hbar\omega_c l^3 = 7.85$ while the dash-dot line is for $g/\hbar\omega_c l^3 = 8.7$.

$\Delta(\mathbf{k}) = |F_{\mathbf{k}nn}|$ or $\Delta(\mathbf{r})$ is given by an obvious generalization to 3D of the results given by Eq. (3.10) and Eq. (3.13). The phase transition between the normal and the mixed state occurs for $n_F \simeq 7.6$ when $g/\hbar\omega_c l^3 = 8.7$ and for $n_F \simeq 9.5$ when $g/\hbar\omega_c l^3 = 7.85$. As can be seen from Fig. 5.3, the oscillations of the attenuation due to the Landau level quantization persist into the mixed state, although they are damped as compared to the normal state oscillations. Eventually, the oscillations die out when the off-diagonal pairing becomes dominant and the diagonal approximation breaks down. This happens for $n_F \gtrsim 11$ for $g/\hbar\omega_c l^3 = 8.7$. This behaviour is equivalent to the damped dHvA oscillations in the mixed state described in chapter 4. However, contrary to the dHvA case, no one has to my knowledge yet confirmed experimentally the theoretically predicted oscillations in the attenuation. Comparing the attenuation for the two coupling strengths in the region $10 \leq n_F \leq 11$, we obtain $\alpha_0(7.85)/\alpha_0(8.7) \simeq 1.9$ and $\alpha_1(7.85)/\alpha_1(8.7) \simeq 2.4$ where $\alpha(g)_i$ is the i'th harmonic of the attenuation for the coupling strength g. From section 3.5, we know that $\langle\Delta(\mathbf{k})\rangle_{\mathbf{k}}$ can be calculated directly from Δ_0 and the coefficient γ in the dispersion law around the gapless points is proportional to $g\Delta_0$. Hence, we can compare the numerical results with the analytical predictions outlined above. If the quasiparticle spectrum is essentially gapped, Eq. (5.24) predicts that $\alpha_0(7.85)/\alpha_0(8.7) = f(\langle\Delta_{7.85}\rangle)/f(\langle\Delta_{8.7}\rangle) \simeq 8.8$. If the attenuation is primarily originating from gapless points in the quasiparticle spectrum, Eq. (5.25) predicts that $\alpha_0(7.85)/\alpha_0(8.7) = [8.7\Delta_0(8.7)/7.85\Delta_0(7.85)]^{2/\eta}$. This gives 2.5 for $\eta = 1$ and 1.6 for $\eta = 2$. Hence, the numerical calculation ($\alpha_0(7.85)/\alpha_0(8.7) \simeq 1.9$) implies (i) that the gapless points dominate the attenuation and (ii) that the dispersion law is somewhere between $\eta = 1$ and $\eta = 2$, since the gapless predictions agree reasonably well with the numerical results while the gapped predictions are qualitatively wrong. We cannot, however, make a quantitative numerical determination of the dispersion law around the gapless points. This is due to the fact that in order to reduce the computation load, which is high in the 3D case, we have to choose a $\mathbf{k}$-mesh with a rather large spacing between the points. The mesh consists of 100×50 points. This means that the gapless regions in the quasiparticle spectrum are only probed by a few $\mathbf{k}$-vectors, thereby prohibiting a quantitative determination of the dispersion law. Likewise, Eq. (5.29) predicts that $\alpha_1(7.85)/\alpha_1(8.7)$ equals 2.5 and 1.6 for $\eta = 1$ and $\eta = 2$ respectively. The $\eta = 1$ prediction of 2.5 agrees well with the numerical result $\alpha_1(7.85)/\alpha_1(8.7) \simeq 2.4$. Again, any quantitative comparison would require a much finer $\mathbf{k}$-mesh. A further complication is that due to the number of Landau levels participating in the pairing (~ 10), the oscillations in the attenuation are quickly damped as the field is lowered, and hence the diagonal approximation is only valid over relatively few oscillations. This problem could be avoided if we were to perform the calculations for experimentally realistic parameters, where there are many more Landau levels in the pairing region. As mentioned in chapter 4, we have not been able to do numerical calculations for experimentally realistic parameters even in 2D; for 3D systems this is totally unfeasible. The above example does show however that the numerical calculations support our analytic theory. In short, the normal state oscillations of the attenuation continue into the mixed state and the damping is dominated by gapless points not too far into the mixed state.

We have therefore derived analytical expressions for both the zeroth and first harmonic of the acoustic attenuation in the mixed state, starting from the microscopic Gor'kov equations. The presence of gapless points enhances the acoustic attenuation above the conventional value for the Meissner state. When $\langle\Delta\rangle \gtrsim 3k_BT$ such that we can ignore the contribution from the gapped part of the spectrum, the temperature dependence of the attenuation is a power law given by $\alpha \propto T^{2/\eta}$. Furthermore, we predict that one should observe oscillations in the signal as the external field is varied. The magnitude of these oscillations should have the same temperature dependence as the average value of the signal. Hence by looking at the temperature dependence of the attenuation, one should be able to detect the presence of the gapless points and extract the dispersion law around these points. This is in contrast to the experimentally well-documented effect of the dHvA oscillations in the mixed state where, as we saw in chapter 4, there is no such simple link between the attenuation of the signal and the quasiparticle spectrum.

5.5 Low Temperature

We will now consider the limit where $k_BT \ll \hbar\omega$. In this limit, only the third delta function in Eq. (5.14), which describes the creation of two quasiparticles will contribute to the damping since there are no quasiparticles present to scatter with the phonon. We first calculate the zeroth harmonic of the attenuation. Using the Poisson identity, making a substitution of variables and using the fact that $v_s \equiv \omega/q \ll v_f$ (v_f is the Fermi velocity), we obtain from Eq. (5.17) that the zeroth harmonic of the attenuation, when $\epsilon(k_z) = k_z^2/2m$, is given by

$$\alpha(q,\omega)_0 = \frac{m\omega}{q\hbar^3\omega_c L_x L_y}\sum_{\mathbf{k}}\int_{\Delta(\mathbf{k})}^{\hbar\omega-\Delta(\mathbf{k})} dE[1-f(E)-f(\hbar\omega-E)]\times$$
$$\frac{E(\hbar\omega-E)+\Delta^2}{\sqrt{(E^2-\Delta^2)((\hbar\omega-E)^2-\Delta^2)}}. \quad (5.31)$$

In the limit $\omega/k_BT \to \infty$ (i.e. zero temperature), this integral can be written as a complete elliptic integral [15] and we obtain

$$\alpha(q,\omega)_0 = \frac{m\omega^2}{4\pi^2\hbar^2\omega_c q}\int d^2\mathbf{k}\mathcal{E}\left(\sqrt{1-4\Delta(\mathbf{k})^2/\hbar^2\omega^2}\right). \quad (5.32)$$

Here $\mathcal{E}(k) \equiv \int_0^{\pi/2}\sqrt{1-k^2\sin^2\theta}d\theta$ is the complete elliptic integral of the second kind [48]. The existence of the gapless points again gives rise to a qualitatively different result for the acoustic attenuation in the mixed state as compared to the Meissner state. This is most easily understood by the observation that there will always be attenuation for any frequency in the mixed state since there are always quasiparticle states with $\Delta(\mathbf{k}) \leq \hbar\omega/2$. Hence, the phonon will always have enough energy to create two quasiparticles. This is in contrast to the Meissner state, where there is no attenuation for $\hbar\omega < 2\Delta$. Thus, a clear experimental signature of these gapless points would be the absence of the discontinuity in the attenuation which is present in the Meissner state [15], when $\hbar\omega = 2\Delta$, and the presence of acoustic attenuation in the mixed state as $\omega \to 0$. We will now show that the frequency dependence of the attenuation gives direct information on the quasiparticle dispersion law around the gapless points. It is again assumed that the dispersion law around a gapless point to leading order is given by $\Delta(\mathbf{k}) = \gamma k^\eta$ ($k = |\mathbf{k}|$) in the region that contributes to the attenuation (i.e for $\Delta(\mathbf{k}) \leq \hbar\omega/2$). Using the variable substitution $x^\eta = 2\gamma k^\eta/\omega$ in Eq. (5.32), we obtain

$$\begin{aligned}\alpha(q,\omega)_0 &= Q_{gl}\frac{m\omega^{2/\eta+2}}{2\pi\hbar^2\omega_c q(2\gamma)^{2/\eta}}\int_0^1 xdx\mathcal{E}(\sqrt{1-x^{2\eta}}) \\ &= Q_{gl}\frac{m\omega^{2/\eta+2}}{2\pi\hbar^2\omega_c q(2\gamma)^{2/\eta}}I_\eta. \end{aligned} \tag{5.33}$$

Since the attenuation for the normal state is $\alpha(q,\omega)_{0,N} = m^2\omega^2/2\pi\hbar^3 q$, we have

$$\frac{\alpha(q,\omega)_0}{\alpha(q,\omega)_{0,N}} = Q_{gl}\left(\frac{\omega}{2\gamma}\right)^{2/\eta}\frac{\hbar I_\eta}{m\omega_c}. \tag{5.34}$$

The frequency dependence $\omega^{2/\eta}$ of the attenuation in the mixed state, as given in Eq. (5.33), can be qualitatively understood from the following simple argument: only quasiparticles with energy less than $\hbar\omega/2$ contribute to the damping as the phonon cannot create quasiparticles with higher energies. Thus to estimate the frequency dependence, we can assume that the attenuation is proportional to $\omega^2\int_0^{(\omega/2)^{1/\eta}} k\,dk \propto \omega^{2/\eta+2}$. This is exactly the frequency dependence given in Eq. (5.33) which was obtained by the more rigorous analysis outlined above. For the same reasons as the $\hbar\omega \ll k_B T$ case, we expect Eq. (5.34) to also be valid in the dirty limit. Thus, as expected, the dispersion law around the gapless points in the spectrum shows up in the frequency dependence of the low T attenuation. Incidentally, the remaining integral in Eq. (5.33) can be solved for various η. We obtain, for instance, $I_1 = 2/3$, $I_2 = \pi^2/16$, $I_{1/2} = 32/45$ etc.

