

# **Hartree–Fock–Bogoliubov Mean-Field Theory for trapped fermionic atoms**

## **Hartree–Fock–Bogoliubov- Molekularfeldtheorie für gefangene fermionische Atome**

A thesis for degree of Master of Science  
submitted by  
Sejung Yong

under supervision of  
Priv.-Doz. Dr. Axel Pelster

Kaiserslautern, March 5, 2024.



RPTU Kaiserslautern-Landau  
Department of Physics

# Abstract

Despite the long history of groundbreaking achievements by many revered researchers, including the celebrated Bardeen–Cooper–Schrieffer (BCS) theory, understanding the nature of fermionic many-body systems remains as a challenge in modern physics. Superconductivity, with its practical significance, serves as a representative example showing the profound and complex nature of the fermionic many-body phenomena. Since the beginning era of the quantum physics, numerous attempts to elucidate this macroscopic quantum phenomenon have led to many foundational advancements in quantum many-body physics and quantum field theory. Nevertheless, superconductivity is still considered not fully understood to this day.

On the other hand, quantum gas physics has undergone remarkable developments in the past few decades, offering possibilities that were previously deemed impossible in solid-state physics. Among these, the BEC-BCS crossover provides a notable experimental platform to study quantum many-body physics. The ability to experimentally control interactions between fermionic atoms has allowed researchers to study within one system BCS superfluidity in one limit and Bose–Einstein condensation as another important macroscopic quantum phenomenon in the other limit.

However, challenges persist. Compared to the relatively well-understood BEC side, the ultracold atomic gas on the BCS side, dominated by fermionic behaviour, appears much more irresponsive to interactions and thermal excitations. Consequently, analysing experimental data obtained in the BCS side poses significant difficulties. For instance, thermometry of fermionic quantum gases remains unclear, with only indirect methods like adiabatic ramping from the BCS- to the BEC-side to measure the temperature of the bosonic gas are known. Addressing these challenges, the present thesis introduces an extended BCS mean-field theory that quantitatively describes the behaviour of fermionic many-body systems more effectively. To this end, we have implemented the Hartree–Fock–Bogoliubov mean-field theory which consists of not only the Bogoliubov pairing channel of usual BCS-type theories, but also the Hartree interaction channel that yields in combination with the pairing channel non-trivial effects in inhomogeneous systems. Particularly noteworthy is the new possibility, based on this theory, to directly measure the temperature of fermionic atoms in the laboratory, a task that has been challenging thus far. Building upon its excellent explanatory power, we argue that this extended mean-field theory brings an important insight in studying fermionic many-body systems.

# Zusammenfassung

Trotz der langen Geschichte bahnbrechender Erfolge vieler geachteter Forscher, einschließlich der gefeierten Bardeen-Cooper-Schrieffer (BCS)-Theorie, bleibt heutzutage das Problem des fermionischen Vielteilchensystems eine der bedeutendsten Herausforderungen in der Physik. Mit ihrer praktischen Bedeutung dient die Supraleitung als ausgezeichnetes Beispiel für die tiefgründige und komplexe Natur des fermionischen Vielteilchensystems. Seit der Anfangszeit der Quantenphysik haben zahlreiche Versuche, dieses makroskopische Quantenphänomen zu klären, zu grundlegenden Fortschritten in der Quanten-Vielteilchenphysik und der Quantenfeldtheorie geführt. Dennoch gilt die Supraleitung bis heute als nicht vollständig verstanden.

Auf der anderen Seite hat die Quantengasphysik in den letzten Jahrzehnten beeindruckende Entwicklungen erlebt und bietet Möglichkeiten, die zuvor in der Festkörperphysik für unmöglich gehalten wurden. Insbesondere der BEC-BCS-crossover liefert besondere experimentelle Realisierungen zur Erforschung der Vielteilchenphysik. Dank der Möglichkeit, Wechselwirkungen zwischen fermionischen Atomen experimentell zu kontrollieren, können Forscher innerhalb eines Systems die BCS-Suprafluidität im einem Grenzfall und die Bose-Einstein-Kondensation als weiteres wichtiges makroskopisches Quantenphänomen im anderen Grenzfall untersuchen.