Again, the attenuation has an oscillatory behaviour as a function of the magnetic field H^{-1} due to Landau levels. From the Poisson identity, we obtain for the first harmonic

$$\alpha(q,\omega)_1 = Q_{gl}\frac{m\omega}{4\hbar^3\omega_c q 2\pi}\sum_{j=-1,1} e^{2\pi i j(n_f-\epsilon(k_z^*)/\hbar\omega_c)}\int kdk$$
$$\iint d\xi d\xi'\delta(E+E'-\omega)\times\left[(1-\xi/E)(1+\xi'/E')+\frac{\Delta(k)^2}{EE'}\right]e^{ij\xi/\hbar\omega_c}. \tag{5.35}$$

We have not been able to solve this integral exactly. However, in the region where the diagonal approximation holds (i.e for $\hbar\omega \lesssim \hbar\omega_c/4$), one can expand the factor $e^{il\xi/\hbar\omega_c}$ to a good approximation. This immediately yields the result that, to leading order in ω/ω_c, the amplitude of the first harmonic varies as $\omega^{2/\eta+2}$. The next correction term will go as $\omega^{2/\eta+4}$.

Hence, we see that the existence of the gapless points in the MBZ has perhaps even more dramatic consequences on the sound attenuation in the low T limit compared to the low ω limit. In contrast to the Meissner state, there is a finite attenuation for any frequency of the sound wave. There will be no discontinuity in the attenuation as a function of the sound wave frequency. Also, as the external field is varied, one should observe oscillations in the attenuation. The dependence of the attenuation on frequency is algebraic and the power-law is determined by the dispersion law around the gapless points. If $\Delta(\mathbf{k}) = \gamma k^\eta$ we obtain $\alpha \propto \omega^{2/\eta+2}$. The absence of the discontinuity in the attenuation should give a direct experimental indication of the presence of the gapless points. The frequency dependence should in principle provide the possibility of experimentally determining the dispersion law for the gapless points. By making the same substitutions as in the $\hbar\omega \ll k_B T$ limit, one can obtain the results for the case $\epsilon(k_z) = t\cos(k_z a_z)$ relevant for layered structures.

5.6 Summary

In this chapter, we have considered the acoustic attenuation in a type-II BCS superconductor at high magnetic fields using both numerical and analytical methods. We have been able to derive simple expressions for the attenuation starting from the microscopic Gor'kov equations. By including the Landau level structure in the formalism from the outset, we avoided some of the problems encountered in earlier theoretical attempts. It was shown that away from the semiclassical regime where the Landau level structure of the electronic states is important, the attenuation will in general be an oscillatory function of the external magnetic field. Furthermore, since the attenuation probes the low lying quasiparticle energies, it is well suited to check the theoretically predicted existence of gapless excitations in the spectrum. Indeed, we showed that the presence of such gapless points makes the attenuation behave qualitatively different as compared to the Meissner state attenuation. For $k_B T \ll \hbar\omega_c$, the attenuation is an algebraic function of the frequency and there is no discontinuity, as opposed to the Meissner state attenuation. For $k_B T \gg \hbar\omega_c$, the attenuation is an algebraic function of the temperature. The exponent of the power law in the two cases is determined by the dispersion law around the gapless points. Thus, the acoustic attenuation provides an observable to test our theoretical understanding of the low energy quasiparticle spectrum in the mixed state. The oscillatory behaviour of the attenuation, the lack of discontinuity at $\hbar\omega = 2\Delta$ for low T and the frequency and temperature dependence of the attenuation should in principle be experimentally detectable; such an experiment would provide confirmation of the existence and nature of the gapless points.

Chapter 6

Convergence properties of the Gor'kov expansion

6.1 Introduction

The Gor'kov expansion of the grand canonical potential in powers of $\Delta(\mathbf{r})$ was described in section 3.7. Since its derivation by Gor'kov in 1959 [47], it has been a cornerstone in the theoretical framework describing superconductors; most standard microscopic calculations of the properties of type-II superconductors near the upper critical field rely on this expansion. For instance, the Ginzburg-Landau theory which is extremely useful when describing many physical phenomena for superconductors with a spatially varying order parameter[1], is derived from the Gor'kov expansion. Furthermore, as we saw in chapter 3 and chapter 4, much of the theory presented in this thesis to handle problems where the quantizing effect of the magnetic field is crucial, is based on the Gor'kov expansion. Surprisingly, it has recently been postulated that the Gor'kov expansion may be invalid when describing type-II superconductors near the upper critical field [8]. It was suggested

[1] Apart, of course, from the phenomena described in this thesis connected to the quantization of the electron motion in a magnetic field.

that there are non-perturbative effects coming from the large (macroscopic) degeneracy $L_x L_y/2\pi l^2$ of the Landau levels describing the electron motion perpendicular to a magnetic field. The degeneracy means that even a small perturbation (e.g. superconducting order) can change the quasiparticle levels significantly as compared to the normal state. This effect, which should be present even close to H_{c2}, has been proposed as a mechanism for the breakdown of the standard perturbation (Gor'kov) theory describing type-II superconductors [8]. The non-perturbative terms should give rise to spectacular observable effects such as exponential tails of residual superconductivity above the usual H_{c2}, the possibility of the superconducting transition being first order, and unusual behavior of the heat capacity, magnetization etc. close to the phase boundary. For $T = 0$, there should be a non-perturbative linear term in the expansion of $\Omega_S - \Omega_N$ in powers of $\Delta(\mathbf{r})$, whereas for $T > 0$ there should be a non-perturbative third order term [7, 8]. As the Gor'kov expansion is an extremely useful theoretical tool when describing superconductors, it is important to certify the validity of such surprising results. If true, they would invalidate numerous theoretical results, including much of the work presented in this thesis. Thus, we will in this chapter examine the convergence radius of the Gor'kov expansion. This is done in order to check the results of ref.[8] and to understand better the formal convergence properties of the Gor'kov expansion. Such an understanding should be very useful taking into consideration the significance of this expansion in the field of theoretical superconductivity. For simplicity, we work in 2D in this chapter and we neglect any finite Zeeman splitting. Note that the above non-perturbative effects are within mean-field theory and have nothing to do with any of the fluctuation effects away from the mean-field solution described in section 2.6. This chapter is basically a more detailed presentation of the results published in Ref. [22].

The chapter is structured as follows: In section 6.2, we present the arguments leading to the conjecture of the invalidity of the Gor'kov expansion.

Also, we provide an expression for the grand canonical potential Ω which is well suited to check the existence of the proposed non-perturbative terms. Then in section 6.3, we examine the zero temperature case. In this limit, we indeed do find non-perturbative terms in the Gor'kov expansion in agreement with Bahcall [8]. The $T > 0$ case is treated in section 6.4. First, in section 6.4.1, we look at the quantum limit where an exact solution for the grand canonical potential is available. We then treat the general case of many Landau levels participating in the pairing in section 6.4.2. It is shown that the non-perturbative terms in the expansion for the grand canonical potential cancel and that the Gor'kov theory is valid for finite T when the order parameter is small. Furthermore, we derive some criteria for the convergence of the Gor'kov expansion. It is examined whether these criteria impose any new restrictions on Ginzburg-Landau theory. In section 6.5, we consider some numerical results in order to check some of the convergence properties of the Gor'kov expansion derived in section 6.4.2. Finally, in section 6.6, we summarize the results presented in this chapter.

6.2 The degeneracy

In this section, we will outline the theoretical considerations leading to the proposal of the non-perturbative terms in the Gor'kov expansion. We will assume that the order parameter forms a vortex lattice as described in section 3.3. From section 3.5, we know that the BdG equations can then be split into a $2N \times 2N$ secular matrix equation for each $\mathbf{k}$, where N is the number of Landau levels participating in the pairing. Also, when $n_F \equiv \mu_F/\hbar\omega_c - 1/2 = n$ (n integer) there is an exact degeneracy between an electron state in the Landau level $n_F + m$ and a hole state in the Landau level $n_F - m$. For clarity, the structure of the BdG equations for a given $\mathbf{k}$ as given by Eq. (3.9), is outlined below when $n_F =$ integer:

$$E^\eta_{\mathbf{k}} \begin{pmatrix} \vdots \\ u^\eta_{n_F-1\,\mathbf{k}} \\ u^\eta_{n_F,\mathbf{k}} \\ u^\eta_{n_F+1\,\mathbf{k}} \\ \vdots \\ \cdots\cdots \\ \vdots \\ v^\eta_{n_F-1\,\mathbf{k}} \\ v^\eta_{n_F,\mathbf{k}} \\ v^\eta_{n_F+1\,\mathbf{k}} \\ \vdots \end{pmatrix} = \left(\begin{array}{ccccc|ccccc} \ddots & & & & & & & & & \\ & -\hbar\omega_c & & & & & & & & \\ & & 0 & & & & & F_{\mathbf{k}NM} & & \\ & & & \hbar\omega_c & & & & & & \\ & & & & \ddots & & & & & \\ \hline & & & & & \ddots & & & & \\ & F^*_{\mathbf{k}MN} & & & & & \hbar\omega_c & & & \\ & & & & & & & 0 & & \\ & & & & & & & & -\hbar\omega_c & \\ & & & & & & & & & \ddots \end{array}\right) \begin{pmatrix} \vdots \\ u^\eta_{n_F-1\,\mathbf{k}} \\ u^\eta_{n_F,\mathbf{k}} \\ u^\eta_{n_F+1\,\mathbf{k}} \\ \vdots \\ \cdots\cdots \\ \vdots \\ v^\eta_{n_F-1\,\mathbf{k}} \\ v^\eta_{n_F,\mathbf{k}} \\ v^\eta_{n_F+1\,\mathbf{k}} \\ \vdots \end{pmatrix}$$