Aber es gibt immer noch eine Herausforderung. Im Vergleich zur relativ gut verstandenen BEC-Seite ist das ultrakalte atomare Gas auf der BCS-Seite, dominiert von fermionischen Verhalten, unempfindlich bezüglich Wechselwirkungen und thermischen Anregungen. Daher stellt die Analyse experimenteller Daten, die auf der BCS-Seite gemessen wurden, erhebliche Schwierigkeiten dar. Beispielsweise bleibt die Thermometrie fermionischer Quantengase unklar, und nur indirekte Methoden wie adiabatisches Rampen von der BCS- zur BEC-Seite sind bekannt, um die Temperatur des bosonischen Gas zu messen. Um diesen Herausforderungen zu begegnen, stellt die vorliegende Arbeit eine erweiterte BCS-Molekularfeldtheorie vor, die das Verhalten fermionischer Vielteilchensysteme quantitativ effektiver beschreibt. Zu diesem Zweck haben wir die Hartree-Fock-Bogoliubov-Molekularfeldtheorie implementiert, die nicht nur den Bogoliubov-Paarungskanal üblicher BCS-Typ-Theorien umfasst, sondern auch den Hartree-Wechselwirkungskanal, der mit dem Paarungskanal kombiniert zu nichttriviale Effekte in inhomogenen Systemen führt. Besonders bemerkenswert ist die neue Möglichkeit, basierend auf dieser Theorie, die Temperatur fermionischer Atome direkt im Labor zu messen, eine Aufgabe, die bisher anspruchsvoll war. Basierend auf ihre ausgezeichnete erklärungskräftige Leistung argumentieren wir, dass diese erweiterte Molekularfeldtheorie einen wichtigen Einblick in die Erforschung fermionischer Vielteilchensysteme bietet.

## **Acknowledgement**

While writing this thesis, I was supported by many other people who helped and encouraged to complete this work, therefore I must take this opportunity to express my gratitude for them.

First of all, my deepest appreciation is dedicated to my supervisor, Priv.-Doz. Dr. Axel Pelster. Joining his group has been the greatest choice in my academic journey. During my work with him, he has been providing not only regular and active discussion for my subject, but also variety of opportunities of visiting conferences, schools, seminars, and participating in scientific research projects. Such valuable guidances offered by him has allowed me to step into the fascinating world of physics. I can not appreciate enough for what I have received from him.

Also thank for Prof. Dr. Artur Widera and his people for kind share of valuable experimental data of his research group. If their support had not been available, my research would have lost its meaning. Especially, I thank Sian Barbosa for his excellent experimental works and collaboration with us.

Furthermore, I would like to express my gratitude to Prof. Dr. Michael Fleischhauer for allowance of the office and letting me join his group seminar.

I am grateful for my colleagues as well. Unfortunately I can not list all of them, but my coworker Nikolai Kaschewski must be appreciated. We have been discussed a lot of time about the topic, and I was greatly helped with it.

Last but not least, I am thankful for the supports of my mother, Milkyung. I have been able to concentrate on my work thanks for her endless supports and understanding.



# Contents

|          |                                                            |           |
|----------|------------------------------------------------------------|-----------|
| <b>1</b> | <b>Introduction</b>                                        | <b>1</b>  |
| 1.1      | Bose–Einstein condensate . . . . .                         | 1         |
| 1.2      | Bardeen–Cooper–Schrieffer theory . . . . .                 | 2         |
| 1.3      | BEC-BCS crossover . . . . .                                | 4         |
| 1.4      | Outline of thesis . . . . .                                | 6         |
| <b>2</b> | <b>Mean-Field Theories for Interacting Fermions</b>        | <b>9</b>  |
| 2.1      | Hartree–Fock–Bogoliubov mean-field approximation . . . . . | 9         |
| 2.1.1    | Model Hamiltonian . . . . .                                | 10        |
| 2.1.2    | Contact s-wave scattering . . . . .                        | 10        |
| 2.1.3    | Hartree–Fock–Bogoliubov approximation . . . . .            | 11        |
| 2.1.4    | Hamiltonian in momentum spectrum . . . . .                 | 12        |
| 2.2      | BCS–Bogoliubov theory . . . . .                            | 13        |
| 2.2.1    | Bogoliubov transformation . . . . .                        | 13        |
| 2.2.2    | BCS–Bogoliubov equations . . . . .                         | 14        |
| 2.3      | Hartree–Fock theory . . . . .                              | 16        |
| 2.3.1    | Hartree–Fock transformation . . . . .                      | 16        |
| 2.3.2    | Hartree- and Fock equations . . . . .                      | 18        |
| 2.4      | Hartree–Fock–Bogoliubov theory . . . . .                   | 19        |
| 2.4.1    | Hartree–Fock–Bogoliubov Hamiltonian . . . . .              | 20        |
| 2.4.2    | Hartree–Bogoliubov equations . . . . .                     | 23        |
| <b>3</b> | <b>Uniform Fermi Gas</b>                                   | <b>25</b> |
| 3.1      | Ideal Fermi gas . . . . .                                  | 25        |
| 3.2      | BCS–Bogoliubov theory . . . . .                            | 27        |
| 3.2.1    | Thermodynamic ensemble . . . . .                           | 27        |
| 3.2.2    | Phase transition . . . . .                                 | 28        |
| 3.2.3    | Condensation . . . . .                                     | 29        |
| 3.2.4    | Superfluidity . . . . .                                    | 32        |
| 3.2.5    | Ground state . . . . .                                     | 33        |
| 3.3      | Hartree theory . . . . .                                   | 35        |
| 3.3.1    | Thermodynamic ensemble . . . . .                           | 36        |
| 3.3.2    | Ground state . . . . .                                     | 38        |
| 3.4      | Hartree–Bogoliubov theory . . . . .                        | 38        |
| 3.4.1    | Thermodynamic ensemble . . . . .                           | 39        |
| 3.4.2    | Phase transition . . . . .                                 | 39        |
| 3.4.3    | Ground state . . . . .                                     | 40        |

## CONTENTS

|          |                                                                           |           |
|----------|---------------------------------------------------------------------------|-----------|
| <b>4</b> | <b>Fermi Gas in Harmonic Trap</b>                                         | <b>43</b> |
| 4.1      | Local Density Approximation . . . . .                                     | 43        |
| 4.2      | Harmonic trap potential . . . . .                                         | 44        |
| 4.3      | Ideal Fermi gas . . . . .                                                 | 45        |
| 4.3.1    | Density profile . . . . .                                                 | 46        |
| 4.3.2    | Ground state . . . . .                                                    | 48        |
| 4.4      | BCS–Bogoliubov theory . . . . .                                           | 48        |
| 4.4.1    | Phase transition . . . . .                                                | 49        |
| 4.4.2    | Density profile . . . . .                                                 | 51        |
| 4.5      | Hartree theory . . . . .                                                  | 53        |
| 4.5.1    | Density profile . . . . .                                                 | 53        |
| 4.5.2    | Ground state . . . . .                                                    | 55        |
| 4.6      | Hartree–Bogoliubov theory . . . . .                                       | 55        |
| 4.6.1    | Phase transition . . . . .                                                | 56        |
| 4.6.2    | Density profile . . . . .                                                 | 58        |
| <b>5</b> | <b>Experiment</b>                                                         | <b>63</b> |
| 5.1      | Method . . . . .                                                          | 63        |
| 5.2      | Data analysis . . . . .                                                   | 64        |
| 5.2.1    | Feshbach magnetic field at 1070 G . . . . .                               | 64        |
| 5.2.2    | Feshbach magnetic field at 977.4 G . . . . .                              | 65        |
| <b>6</b> | <b>Conclusion</b>                                                         | <b>71</b> |
| <b>7</b> | <b>Outlook</b>                                                            | <b>73</b> |
| 7.1      | Low-dimensional system . . . . .                                          | 73        |
| 7.2      | Spin polarisation . . . . .                                               | 74        |
| 7.3      | Generalisation of the Hartree–Fock–Bogoliubov mean-field theory . . . . . | 74        |
|          | <b>Appendices</b>                                                         | <b>77</b> |
| <b>A</b> | <b>Polylogarithm</b>                                                      | <b>79</b> |
| <b>B</b> | <b>Hypergeometric Function</b>                                            | <b>87</b> |

# Chapter 1

## Introduction

Constructing a theory for interacting many-body system is challenging. While behaviours of non-interacting many particles can be described via the statistics of many statistically independent particles, any interaction between the particles raises the difficulty of describing the system substantially, and this class of problem is known as the *many-body problem*. Non-interacting particles exist only in the ideal world imagined by physicists, but in reality particles interact with each other. Also, interesting physical problems usually require to handle with a large number of particles. As an example taken from condensed matter physics, a  $1\text{ cm}^3$  volume of typical metal contains almost  $10^{23}$  free electrons. Therefore, the many-body problem has held significant importance in the history of physics.

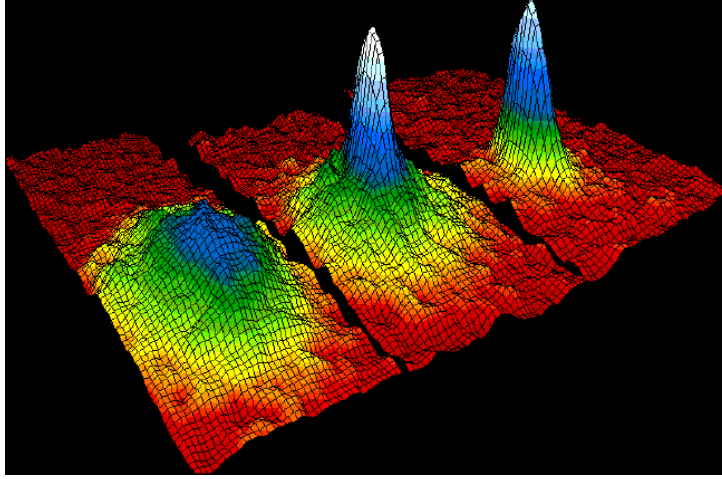
Moreover, the combination of the many-body physics and quantum mechanics turns out to be a rich ground for the fascinating *quantum many-body physics*. In many cases a quantum many-body Hamiltonian of a vast number of interacting particles can be transformed to a Hamiltonian of weakly- or non-interacting quasiparticles, allowing one to find an approximate solution of the underlying quantum many-body problem. Here, the many-body Hamiltonian formulated with microscopic fundamental interactions of individual constituent particles leads to the observation of macroscopic quantum phenomena [1]. Furthermore, while macroscopic quantum phenomena are typically induced by interactions, simply applying quantum statistics to many particles is also sufficient to produce a macroscopic phenomenon. Prominent examples are Bose–Einstein condensation and superconductivity, which are both manifest at very low temperatures close to zero. Since these important phenomena represent the basis of the topic of this thesis, we introduce in the following their historical context.