The normal state degeneracy between the electron Landau levels $n_F + m$ and the hole Landau level $n_F - m$ means that even a small order parameter, giving a small but finite $F_{\mathbf{k}n_F+m\,n_F-m}$, will cause a strong mixing between these two levels. To lowest order, the pairing splits each Landau level into two levels with energies $m\hbar\omega_c \pm |F_{\mathbf{k}n_F+m\,n_F-m}|$ with the $\pm$ coming from the two solutions to the degenerate 2×2 problem. For the filled levels below the chemical potential, the number of occupied states shifted up in energy equals the number of states shifted down. However, for the partially filled Landau level right at the chemical potential, more particles will reside in the levels shifted down in energy since the levels shifted up will be depleted due to the Fermi factor. Thus, we expect this effect to give a term *linear* in $\Delta(\mathbf{r})$ for the energy difference between the superconducting and the normal state. Schematically:

$$E_S - E_N = -\sigma\Delta + \alpha\Delta^2 + \mathcal{O}(\Delta^3). \tag{6.1}$$

From section 3.7, we know that the Gor'kov expansion only produces terms of even order in $\Delta(\mathbf{r})$ [see, for instance, Eq. (3.22) or Eq. (4.4)]. Thus, the linear term $-\sigma\Delta$ is non-perturbative in the sense that it cannot be obtained by a summation of a finite number of terms in the Gor'kov expansion. It seems the Gor'kov expansion does not work. This is in essence the argument leading to the postulate of the failure of the Gor'kov theory for type-II superconductors close to H_{c2} [8]. In order to examine the argument given above in detail, it is convenient to use the following expression for the difference in the grand canonical potential [12]:

$$
\begin{aligned}
\Omega_S - \Omega_N = &\frac{1}{g}\int d^2r|\Delta(\mathbf{r})|^2 \\
&- 2k_BT\sum_{\eta\,\mathbf{k}\in\mathrm{MBZ}}\ln[\cosh(\beta E^{\eta}_{\mathbf{k}}/2)] + 2k_BT\mathcal{D}\sum_n \ln[\cosh(\beta\xi_n/2)]
\end{aligned}
\tag{6.2}
$$

with, as usual, $\mathcal{D} = \frac{L_xL_y}{2\pi l^2}$ being the degeneracy of each Landau level and $\xi_n = (n - n_F)\hbar\omega_c$. Equation (6.2) which can be derived by calculating $\langle\hat{H}_{mean}\rangle$ using the canonical transformation given in Eq. (2.6), gives the grand canonical potential solely in terms of the quasiparticle energies. This is very useful as we can calculate these quasiparticle energies directly from the BdG equations, taking into account the possible degeneracy between electron and hole levels. In that way, we can obtain an expression for $\Omega_S - \Omega_N$ using Eq. (6.2) which includes the possible non-perturbative effects predicted above. By comparing the resultant expression with the one obtained from the standard Gor'kov expansion, we can check the validity and convergence properties of the Gor'kov theory for type-II superconductors in high magnetic fields. For notational simplicity, we use the approximation $\Delta_{j\neq 0} = 0$ such that the Gor'kov expansion for the grand canonical potential is given by Eq. (4.4). None of the conclusions in this chapter are altered when this restriction is relaxed.

6.3 Zero temperature

First, we consider the case $T = 0$ for which the grand canonical potential is equal to the ground state energy. It turns out that there are non-perturbative terms in the expression for the energy in this limit. To illustrate the origin of the non-perturbative effect for $T = 0$, it is sufficient to examine the case when only one Landau level participates in the pairing (quantum limit) and n_F is an integer. The BdG equations then reduce to the diagonalization of the simple 2×2 matrix $\left(\begin{smallmatrix} 0 & F \\ F^* & 0 \end{smallmatrix}\right)$. The positive energy solution is $E_{n_F\mathbf{k}} = |F_{\mathbf{k}n_Fn_F}|$ and Eq. (6.2) reduces to:

$$E_{gS} - E_{gN} = \frac{1}{g}\int d^2r|\Delta(\mathbf{r})|^2 - \sum_{\mathbf{k}} E_{n_F\mathbf{k}} \tag{6.3}$$

From Eq. (3.13) and Eq. (3.10), we have $|F_{\mathbf{k}n_Fn_F}| \propto \Delta_0 \propto |\Delta(\mathbf{r})|$. Hence, we conclude that there is a linear term in $|\Delta(\mathbf{r})|$ for the ground state energy of the superconductor in the mixed state. This is the non-perturbative linear term mentioned in section 6.2. The result is unaltered when we allow many Landau levels to participate in the pairing. Hence, we confirm the result obtained by Bahcall [8] that for $T = 0$, the ground state energy has a term linear in $\Delta(\mathbf{r})$ making any finite Gor'kov expansion invalid. It is simply a trivial consequence of the fact that we have to take the $T \to 0$ limit $k_BT\ln[2\cosh(\beta E_{N\mathbf{k}}2)] \to E_{N\mathbf{k}}/2$ before we perturbatively expand the result in the size of the order parameter. It is of no surprise that the Gor'kov expansion breaks down in the limit $T = 0$ as it is well known to be a high temperature expansion.

6.4 Finite temperature

6.4.1 Quantum limit

The situation is different for finite temperature. It is now possible to expand $\ln[2\cosh(\beta E_{N\mathbf{k}}/2)]$ in powers of the order parameter and then check if we obtain any non-perturbative terms. For notational simplicity, we will in this section do the calculation in the quantum limit when only one Landau level participates in the pairing. In section 6.4.2, we will treat the slight modifications in our result when more than one Landau level is within the pairing width. The 2×2 matrix for a general n_F in the quantum limit is $\left(\begin{smallmatrix} \xi_n & F \\ F^* & -\xi_n \end{smallmatrix}\right)$ with ξ_n being the energy of the single Landau level within the pairing width. The quasiparticle energy is now, from section 3.6, given as $E_{n\mathbf{k}} = \sqrt{\xi_n^2 + |F_{\mathbf{k}nn}|^2}$. Using this result for the energy, Eq. (6.2) yields an exact expression for the grand canonical potential in the quantum limit. In order to compare this result with the Gor'kov expansion, we need to expand $\ln[\cosh(\beta E_{n\mathbf{k}}/2)]$ in powers of $|F_{\mathbf{k}nn}|^2$. Also, since we have the exact solution for the grand canonical potential, we can determine the convergence radius for a power series in the strength of the order parameter. Writing $\beta E_{n\mathbf{k}}/2 = \sqrt{\epsilon^2 + z^2}$ where $\epsilon \equiv \beta\xi_n/2$ and $z = \beta|F_{\mathbf{k}nn}|/2$, we are led to consider the analytic properties of the function $\ln[\cosh(\sqrt{\epsilon^2 + z^2})]$. From the theory of analytic functions, we know that if a function $f(z)$ is analytic in some area $\mathcal{W}$ in the complex plane $z \in \mathcal{C}$, then it can be written as a power series in the variable $z - a$ with $a \in \mathcal{W}$. The radius of convergence r_0 of this series is at least the minimum distance from the point a to the edge of the area $\mathcal{W}$. Thus, the poles and branch cuts in the complex plane $z \in \mathcal{C}$ of the function $\ln[\cosh(\sqrt{\epsilon^2 + z^2})]$ determine the convergence radius r_0 for a power series in z. A simple analysis gives $r_0 = \sqrt{\epsilon^2 + \pi^2/4}$. The requirement for the convergence of a perturbation series for $\ln[2\cosh(\beta E_{N\mathbf{k}}/2)]$ in powers of

$|F_{\mathbf{k}nn}|$ is then

$$|F_{\mathbf{k}nn}| \leq \sqrt{\xi_n^2 + \pi^2(k_B T)^2}. \qquad (6.4)$$

This requirement is most restrictive when the Landau level is at the chemical potential ($\xi_n = 0$). We then have $E_{\mathbf{k}} \leq k_B T\pi$. Furthermore, by calculating the Taylor expansion of $\ln[\cosh(\sqrt{\epsilon^2 + z^2})]$, we see that there will appear only even powers of $|F_{\mathbf{k}nn}|$ in the series. This is true for general μ_F (i.e also when $\xi_n = 0$). So we can immediately rule out any non-perturbative cubic term in the expression for $\Omega_S - \Omega_N$, thereby disproving the predictions based on a numerical analysis [7, 8]. We can now expand the exact expression given by Eq. (6.2) for the grand canonical potential with $E_{n\mathbf{k}} = \sqrt{\xi_n^2 + |F_{\mathbf{k}nn}|^2}$ in powers of $|F_{\mathbf{k}nn}|^2$ and compare the resulting perturbation series with the Gor'kov expansion as given in Eq. (4.4)[2]. This would rigorously check the validity of the Gor'kov expansion for type-II superconductors close to H_{c2}. We find (not surprisingly) that the two expansions of $\Omega_S - \Omega_N$ agree term by term. We have therefore, within the quantum limit, disproven the rather serious claim that the Gor'kov expansion is invalid even for finite T due to the degeneracy of the Landau levels. Also, we have derived the result that the convergence of the Gor'kov expansion is determined by Eq. (6.4). From this, it is clear that the Gor'kov expansion is a high temperature series; the breakdown of the theory for $T = 0$ as described in section 6.3 is of no surprise. Furthermore, for finite T, we expect the Gor'kov series first to become unreliable when there is a Landau level at the chemical potential. This is because the requirement in Eq. (6.4) is most restrictive when $\xi_n = 0$. This conclusion is supported further by the fact shown in chapter 4 that superconductivity, and thereby the change in the quasiparticle energies, is enhanced when there is a Landau level at the chemical potential, making a

[2]Note that we use Eq. (3.13) to express the expansion in $|F_{\mathbf{k}nn}|^2$ in terms of an expansion in Δ_0^2.

perturbative theory less reliable.