### 1.1 Bose–Einstein condensate

Bose–Einstein condensatation is an unique one among known macroscopic quantum phenomena, because it purely results from quantum statistical nature of many-body system free of any interaction. Here, a fraction of bosonic particles or quasiparticles macroscopically occupies the lowest energy state below a certain critical temperature due to their quantum statistics.

The theoretical prediction of Bose–Einstein condensate dates back a century. In 1924, S. N. Bose discussed the statistics of photons by considering photons as indistinguishable particles [2]. In order to get his paper accepted by a journal, Bose sent a letter to A. Einstein. Einstein noticed the profound impact of Bose’s work, and helped to publish it, even himself translated it to German. Inspired by the paper of Bose, Einstein extended the new statistics of non-interacting indistinguishable massless to massive particles. However his calculation led to the perplexing consequence that under a certain condition the indistinguishable particles occupy the same volume, or in other words, the system volume is filled with the particles in the same state. Initially

## 1.2. BARDEEN–COOPER–SCHRIEFFER THEORY



**Figure 1.1:** Iconic image of Bose–Einstein condensate. As the temperature drops from the left to the right, a narrow peak appears in the velocity distribution of atoms. This peak indicates the presence of the macroscopically occupied ground state. Figure is taken from [6].

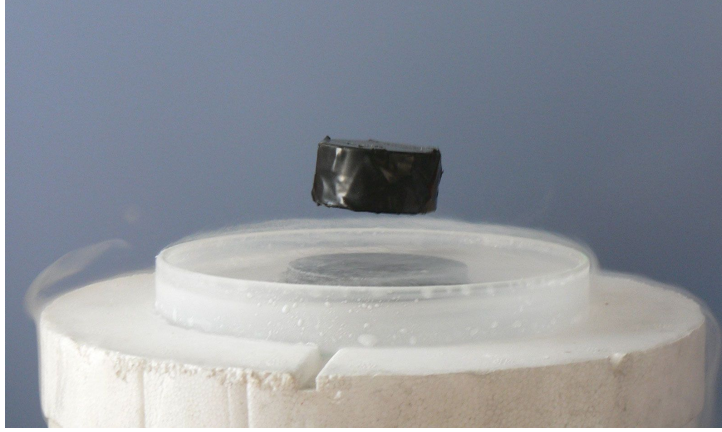
this was a paradox to Einstein, as he expresses at the concluding remark of his paper in 1924: “In the end, I want to draw attention to the paradox that I do not have a solution.” [3]. Today, this conclusion is no more considered as a paradox, but appreciated as a genuine new state of matter, the *Bose–Einstein condensate* (*BEC*).

Despite this earlier theoretical prediction, scientists had to wait many years for an experimental realisation of the BEC. In 1930s  $^4\text{He}$  was found to be superfluid below the temperature of 2.2K, the so-called *lambda temperature*, and possible link between the superfluidity of bosonic  $^4\text{He}$  and BEC was suggested. But due to its high density and non-negligible interaction,  $^4\text{He}$ -superfluid is not considered as an evidence of BEC. As this story tells us, it is not straightforward to observe BEC in reality because there are several problems. According to the theory, BEC should happen at very low temperatures, and cooling techniques at such extreme temperatures rely on the properties of particles in the gas phase. However an ultracold atomic gas tends to liquify and eventually crystallise before the BEC is observed. To avoid this problem, three-body collisions in the gas have to be suppressed, meaning that the density should be kept low. But again at such low densities, two-body scattering also happens rarely, thus thermalisation takes longer time. Moreover the lower density leads to a further lower critical temperature, making the cooling even more challenging. After the introduction of innovative experimental techniques like magnetic trapping, laser cooling, and evaporative cooling, the BEC of  $^{87}\text{Rb}$  atomic cloud was finally observed in 1995 by C. Wieman and E. Cornell [4], see Fig. 1.1. Closely after to this, W. Ketterle also observed a BEC of  $^{23}\text{Na}$  atoms [5]. The Nobel prize in physics of the year 2001 was awarded to Wieman, Cornell and Ketterle for their groundbreaking work. While Wieman and Cornell were the first scientists observed BEC, Ketterle also won the Nobel prize for his contribution of demonstrating an important property of BEC. By measuring the interference pattern of two independent BECs, he showed that the BEC is actually a coherent macroscopic wave function [7].

## 1.2 Bardeen–Cooper–Schrieffer theory

So far we have been tracing back the history of a Bose–Einstein condensate, which is about a phase transition emerging from quantum statistics. However contrary to bosons, there is no such thermodynamic phase transition for fermions, because a phase transition of fermions is always induced by the interaction between particles. Arguably the most well-known macroscopic

## 1.2. BARDEEN–COOPER–SCHRIEFFER THEORY



**Figure 1.2:** Demonstration of the Meissner–Ochsenfeld effect. A magnet levitates over a superconductor cooled under the critical temperature. Figure is taken from [18].

quantum phenomenon in this respect is *superconductivity*, i.e. the conduction of electric charge without resistance. In contrast to BEC, superconductivity was discovered in an unpredicted way like many groundbreaking discoveries in the history of science. Around the end of 19th century, a big scientific quest at the time was liquefying gases. This challenge initiated the new field of physics of cryogenics, i.e. the low temperature physics. Reaching at 20.28 K, hydrogen gas was liquefied by Sir J. Dewar in 1898. However, at this low temperature helium remained still gaseous, and the race to the liquefying helium went on. The winner was H. K. Onnes, as he successfully liquefied helium gas at around 4.2 K in 1908. With his excellent cryogenic technique, Onnes tackled big question at that time, namely the behaviour of resistance of metals at the zero-temperature. It was already known that the resistance of a metal drops with decreasing temperature, but the resistance i.e. electron scattering in metal at the absolute zero was an intriguing question. There were three different predictions: Dewar insisted that the resistance drops continuously to zero because the vibration in metal vanishes, whereas Lord Kelvin argued for an infinite resistance due to the loss of mobility of electrons. Earlier to them, A. Matthiessen had claimed that the resistance becomes flat curve at a non-zero value [8]. Onnes was convinced by Kelvin’s argument, but when he conducted the cooling experiment on mercury he observed a vanishing resistance even before reaching the absolute temperature, which was unexpected. This was also different from predictions both of Dewar and Matthiessen, since the resistance indeed vanishes but abrupt at a non-zero critical temperature. It was the discovery of a completely new kind of phenomenon, namely superconductivity, in 1911 by Onnes [12]. That measuring of the vanishing resistance of an extremely cooled metal is not just a measurement error but a new physical phenomenon, as demonstrated by the *Meissner–Ochsenfeld effect* discovered by W. Meissner and R. Ochsenfeld in 1933 [16], see Fig. 1.2. Here, one observes the expulsion of an external magnetic field from a superconductor below its critical temperature which is a consequence of the vanishing resistance in the superconductor.

Unexpected discoveries bring new questions. In this case, the question was how the electron conduct charge without being disrupted by a lattice vibrations in a metal at finite temperature. The question remained unanswered for long time. F. London correctly acknowledged the importance of quantum mechanics related to superconductivity, suggesting that there might be an underlying single coherent superconductivity wave function, which today called *superconducting order parameter* [17], instead of a wave function of a single electron. Therefore he phrased superconductivity with the term *macroscopic quantum phenomenon* [8]. The following question is then, how the macroscopic wave function is formed. The idea has been suggested that if two electrons can form a pair, then the pair of two fermionic electrons can be regarded as a com-

### 1.3. BEC-BCS CROSSOVER

posite boson and thus is subject to the bosonic condensation. But to be able to form a pair of electrons, the Coulomb repulsion between electrons must be overcome. Regarding this problem, the idea of an effective attractive interaction between two electrons mediated by ions in a crystal leading to a change of the ground energy of fermions is suggested first by H. Fröhlich in 1950 [13]. This idea was highly speculative, but it turns out that experiments with metals of different isotopes the superconductivity is affected by the mass of crystal ions [14], which supports the argument of Fröhlich. Still a decisive theoretical evidence for the existence of bound electron pairs was missing, but once the effective attractive potential between electrons is assumed, the final step is to show the energetically favourable ground state with bound electron pairs. In 1956, L. Cooper came with the idea of a pair of opposite spins, the *Cooper pair*, to handle the Pauli exclusion between electrons, showing that a bound state exists for such a pair of electrons interacting via arbitrarily weak attractive interaction. Finally a year later, in 1957, Bardeen, Cooper and Schrieffer successfully provided the microscopic description of superconductivity in terms of the Cooper pairing [15]. This theory could explain experimental results very well and was soon famed as the *BCS theory*. In 1972 Bardeen, Cooper and Schrieffer were awarded the Nobel prize for their BCS theory. Today, the BCS theory is not only restricted to superconductivity, but generalised for interacting fermions to be used in various fields in physics, for instance to describe the elementary excitation spectrum of nuclei in nuclear physics [23] or to explain the fermionic superfluidity in quantum gas physics, as is discussed in the subsequent section.