6.4.2 Several Landau levels

The above conclusions are essentially unaltered when there is more than one Landau level participating in the pairing. As the convergence radius for the Gor'kov series is smallest when the chemical potential is at a Landau level, we will here consider the case of n_F integer. The structure of the calculation is the same as in section 6.4.1. We calculate the quasiparticle energies from Eq. (3.9) perturbatively in $F_{\mathbf{k}nm}$ using both degenerate and non-degenerate perturbation theory. Then, we expand $\ln[2\cosh(\beta E_{N\mathbf{k}}/2)]$ in powers of the order parameter. The only complication is that we now obtain both even and odd powers of $F_{\mathbf{k}nm}$ in the expression for the quasiparticle energies. For instance, we saw in section 6.2 that the first order correction to the energy is $\pm|F_{\mathbf{k}n_F+m\,n_F-m}|$. There are also terms of order $3, 5$ etc. in the expression for the quasiparticle energy. It is therefore not *a priori* clear that an expansion from Eq. (6.2) involving both degenerate and non-degenerate perturbation theory will reproduce the Gor'kov expansion with only even powers in $|F_{\mathbf{k}nm}|$. As the actual expansion is a long and tedious calculation, I will not reproduce it here. Instead, I will simply mention its main conclusions: it turns out that the odd terms cancel in the expression for $\Omega_S - \Omega_N$. The reason is, as we saw for the first order term in section 6.3, that there are two quasiparticle levels when $\xi_n \neq 0$ for which the odd powers in the expression for the energy have opposite signs. There is only one positive energy solution for the case $\xi_{n_F} = 0$ though. This was indeed the origin of the non-perturbative effect for $T = 0$. However, for finite T, the odd terms from this solution vanish in the expression for $\Omega_S - \Omega_N$ due to the fact that $\partial_x^{2l+1} \ln[\cosh(x)]|_{x=0} = 0$ where l is an integer. The calculation reveals that we indeed recover the standard terms in the Gor'kov series.

In order to examine the convergence properties of the Gor'kov expansion, we write $\beta E_{n\mathbf{k}}/2 = \beta(\xi_n + \delta E)/2 = \epsilon + z$. This leads us to consider the

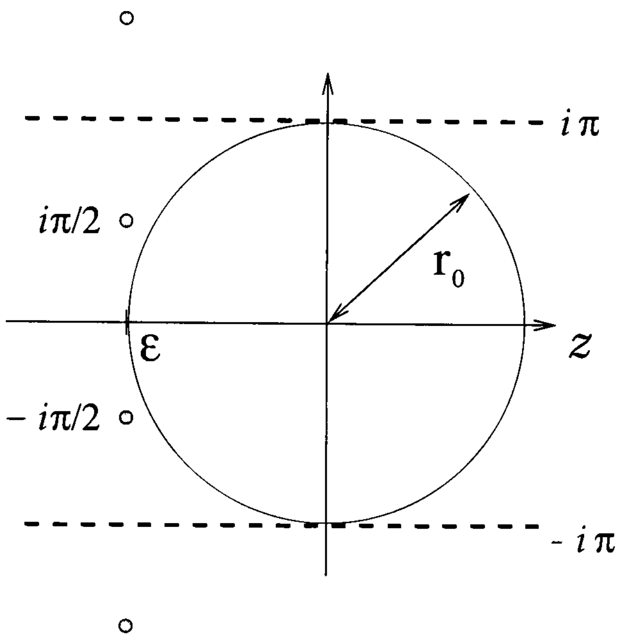


Figure 6.1: The analytic properties of $\ln[\cosh(\epsilon+z)]$ with $z \in \mathcal{C}$. There are two branch cuts at $\mathrm{Im}(z) = \pm i\pi$ and poles at $z = i\pi/2 + in\pi - \epsilon$ with n integer. The convergence radius r_0 for a power series in z is indicated on the figure.

analytic properties of $f = \ln[\cosh(\epsilon+z)]$. The function f has poles for $\cosh(\epsilon+z) = 0$ and a branch cut for $\arg[\cosh(\epsilon+z)] = \pm\pi \Leftrightarrow \mathrm{Im}(z) = \pm i\pi$. The analytic properties of f in the complex plane are illustrated in Fig. 6.1. We see from this that the convergence radius r_0 for a power series in z is $r_0 = \min(\sqrt{\epsilon^2+\pi^2/4}, \pi)$. Thus, a sufficient condition for the convergence of the Gor'kov series is

$$|E_{n\mathbf{k}} - \xi_n| \leq \min\left(2k_BT\pi, k_BT\sqrt{\beta^2\xi_n^2+\pi^2}\right) \tag{6.5}$$

which has to hold for each quasiparticle level within the pairing region. We expect that the Gor'kov theory breaks down when significant portions of the quasiparticle bands lie outside the regions defined in Eq. (6.5). So we have disproven the claim that the Gor'kov expansion is invalid for a finite temperature. The non-perturbative terms cancel in the expression for $\Omega_S - \Omega_N$

and the resulting Gor'kov series in even powers of Δ has a finite convergence radius for $T > 0$. Again, from Eq. (6.5), we clearly see that the Gor'kov theory is a high temperature expansion.

As a first approximation, we can take $|E_{n\mathbf{k}} - \xi_n| = |F_{\mathbf{k}n_F+m\,n_F-m}|$ when the chemical potential is at a Landau level. Using Eq. (3.10), Eq. (3.12), Eq. (3.13), and Eq. (A.1), we can after some algebra transform Eq. (6.5) into the requirement:

$$\langle|\Delta(\mathbf{r})|^2\rangle \equiv \frac{1}{L_x L_y}\int d^2r|\Delta(\mathbf{r})|^2 \leq 2\sqrt{\pi n_F}\pi^2(k_BT)^2 \tag{6.6}$$

This condition gives $\sqrt{\langle|\Delta(\mathbf{r})|^2\rangle}/n_F^{1/4} \leq \sqrt{2}\pi^{5/4}k_BT \simeq 1.9\pi k_BT$ Based on an extensive numerical analysis, Norman *et al.* [83] suggested that a crossover from a perturbative to a non-perturbative regime should occur for $\sqrt{\langle|\Delta(\mathbf{r})|^2\rangle}/n_F^{1/4} = 2\pi k_BT$ in almost precise agreement with Eq. (6.6). Thus, our analytical conditions for the convergence radius of the Gor'kov expansion seem to be verified by a numerical analysis.

As mentioned in section 6.1, Ginzburg-Landau theory can be derived from the microscopic Gor'kov expansion under certain semiclassical conditions [42]. This theory is widely used when solving problems connected to type-II superconductors near the upper critical field. Since we have now established a criterion for the convergence of the Gor'kov expansion, it would be of interest to restate Eq. (6.6) in terms of Ginzburg-Landau parameters. In that way, we can examine if the convergence radius of the Gor'kov expansion introduces a new constraint on the validity•of Ginzburg-Landau theory. From the derivation of the Ginzburg-Landau theory from BCS theory, there is a precise link between the Ginzburg-Landau constants and the microscopic parameters [42]. The Ginzburg-Landau wave function $\Psi(\mathbf{r})$ is given by $\Psi(\mathbf{r}) = \left(\frac{7\xi(3)n}{8(\pi k_BT_c)^2}\right)^{1/2}\Delta(\mathbf{r})$ where $\zeta(x)$ is Riemann's Zeta function and n is the density of electrons. Close to the upper critical field, we have for the spatial average $\langle|\Psi(\mathbf{r})|^2\rangle = -\frac{\alpha}{\beta}\frac{1-H/H_{c2}}{\beta_A(1-1/2\kappa^2)}$ [34] with κ being the Ginzburg Landau parameter and β_A the Abrikosov parameter[3]. We have $\beta_A = 1.16$ for a triangular lattice. Here $\alpha = -\frac{6\pi^2(k_BT_c)^2}{7\xi(3)\epsilon_F^0}(1-T/T_c)$ and $\beta = \frac{6\pi^2(k_BT_c)^2}{7\xi(3)\epsilon_F^0 n}$ are the usual Ginzburg-Landau constants. Using these relations and $H_c(T)^2 = 4\pi\alpha^2/\beta$, we can after some algebra rewrite Eq. (6.6) as

$$\frac{H_{c2}-H}{H_c(0)} \leq \sqrt{n_F}\pi^{1/2}[7\zeta(3)]^{1/2}\beta_A e^{\gamma}(\kappa - \frac{1}{2\kappa})\left(\frac{T}{T_c}\right)^2 \tag{6.7}$$

where γ is Euler's constant. Fortunately, this restriction is always fulfilled for type-II superconductors within the normal range of validity of the Ginzburg-Landau equations (i.e $|T - T_c|/T_c \ll 1$). We conclude that the convergence criteria for the Gor'kov series does not introduce any new restrictions on the validity of Ginzburg-Landau theory.