### 1.3 BEC-BCS crossover

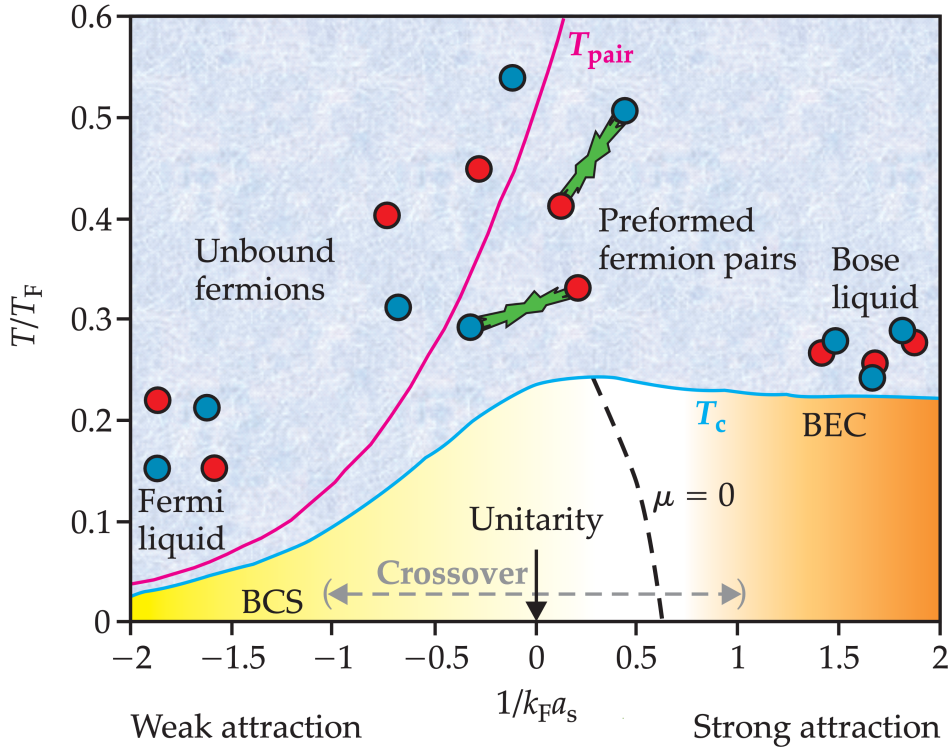
As already hinted in the previous section, theoretical explanation of the macroscopic phenomenon of fermions is connected with the idea of BEC. In fact, many pre-BCS theories of superconductivity were inspired by the BEC theory, although Bardeen, Cooper, and Schrieffer themselves disavowed the connection between superconductivity and BEC [55]. And they are, indeed, different. While the analogy of superfluidity as a condensation of electron pairs pictures the pair as point-like bosons without any internal structure, it turned out that in the BCS theory Cooper pairs are overlapping correlated particles with large correlation distances. To make the analogy work, one would need a very strong attraction that brings the fermions close together, where one can apply the generalised concept of BEC for closely paired fermion-dimer molecules. The theoretical framework for such a BEC of Cooper pairs via variable interaction is called the *BEC-BCS crossover*.

Nonetheless, the original BCS theory was essentially a weak-interaction theory, being restricted to the weakly interacting BCS-limit. In superconducting metals the BCS theory offers a good description of superconductivity, since weak effective attractive interactions between electrons in a metal imply larger Cooper pair radius compared to the average distance between electrons. While the task of extending the BCS theory to arbitrarily strong interaction is not a trivial task, for the dilute ultracold atoms a relatively simple approach of generalising the BCS theory is available. In this approach the BCS wave function becomes formally identical to the BEC of Cooper pairs with a smaller Cooper pair radius compared to the average interparticle distance in the strongly interacting BEC limit. The intermediate crossover regime is determined by using variational ansatz for the wave function over the whole interaction strength range [21].