6.5 Numerical analysis

Finally, we will briefly consider numerical results in order to check some of the statements above. We compare our fourth order perturbative results for $\Delta(\mathbf{r})$ derived from Eq. (4.5) with the exact numerical solution of the BdG equations. This was already done in some detail in section 4.4 where the parameters $\omega_D/\omega_c = 5$, $\frac{g}{\hbar\omega_c l^2} = 8.2$ and $k_BT/\hbar\omega_c = 0.28$ when $n_F = 12$ were used. We saw that there was relatively good agreement between the Gor'kov expansion and the exact solution close to H_{c2} thereby confirming the validity of the perturbation theory. Also, we note from Fig. 4.3 with $n_F \gtrsim 12$ that the perturbative result tends to differ most from the exact solution when the chemical potential is at a Landau level. This conclusion is confirmed by solving the BdG equations with various sets of parameters [22]. It is in agreement with the remarks made in section 6.4.1 and section 6.4.2 that the Gor'kov expansion is expected to break down first when there is a Landau level at the chemical potential.

[3] This equation directly gives the much used relation $\Delta(H) = \Delta(0)\sqrt{1 - H/H_{c2}}$.

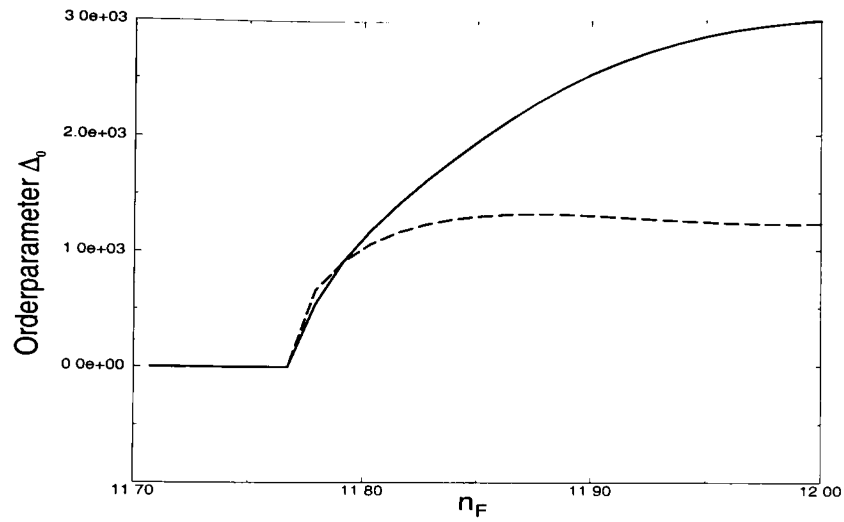


Figure 6.2: The order parameter Δ_0 vs n_F calculated numerically (solid line) and perturbatively to fourth order in Δ_0 (dotted line) for $\omega_D/\omega_c = 5$, $\frac{g}{\hbar\omega_c l^2} = 7.0$ and $k_BT/\hbar\omega_c = 0.05$ when $n_F = 12$.

To illustrate the temperature dependence of the convergence radius of the Gor'kov series, we plot in Fig. 6.2 Δ_0 as a function of n_F for a very low temperature. As can be seen, the perturbation series breaks down much earlier ($\Delta_0 \sim 1000$) for this low temperature in agreement with Eq. (6.5). In Fig. 6.3, we plot the lowest quasiparticle level along the high symmetry $K - M$ direction in $\mathbf{k}$-space when $n_F = 12$ for the parameters used in Fig. 6.2[4]. The horizontal line gives the boundaries for $E_{\mathbf{k}} - \xi_{n_F}$ calculated from Eq. (6.5). As expected, there are large parts of the quasiparticle band in $\mathbf{k}$-space lying outside the region of convergence of the perturbation expansion. This explains the observed discrepancies between perturbation theory and the exact numerical result. Thus, the numerical results presented here and by other authors [22, 83] seem to confirm the convergence properties of the Gor'kov expansion derived in this chapter.

[4]The line $K - M$ in the MBZ is defined in section 3.5.

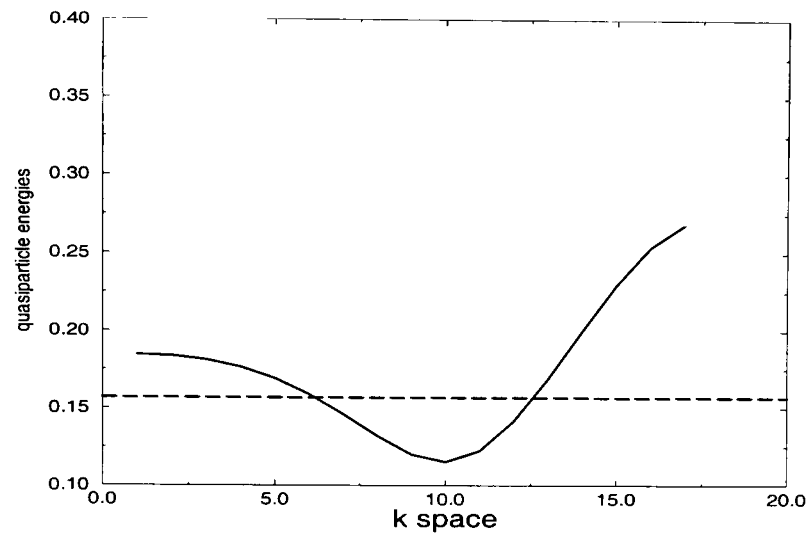


Figure 6.3: The lowest quasiparticle band in units of $\hbar\omega_c$ along a high symmetry line in **k**-space for $n_F = 12$. The dashed line marks the boundary defined by Eq. (6.5).

6.6 Summary

In conclusion, we have in this chapter examined the convergence properties of the Gor'kov expansion. Recently, it was claimed that this expansion is invalid for type-II superconductors close to H_{c2} due to the large degeneracy of the Landau levels. It is important to establish whether such a claim is true since the Gor'kov theory is widely used to calculate properties of superconductors in magnetic fields. We find, in agreement with Bahcall [8], that for $T = 0$ there is indeed a non-perturbative term linear in $\Delta(\mathbf{r})$ in the expression for the grand canonical potential. For finite T, our conclusion is that although the degeneracy of the Landau levels gives large effects on the quasiparticle wave functions even for a weak superconducting order, these effects cancel in the expression for the grand canonical potential and the Gor'kov expansion is in fact correct. We have therefore ruled out the possibility of a non-perturbative third order term in the expression for the grand canonical potential. Also, we have derived some convergence criteria for the Gor'kov expansion; the minimum range of validity is given by Eq. (6.5) which indicates that Gor'kov theory is essentially a high temperature expansion. This requirement is always fulfilled within the range of validity of the Ginzburg-Landau equations leading to no inconsistencies. Furthermore, we have the usual requirement $|E_{n\mathbf{k}} - \xi_n| \ll \hbar\omega_c$ for perturbation theory to work. We conclude that the Gor'kov expansion is expected to breakdown first when the chemical potential is at a Landau level. Our results are confirmed by a comparison between the results of an exact numerical solution to the BdG-equations and a Gor'kov series to fourth order in the order parameter, and they agree with the conjecture of Norman *et al.* [83].

Chapter 7

Summary and outlook

7.1 Review of main results obtained

In this thesis, we have studied clean type-II superconductors in the mixed state in high magnetic fields and low temperatures such that the semiclassical approximation breaks down. The physics of the mixed state is characterized by the competition between the tendency of the electrons to form Cooper pairs and to reside in Landau levels. This is the origin of a number of interesting phenomena, and an understanding of this subject is important both from a fundamental point of view and for practical applications.

We have considered several aspects of the physics in the mixed state. Within the mean field approximation, the order parameter $\Delta(\mathbf{r})$ is known to form a vortex lattice. This symmetry puts strict limitations on the functional form of order parameter and it can be parametrized by a finite set of variables. Using this, we were able to develop an algebra which simplifies the analysis considerably; the Gor'kov expansion for the grand canonical potential was found to reduce to a simple polynomial in the variables parametrizing the order parameter. The problem of determining $\Delta(\mathbf{r})$ self-consistently was shown to be equivalent to the much easier task of minimizing this polynomial with respect to these variables. The critical temperature determined from the sign shift of the lowest order term in the Gor'kov expansion was shown to be maximum when the Cooper pairs acquired a minimum in the kinetic energy.

The algebra developed to describe type-II superconductors in the mixed state was used to construct a theory for the experimentally observed damped dHvA oscillations in the mixed state. An inherent feature of the theory is the self-consistent determination of the order parameter. This seems important as the order parameter was found to be an oscillatory function of the magnetic field; these oscillations must be included in any consistent theory for the dHvA-effect. The theory which is based on the Gor'kov expansion, was compared to an exact numerical solution and we found good agreement close to H_{c2}. A physical interpretation of the damping of the oscillations emerged naturally from the formalism; the superconducting condensation energy oscillates in anti-phase with the normal state energy since the instability towards superconductivity is enhanced whenever there is a Landau level at the chemical potential such that the density of states for gapless normal state excitations is large. The difference between the cases of constant chemical potential and a fixed number of particles was considered. By simplifying the theory in the limit of many Landau levels participating in the Cooper pairing, we were able to predict the dependence of the damping of the dHvA oscillations in the mixed state on parameters such as a finite Zeeman term, the temperature, and the magnetic field. We compared our theoretical predictions with experimental data on the quasi-2D organic superconductor κ-$(ET)_2Cu(NCS)_2$ and found good agreement.

A theory for the attenuation of longitudinal sound waves in the clean limit of type-II superconductors in the mixed state was presented. Contrary to many earlier attempts, the algebra set up in this thesis enabled us to derive physically reasonable results from the microscopic BdG equations. The attenuation was shown to be an oscillatory function of the external magnetic field close to H_{c2}. Since the attenuation probes the low lying density of states, the presence of gapless points in the quasiparticle spectrum was predicted to have a fundamental influence on the attenuation. In contrast to the Meissner state, there is no discontinuity in the attenuation as a function of frequency in the limit of low temperature. Furthermore, the frequency and temperature dependence of the attenuation was found to yield information on the dispersion law around these gapless points in the limit of low temperature and low frequency respectively. As the existence of the gapless quasiparticle excitations follows directly from the formalism for type-II superconductors in a strong magnetic field, we suggested that a measurement of the attenuation of a longitudinal sound wave in the mixed state should provide a fundamental check of our theoretical understanding of the interplay between magnetic fields and superconductivity.

Some aspects concerning the convergence properties of the Gor'kov expansion were derived. This rather formal analysis was performed in the light of recent predictions of the breakdown of the Gor'kov theory when describing type-II superconductors in high magnetic fields. The origin of the breakdown was claimed to be due to the large degeneracy of the Landau levels in the normal state. This degeneracy makes the system very sensitive to any small, but finite, order parameter and perturbative description is questionable. Indeed, for $T = 0$, we showed that the expression for the ground state energy of the superconductor contains a non-perturbative term not included in any finite Gor'kov series. However, for finite temperature, we found that the non-perturbative terms cancel and that the Gor'kov expansion yields correct results close to the upper critical field H_{c2}. We disproved the claim that the Gor'kov expansion is invalid at finite T for type-II superconductors close to the upper critical field, thereby establishing the validity of a large body of published work on the properties of the mixed state (including parts of this thesis). In fact, the Gor'kov series was shown to be a high temperature expansion in the sense that it is convergent if the change δE of the quasiparticle energies in the mixed state, as compared to the normal state, is such that

$\delta E \lesssim k_B T$.

7.2 Possible future research

Since the interplay between superconductivity and external magnetic fields gives rise to such a rich variety of phenomena, there are several natural extensions of the research presented in this thesis. I will here describe some of these:

- **Extension of the theory of the dHvA effect to three dimensions.** As noted in chapter 4, we were unable to perform a very strict comparison between our theory and experimental data due to the observed spread in the upper critical field H_{c2} for the quasi-2D crystal κ-$(ET)_2Cu(NCS)_2$. An immediate continuation of my research would be to extend my theory of the dHvA effect in the mixed state to 3D systems. As mentioned in section 4.10.5, Janssen *et al.* [61] have performed a series of beautiful dHvA experiments on the 3D materials V_3Si and 2H-$NbSe_2$. They compare their results with a number of theoretical predictions for the damping of the dHvA oscillations in the mixed state. The conclusion is that *none* of the present theories for 3D materials can reproduce the experimental data for both materials. It would therefore be very interesting to extend the theory presented in chapter 4 to 3D systems, thus enabling a comparison with the high quality experimental data. In fact, I have been contacted by one of the authors of ref. [61] who requested me to embark on such an extension [101].

- **Calculation of the Local Density of States.** Recently, Hess *et al.* [55, 56, 57] have managed to perform a series of elegant Scanning Tunneling Microscopy measurements of the local density of states (LDOS) around a vortex core for the type-II superconductor 2H-$NbSe_2$. Their results yield detailed information on the structure and energy of the quasiparticle states bound within the vortex core. This has sparked a number of theoretical investigations of the LDOS in the mixed state. Gygi *et al.* calculated the LDOS obtained from a solution to the BdG equations in the case of an isolated vortex [51]. However, the STM experiments are usually performed in a high magnetic field where the distance between the vortex cores is relatively short and the overlap of the vortices cannot be neglected. Therefore, in a later publication, they put in by hand the influence of the vortex lattice by introducing an arbitrary perturbation term in the BdG equations [52]. A more rigorous calculation of the LDOS including the influence of the vortex lattice was presented by Hayashi *et al.*[54, 60]. Their calculation is based on a solution to the semiclassical Eilenberger equations and does not include the quantum effects of the magnetic field. But, as we have seen in this thesis, the presence of the dHvA oscillations in the mixed state of a number of superconductors indicate that it is important to include the Landau level structure of the normal state spectrum when calculating properties of the quasiparticle states. By using the theoretical framework outlined in this thesis, it should be straightforward to calculate the LDOS including the Landau levels from the outset.

- ***d*-wave superconductivity.** This thesis has exclusively considered superconductors with an isotropic (s-wave) pairing. In recent years, strong evidence has been presented that the High T_c's have an unconventional pairing symmetry such as pure $d-$wave or more exotic mixtures [5]. As the High T_c's have a very high upper critical field H_{c2}, experiments are being performed in their mixed state. This means that the interplay between high magnetic fields and superconductivity with an unconventional pairing symmetry is a relevant problem to investigate. Thus, an interesting project would be to generalize some of the results presented in this thesis to cases such as $d-$wave pairing. For example, from chapter 5, we expect the inherent gapless points of a $d-$wave superconductor to have measurable consequences on the acoustic attenuation.

- **Lattice melting.** As mentioned in section 2.6, mean field theory is expected on general grounds to break down close to the upper critical field. This breakdown should be accompanied by the melting of the vortex lattice; it simply loses its regular lattice structure as the vortices start to move in the plane perpendicular to the magnetic field. For many low temperature superconductors, the melting occurs unobservably close to H_{c2}. However, in High T_c's, with their short coherence length, high critical temperature and low dimensionality, there is sufficient thermal energy to induce melting well below T_c [14]. This gives rise to a wealth of interesting problems such as how the thermal energy, the vortex-vortex interaction, pinning and interlayer coupling determines the various phases (pancake phase, disentangled and entangled vortex liquid) [31]. To address such questions, we would have to include the effect of fluctuations of the order parameter away from the mean field solution in the theory presented in the preceding chapters. In that way, we could investigate the question of the vortex lattice melting including the quantum effects of the magnetic field right from the beginning.

- **BCS state in a magnetic trap.** Another exciting project is the question of a BCS state for a gas of ultra-cold atoms in an external trap. This problem emerged naturally after the impressive experimental achievement of Bose-Einstein condensation in the trapped Bosonic systems ^{87}Rb, ^{7}Li, and ^{23}Na [4, 17, 33]. The main candidates for achieving a BCS transition in a trap are the fermionic atoms ^{40}K and ^{6}Li. Several groups both in Europe and in the United States are now experimentally investigating the problem of forming a BCS state with these atoms. A problem of obvious importance to experimentalists is how to observe the formation of the superfluid. In the Bose-Einstein case, the formation of the condensate could be observed by measuring the momentum distribution or by looking at the excitations of the condensate. In the fermionic case, the problem seems to be somewhat more complicated. Due to the Pauli exclusion principle, one cannot macroscopically populate the quasiparticle excitations making them easily observable. Also, it is not obvious that the momentum distribution will change significantly in the BCS state as compared to the normal state. Hence, the development of a microscopic theory for a superfluid in a trap and for the various experimentally measurable quantities is desirable. The external trapping potential can, to a good approximation, be represented by a simple harmonic oscillator potential. As the motion of a particle in a harmonic potential is closely linked to that of a charged particle in a magnetic field, much of the formalism developed through my research on superconductivity in high magnetic fields can be carried over to the problem of the BCS state in a trap. I am therefore at the moment heavily involved in research into this area. A major problem has been the development of a renormalizable theory for an interacting trapped Fermi gas. Since there is no natural cutoff ω_D for the effective interaction in the case of trapped atoms, one has to remove the ultraviolet divergence in a somewhat more careful way [21]. The primary objective of such a theory is to calculate various observables such as the density distribution, the energy, heat capacity, and the quasiparticle excitations. In that way, we hope/expect to identify an observable which will change significantly at the phase transition. I have also examined the properties of a gas of interacting fermions in a trap in the normal state [20]. These properties are important to understand in order to achieve superfluidity and to be able to compare the properties of the two states. There are, of course, numerous other interesting theoretical challenges. These involve a calculation of the collective modes (Goldstone modes) and their damping for a trapped BCS state, the formation of vortices in such a state, extension of the theory to include time-dependent problems, etc. Also, as one can cool ^{6}Li with the bosons ^{7}Li, it would be relevant to develop a theory for a system of bosons mixed with fermions in a magnetic trap.

Appendix A

Calculation of the oscillatory terms

In this section, I will outline the derivation of some approximate expressions for the coefficients a_2 and g_2. We are interested in how a_2 and g_2 depend on the parameters n_F, ω_D, T, the spin and on the external magnetic field. It turns out that it is fairly straightforward to extract this dependence. First, we note the following approximate identity coming from the law of large numbers:

$$B_0^{n_1,n_2} \simeq \frac{1}{\sqrt[4]{\pi n_1}} e^{-(n_1-n_2)^2/8n_1} \simeq \frac{1}{\sqrt[4]{\pi n_F}} e^{-(n_1-n_2)^2/8n_F} \tag{A.1}$$

where we have assumed that $|n_1 - n_2|/n_1 \ll 1$ and $n_1 \simeq n_F$ (i.e $\omega_D/\omega_c \equiv 2\sigma \ll n_F$). Using this formula, Eq. (3.29), and the Poisson identity Eq. (4.2), we obtain the following integrals for $\alpha(H)$:

$$\hbar\omega_c \sum_{n_1,n_2} B_0^{n_1\,n_2 2} \frac{\tanh(\beta\frac{\xi_{n_1}}{2}) + \tanh(\beta\frac{\xi_{n_2}}{2})}{\xi_{n_1} + \xi_{n_2}} w^2(n_1) w^2(n_2) =$$

$$\sum_{l,m} e^{2\pi i n_F(m-l)} \iint dx\, dy e^{2\pi i(mx-ly)} \frac{e^{-\frac{(x-y)^2}{4n_F}}}{\sqrt{\pi n_F}} \frac{\tanh(\beta\frac{\xi_x}{2}) + \tanh(\beta\frac{\xi_y}{2})}{x+y} w^2(x) w^2(y)$$

$$= \sum_{l,m} I_{l,m} e^{2\pi i n_F(m-l)} \tag{A.2}$$

where $\xi_x = \hbar\omega_c x$ and $w(x) = e^{-(\xi_x/0.5\hbar\omega_D)^2} = e^{-x^2/\sigma^2}$. Also, we have neglected a finite Zeeman term for the moment. To estimate $I_{l,m}$ where $(l,m) \neq (0,0)$, we write the integral in the form:

$$I_{l,m} = \frac{2k_B T}{\hbar\omega_c} \sum_\nu \iint dx\, dy \frac{e^{-(x-y)^2/4n_F}}{\sqrt{\pi n_F}} \frac{e^{-2(x^2+y^2)/\sigma^2 + 2\pi i(mx-ly)}}{(x - i\omega'_\nu)(y + i\omega'_\nu)} \tag{A.3}$$

where $\omega'_\nu = \omega_\nu/\omega_c$. The 1'st harmonic of $\alpha(H)$ comes from the terms with $|l-m| = 1$. Taking $m = 1$ and $l = 0$ yields the integral:

$$\int dx \frac{e^{2\pi i x - 2x^2/\sigma^2}}{x - i\omega'_\nu} \int dy \frac{e^{-2y^2/\sigma^2 - (x-y)^2/4n_F}}{y + i\omega'_\nu} \tag{A.4}$$