The variational approach to the BEC-BCS crossover was first implemented by D. M. Eagles in 1969. He considered a dilute electron gas motivated by experiments of superconductor  $\text{SrTiO}_3$  doped with Zr and realised that the radii of Cooper pairs are sufficiently small compared to the average electron distance, so the Cooper pairs can be seen as tightly bound bosonic dimers. Eagles calculated the BCS order parameter equation in terms of the interaction strength as well as the particle number equations over whole crossover regime [19]. In 1980, A. Leggett investigated



### 1.3. BEC-BCS CROSSOVER

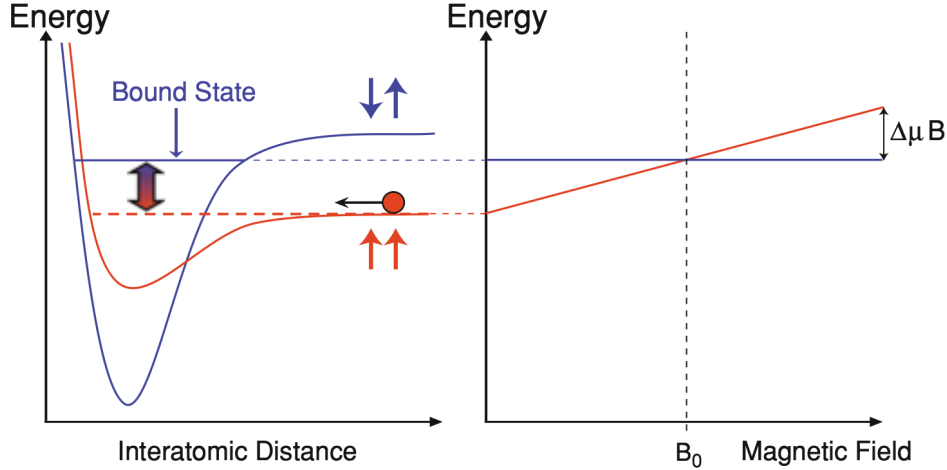


**Figure 1.3:** Phase diagram of BEC-BCS crossover where BCS-limit and BEC-limit are represented as a limit of inverse scattering parameter  $(k_F a_s)^{-1} \rightarrow -\infty$  and  $(k_F a_s)^{-1} \rightarrow +\infty$ , respectively. The pairing temperature  $T_{\text{pair}}$  for the formation of Cooper pairs is calculated by a mean-field approach, and the temperature  $T_c$  for emergence of phase coherence between the Cooper pairs is calculated including beyond-mean-field corrections. Figure is taken from [23].

the crossover problem of a dilute ultracold Fermi gas with s-wave scattering as the interaction model motivated by  $^3\text{He}$  experiments at the time [20]. In his study, Leggett introduced the scattering parameter  $k_F a_s$  and considered the change of the chemical potential  $\mu$  and the BCS order parameter  $\Delta$  as a function of the dimensionless parameter  $k_F a_s$ . This parameter is key to study the BEC-BCS crossover problem, since it corresponds to the ratio between the Cooper pair radius and interparticle distance, thus the macroscopic behaviour of the collective wave function.

Eagle's and Leggett's pioneering work dealt both with a mean-field theory at  $T = 0$ . The phase transition at finite temperatures over the crossover range was first studied by P. Nozières and S. Schmitt-Rink in 1985 [22]. They found a different behaviour of the phase transition temperature in two extreme regimes, i.e. a BCS-like behaviour in the weakly interacting BCS-limit and a BEC-like behaviour in the strongly interacting BEC-limit. Most importantly, they showed that the transition temperature turns out to be a smooth function in the intermediate crossover regime. Still the thermal excitation of collective modes was the pending question from their theory. C. A. R. Sá de Melo, J. Engelbrecht and M. Randeria finally determined the transition temperature  $T_c$  over the whole crossover range in 1993 by adopting a beyond-mean-field approach on the basis of functional integration [30], see Fig. 1.3.

While the effective electron-phonon interaction in metals is difficult to control, in quantum gas physics one has the unique possibility of tuning the interaction between the particles by the *Feshbach resonance* technique. The Feshbach resonance technique is available for atomic particles where collision processes consists of at least two energetically different channels: one associated



**Figure 1.4:** Energy diagram for open and closed channels at a Feshbach resonance. Atoms enter a two-body scattering event via an open channel (red) where the collision process is coupled to the closed channel (blue) corresponding to the bound state, as shown on the left side. The energetic difference between the channels can be controlled by varying the magnetic field  $B$ , where the resonance is at  $B_0$  as shown in the right side. Figure is taken from [21].