We approximate this integral by:

$$\int dx \frac{e^{2\pi i x}}{x - i\omega'_\nu} \int dy \frac{e^{-(y-x)^2/4n_F}}{y + i\omega'_\nu} \tag{A.5}$$

since we have assumed $8n_F \ll \sigma^2$. The integral can be solved exactly and we obtain:

$$I_{0,1} =$$

$$\frac{4k_BT\pi^2}{\hbar\omega_c\sqrt{\pi n_F}}\sum_{\nu\geq 0} e^{-2\pi\omega'_\nu}\left([1-\Phi(\omega'_\nu/\sqrt{n_F})]e^{\omega'^2_\nu/n_F} + e^{t_\nu^2}[(1-\Phi(t_\nu))]e^{-4\pi^2 n_F}\right)$$

$$\simeq \frac{4k_BT}{\hbar\omega_c\sqrt{\pi n_F}}\pi^2 e^{-2\pi^2\frac{k_BT}{\hbar\omega_c}} \quad \text{(A.6)}$$

where $\Phi(x) \equiv 2\pi^{-1/2}\int_0^x e^{-s^2}ds$ is the error function and $t_\nu = (\omega'_\nu + 2\pi n_F)/\sqrt{n_F}$. Here we have used that $\exp(-2\pi\omega_{\nu\neq 0}) \ll \exp(-2\pi\omega_{\nu=0})$ for $2\pi^2 k_BT/\hbar\omega_c \gtrsim 1$, $\exp(-4\pi^2 n_F) \ll 1$, and $n_F^{-1/2}\omega'\nu = 0 \ll 1$. So, in this temperature range the dominant contribution to the 1'st harmonic comes from the lowest Matsubara frequency, which makes our approximation above self-consistent. Note, that in this temperature regime only the 1'st harmonic of the oscillations is important in agreement with the comments at the end of section 4.7. The contribution to the 1'st harmonic from the $|l-m| = 1$ term given $l, m \neq 0$ can be calculated in the same way; it is proportional to $\exp(-2\pi^2 mk_B\hbar\omega_c)$ and therefore negligible for $2\pi^2k_BT/\hbar\omega_c \gtrsim 1$ in agreement with the results obtained by Gruenberg and Gunther [50]. After some algebra, the calculations outlined above combined with Eq. (3.29) lead to the following result:

$$a_2 \simeq \frac{g^2\left(\frac{a_x}{l}\right)2\pi}{L_xL_yl^2\sqrt{\pi n_F}}\frac{k_BT}{(\hbar\omega_c)^2}e^{-2\pi^2\frac{k_BT}{\hbar\omega_c}} \quad \text{(A.7)}$$

The above result that a_2 is proportional to $1/\sqrt{n_F}$ and $k_BTe^{-2\pi^2\frac{k_BT}{\hbar\omega_c}}$ and independent of ω_D is still correct even when $\sigma^2 \ll 8n_F$, as long as $\min(\sigma, \sqrt{n_F}) \gg 1$ and $2\pi^2k_BT/\hbar\omega_c \gtrsim 1$.

We can now easily calculate the effect of a finite Zeeman term. Inclusion of spin is simply equivalent to making the substitution $x \rightarrow x + \frac{g^*m}{4m_0}$ and $y \rightarrow y - \frac{g^*m}{4m_0}$ in the integrals $I_{l,m}$. This results in a reduction factor $\cos(\pi\frac{g^*m}{2m_0})$ in Eq. (A.7) if $\min(\sqrt{n_F}, \sigma) \gg g^*$. This reduction factor is the same as for the normal state oscillations.

The calculations for g_2 are very similar to the ones above. Using Eq. (3.30) and the Poisson formula, we end up with the following integrals determining the dependence of γ on n_F, T, ω_D and the magnetic field:

$$\sum_{\substack{l_1,l_2,l_3,l_4 \\ \nu}} \frac{k_B T}{n_F} e^{2\pi i n_F(l_1+l_3-l_2-l_4)}$$
$$\times \int dx_1 \ldots dx_4 \frac{e^{-(x_1-x_4)^2+(x_3-x_2)^2+(x_1-x_2)^2+(x_3-x_4)^2]/8n_F}}{(i\omega'_\nu - x_1)(i\omega'_\nu + x_2)(i\omega'_\nu - x_3)(i\omega'_\nu + x_4)}$$
$$\times e^{-2(x_1^2+x_2^2+x_3^2+x_4^2)/\sigma^2} e^{2\pi i(l_1x_1+l_3x_3-l_2x_2-l_4x_4)} \Xi_{x_1+x_2,x_3+x_4}^{x_1+x_4,x_2+x_3} \tag{A.8}$$

where $\Xi_{j_3,j_4}^{j_1,j_2}$ is given in Eq. (3.32). Contributions to the 1'st harmonic of g_2 come from the terms with $|l_1 + l_3 - l_2 - l_4| = 1$. As in the case for a_2, we can neglect the terms with more than one l_i different from zero when $2\pi^2 k_B T/\hbar\omega_c \gtrsim 1$. Although we do not have any simple expression for $\Xi_{x_1+x_2,x_3+x_4}^{x_1+x_4,x_2+x_3}$, we can still extract the dependence on T, ω_D, and n_F. This is because the integral over $x_2 \ldots x_4$ does not vary appreciably with x_1 on a scale $\mathcal{O}(\omega'_{\nu=0})$. Using the result $\int dx \frac{exp(2\pi i x_1)}{i\omega' - x_1} f(x_1) \propto f(0)e^{-2\pi\omega'}$ $(\omega' > 0)$ for any well-behaved function $f(x)$ which varies slowly for $x \lesssim \omega'$ and taking $l_1 = 1,\ l_2 = l_3 = l_4 = 0$, we get the integral:

$$\frac{k_B T}{n_F} \int dx_1 \frac{e^{2\pi i x_1}}{i\omega'_\nu - x_1} \int dx_2 \ldots dx_4 \frac{e^{-[x_4^2+(x_3-x_2)^2+x_2^2+(x_3-x_4)^2]/8n_F}}{(i\omega'_\nu + x_2)(i\omega'_\nu - x_3)(i\omega'_\nu + x_4)}$$
$$\times e^{2(x_2^2+x_3^2+x_4^2)/\sigma^2} \Xi_{x_2,x_3+x_4}^{x_4,x_2+x_3} \tag{A.9}$$

The factors $(i\omega'_\nu \pm x_j)^{-1}$ in the integrand makes the integral largely independent of any long range behaviour determined by σ and n_F as long as $|\omega'_\nu| \ll \min(\sigma, \sqrt{n_F})$. We therefore conclude that g_2 is independent of ω_D and that it only depends on n_F through the n_F^{-1}-factor coming from the four $B_0^{N,M}$ coefficients. We also obtain that g_2 is proportional to $k_B T \exp(-2\pi^2 \frac{k_B T}{\hbar\omega_c})$. The proportionality constant is found through an exact evaluation of γ given in Eq. (3.30). We obtain:

$$g_2 \simeq \frac{\left(\frac{g}{\hbar\omega_c}\right)^4 27}{n_F(L_xL_y)^3 l^2} k_B T e^{-2\pi^2 \frac{k_B T}{\hbar\omega_c}} \tag{A.10}$$

Again, the effect of spin provide an additional $\cos(\pi \frac{g^* m}{2m_0})$ in Eq. (A.10). It is not surprising that the oscillatory terms a_2 and g_2 are independent of the pairing width ω_D since the oscillations are a consequence of the individual Landau levels going through the chemical potential. Likewise the $1/\sqrt{n_F}$ and $1/n_F$ dependence reflect the fact that the probability for two electrons, each with energy $(n+1/2)\hbar\omega_c$, to form a pair with minimum COM energy is proportional to $1/\sqrt{n}$ for high quantum numbers, as can be seen from Eq. (A.1). This proportionality can be explained via simple phase-space considerations. We have tested the dependence of a_2 and g_2 on the different parameters n_F, ω_D and T by evaluating Eq. (3.29)-(3.30) numerically, and we find excellent agreement with our approximate forms.

Appendix B

Calculation of the smooth terms

In this appendix, we will extract the dependence of a_1 and g_1 on n_F, T, σ and spin. This is considerably harder than for a_2 and g_2 because we do not have any oscillatory factor in the relevant integrals that would make the long range behaviour of the remaining integrand insignificant. It turns out, that it is still fairly straightforward to derive the temperature and spin dependence of a_1 and g_1, whereas we have to make some rather drastic approximations to obtain the dependence on n_F and σ for g_1.

The smooth part (zeroth harmonic) of $\alpha(H)$ comes from the terms $I_{l,l}$ in Eq. (A.2). We first look at the term $l = m = 0$. Making the variable substitution $v = \frac{x+y}{\sigma\sqrt{2}}$, $u = \frac{x-y}{\sigma\sqrt{2}}$, we get the following integral:

$$I_{0,0} = \frac{\sigma}{\sqrt{2\pi n_F}} \int du \int dv e^{-(\frac{\sigma^2}{2n_F}+2)u^2} \{\tanh[K\sigma(v+u)] + \tanh[K\sigma(v-u)]\} \frac{e^{-2v^2}}{v} \tag{B.1}$$

where $K\sigma = \beta\hbar\omega_c\sigma/2\sqrt{2} \gg 1$ determines the temperature dependence of the integral. Since K is only important around the region $v \simeq 0$ which does not contribute significantly to the integral, we conclude that $I_{0,0}$ is independent of the temperature to a very good approximation. Calculations similar to the ones in appendix A show that for $2\pi^2 k_B T/\hbar\omega_c \gtrsim 1$, we can neglect the contribution to the zeroth harmonic from the $I_{l,l}$-terms where $l \neq 0$; we conclude that a_1 for is independent of the temperature for temperatures that are not too high. We have checked this independence against the exact result given in Eq.(3.29) and found very good agreement. To obtain the dependence on n_F and σ, we make the simplification

$$\frac{\tanh[K\sigma(v+u)] + \tanh[K\sigma(v-u)]}{v} \simeq \begin{cases} 0 & \text{if } |v| < |u| \\ \frac{2}{|v|} & \text{if } |v| > |u| \end{cases} \tag{B.2}$$

which is a very good approximation since $K\sigma \gg 1$. It is exact for $T = 0$. The resulting integral can then be solved and we obtain:

$$I_{0,0} \simeq \frac{4}{\sqrt{1 + n_F/\sigma^2}} \ln\left(\sqrt{\frac{\sigma^2}{4n_F} + 1} + \sqrt{\frac{\sigma^2}{4n_F} + 2}\right) \simeq 2\ln(\frac{\sigma^2}{n_F}) \tag{B.3}$$

where we have assumed $\sigma^2 \gg 4n_F$. This yields the result

$$a_1 \simeq \frac{g^2\left(\frac{a_x}{l}\right)}{4\pi L_x L_y l^2 \hbar\omega_c}. \tag{B.4}$$

The expression for a_1 is independent of any spin effects for $\min(\sqrt{n_F}, \sigma) \gg g^*$. We have again checked the independence of a_1 on n_F, σ, and spin against the exact result obtained from Eq. (3.29) and we find very good agreement.

The dependence of g_1 on n_F, σ, and T is determined by the integrals in Eq. (A.8) for which $l_1 - l_2 + l_3 - l_4 = 0$. Again, it turns out that for $2\pi^2 k_B T/\hbar\omega_c \gtrsim 1$ we can neglect the contribution to g_1 from the terms with $l_1 - l_2 + l_3 - l_4 = 0$ and $\max(|l_1|, |l_2|, |l_3|, |l_4|) > 0$. Using Eq. (3.31), we can rewrite the integral with $l_1 = l_2 = l_3 = l_4 = 0$ as

$$\int dx_1 \ldots dx_4 \frac{\hbar\omega_c}{2} \left[\frac{1}{x_3 - x_1} \left(\frac{\tanh(Kx_1/2)}{(x_1+x_2)(x_1+x_4)} - \frac{\tanh(Kx_3/2)}{(x_3+x_2)(x_3+x_4)} \right) \right.$$
$$\left. + \frac{1}{x_4 - x_2} \left(\frac{\tanh(Kx_2/2)}{(x_1+x_2)(x_2+x_3)} - \frac{\tanh(Kx_4/2)}{(x_4+x_1)(x_4+x_3)} \right) \right] \times$$
$$e^{[(x_1-x_4)^2+(x_3-x_2)^2+(x_1-x_2)^2+(x_3-x_4)^2]/8n_F - 2(x_1^2+x_2^2+x_3^2+x_4^2)/\sigma^2} \Xi^{x_1+x_4, x_2+x_3}_{x_1+x_2, x_3+x_4} \tag{B.5}$$

where $K = \hbar\omega_c/k_B T$ determines the temperature dependence. Again for $\min(\sqrt{n_F}, \sigma) \gg g^*$, g_1 will be independent of spin effects. As in the case of a_1, it is fairly straightforward to see that since $1/K \ll \min(\sqrt{n_F}, \sigma)$, the integral and therefore g_1 are independent of the temperature to a very good approximation. We have checked this independence against the exact result given in Eq. (3.30) and we find excellent agreement.

To make any progress in determining the dependence of g_1 on σ and n_F, we need some simple expression for $\Xi^{n_1+n_4, n_2+n_3}_{n_1+n_2, n_3+n_4}$. As a rough approximation, we make the following simplification to:

$$\Xi^{n_1+n_4, n_2+n_3}_{n_1+n_2, n_3+n_4} \sim (\delta_{n_1,n_3} + \delta_{n_2,n_4}) \frac{L_x L_y}{4\pi a_x^2} \tag{B.6}$$

This is based on the expression

$$\Xi^{j_1,j_2}_{j_3,j_4} = \sum_{\mathbf{k} \in MBZ} \chi_{j_1}(\mathbf{k}) \chi_{j_2}(\mathbf{k}) \chi^*_{j_3}(\mathbf{k}) \chi^*_{j_4}(\mathbf{k}). \tag{B.7}$$

and the fact that $\chi_{j_1}(\mathbf{k})\chi^*_{j_2}(\mathbf{k})$ in general is a complex number for $j_1 \neq j_2$. When the $\mathbf{k}$-sum is performed the phase factor will change 'randomly' and make the sum approximately zero. Physically it corresponds to ignoring cases where electrons in four different Landau levels interact. Using this simplification, Eq. (A.1) and the Poisson formula, we get from Eq. (3.30) the following integral determining the dependence of g_1 on n_F and σ:

$$\sum_{\omega'_\nu} \frac{k_B T}{n_F} \int dx dx_2 dx_4 \frac{e^{-[(x-x_2)^2+(x-x_4)^4]/4n_F}}{(i\omega'_\nu - x)^2(i\omega'_\nu + x_2)(i\omega'_\nu + x_4)} e^{-2(2x^2+x_2^2+x_4^2)/\sigma^2}$$
$$= \sum_{\omega'_\nu} I_{\omega'_\nu} \tag{B.8}$$

where $\omega'_\nu = \omega_\nu/\omega_c$. We have again assumed $2\pi^2 k_B T/\hbar\omega_c \gtrsim 1$. Assume now that $8n_F \ll \sigma^2$. Then we can approximate the integrals by:

$$I_{\omega'_\nu} \simeq \frac{k_B T}{n_F} \int dx \frac{e^{-x^2/2n_F}}{(i\omega'_\nu - x)^2} \int dx_2 \frac{e^{-x_2^2/4n_F}}{i\omega'_\nu + x_2} \int dx_4 \frac{e^{-x_4^2/4n_F}}{i\omega'_\nu + x_4} \tag{B.9}$$

We will now show, that in this approximation the sum of the integrals is largely independent of n_F and therefore $g_1 \propto 1/n_F$. The integral can be solved, and we get:

$$I_{\omega'_\nu} = \frac{k_B T}{n_F^{3/2}} \left(-\frac{\pi|\omega'_\nu|}{\sqrt{n_F}} e^{\omega'^2_\nu/2n_F}[1 - \Phi(\frac{|\omega'_\nu|}{\sqrt{2n_F}})] + \sqrt{2\pi} \right)$$
$$\times \pi^2[1 - \Phi(\frac{|\omega'_\nu|}{2\sqrt{n_F}})]^2 e^{\omega'^2_\nu/2n_F} \tag{B.10}$$

where we again have $\Phi(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^x dt e^{-t^2}$. We can then write Eq. (B.8) on the form

$$\frac{\hbar\omega_c}{2\pi n_F} \Delta x \sum_{x_n} \left\{ -\pi x_n e^{x_n^2/2}[1 - \Phi(\frac{x_n}{\sqrt{2}})] + \sqrt{2\pi} \right\} \pi^2 [1 - \Phi(\frac{x_n}{2})]^2 e^{x_n^2/2} \tag{B.11}$$

where $x_n = \frac{\omega_n}{\omega_c \sqrt{n_F}}$ and $\Delta x = \frac{2\pi k_B T}{\hbar\omega_c\sqrt{n_F}}$. Since $\Delta x \ll 1$, we can approximate this sum by an integral and we conclude that g_1 is independent of the temperature in agreement with the result above. Furthermore, we obtain $g_1 \propto 1/n_F$ for n_F large and g_1 independent of σ. When $\sigma^2 \gg 8n_F$ does not hold, the calculation is the same as above. We just have to substitute $1/4n_F$ with $1/4n_F + 2/\sigma^2$ in the integrals. The $1/n_F$ dependence coming from the $B_0^{j_1\, j_2}$ factors in

Eq. (3.30) is unaltered and we still get that $g_1 \propto 1/n_F$ for $\min(\sqrt{n_F}, \sigma)$ large and that g_1 is independent of σ and the temperature. By calibrating g_1 through an exact evaluation based on Eq. (3.30), we obtain:

$$g_1 \simeq \frac{g^4}{(L_x L_y)^3 l^2 (\hbar\omega_c)^3 5.4 n_F} \tag{B.12}$$

It should be noted that the dependence of g_1 on n_F and σ in the above expression is only approximate and rests on the various simplifications made. We have tested the above expression against the exact result and we find that the dependence on n_F and σ fits to an accuracy of 20%.

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