to the scattering state, the so-called open channel, and another one corresponding to the bound state, the closed channel, see Fig. 1.4. The tuning of the interaction is realised by applying an external magnetic field  $B$ . Due to the Zeeman shift  $\Delta E = -\Delta\mu \cdot B$  between associated atomic hyperfine states for open and closed channels with the magnetic momentum difference  $\Delta\mu$ , a change of  $B$  yields a changing energy difference between those channels. For the resonance width  $\Delta B$  and the resonant magnetic field strength  $B_0$  the scattering length  $a_s$  is given by:

$$a_s(B) = a_{bg} \left( 1 - \frac{\Delta B}{B - B_0} \right), \quad (1.1)$$

where  $a_{bg}$  denotes the background scattering length in the absence of the coupling to the closed channel [21]. The Feshbach resonance technique is the ideal tool for experimental investigation of the BEC-BCS crossover, because it enables an experimental control of the interaction parameter  $k_F a_s$  in a dilute ultracold atomic gas. The experimental realisation of the BEC-BCS crossover by means of the Feshbach resonance was published by three experimental groups in 2003, where the Grimm group in University of Innsbruck and the Ketterle group in MIT used  $^6\text{Li}$  [24, 25], whereas the Jin group in JILA used  $^{40}\text{K}$  atoms [26]. Elusive experimental proof for fermionic superfluidity was supported by the observation of vortices in the BCS-regime in 2005 [27]. At the RPTU Kaiserslautern-Landau, an experimental platform for investigating BEC-BCS crossover is available in the Widerra research group [28].

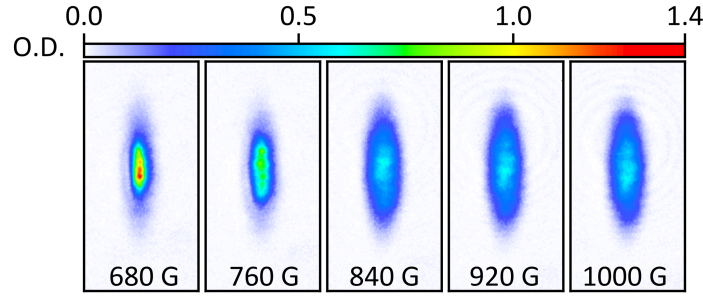
## 1.4 Outline of thesis

Our objective is to understand the many-body problem of trapped interacting fermions theoretically. Based on this, we apply the theory to analyse the experimental data of the Widerra research group. The preprint of the research has been released as a short letter [11], and the present thesis offers extensive discussions and analysis that is left out in the letter.

In the framework of the BEC-BCS crossover of  $^6\text{Li}$  atoms in a harmonic trap, we concentrate ourselves to the fermionic BCS-side of the crossover, which has been less studied so far compared to the bosonic BEC-side, where the latter is well understood by means of the Gross-Pitaevskii



## 1.4. OUTLINE OF THESIS



**Figure 1.5:** Density distributions of trapped  ${}^6\text{Li}$  atoms as optical absorption images at various magnetic field strengths  $B$ , i.e. various dimensionless interaction parameter  $k_F a_s$ . The left side shows the strongly interacting BEC-limit, and the right side corresponds to the weakly interacting BCS-limit, where the resonant magnetic field strength is at  $B_0 \approx 840$  G in the middle. Figure is taken from [28].

theory. Although the BCS-limit represents a weakly interacting case, surprisingly it is somewhat difficult to analyse the experimental data based on the BCS theory. As presented in Fig. 5.1, in the BEC-limit the trapped gas shows the characteristic peak of a BEC. However the BCS-regime raises intriguing questions, as the density profiles are largely featureless there due to the Pauli principle. The insensitivity to interaction strength and thermal excitations on the BCS side renders the quantitative analysis of a Fermi gas in the BCS-limit intractable [11]. Consequently, indirect evidence, such as the presence of vortices, is often considered as an indicator for a superfluidity onset in the BCS regime. Regarding on this challenge, we will establish a theory enables a complete thermodynamic analysis of the interacting fermions on the BCS-side. Specifically, we construct a mean-field theory for a simple description of the fermionic many-body system, which allows a direct quantitative analysis of experimental data.

To achieve our goal effectively, the thesis is composed of seven chapters including this introduction. In chapter 2, we begin with formulating the mean-field models and derive their essential mean-field equations, which are the objects of our study. These mean-field models are then studied for the homogenous case in the following chapter 3. Therein we calculate concrete physical quantities for each models and compare them with respects from the literature. In view of the experimental situation, in chapter 4 we extend the homogeneous gas theory to the theory of the trapped gas in a harmonic potential. Theoretically this is the most important part of the thesis, since our mean-field theory predicts results which considerably different from the well-established usual BCS-type theories in the field. These new predictions are then tested on basis of the experimental data in the following chapter 5. Finally in the last two chapters 6 and 7, we draw a conclusion of the work and suggest future directions for further studies.

#### 1.4. OUTLINE OF THESIS

## Chapter 2

# Mean-Field Theories for Interacting Fermions

The exploration of a physical system requires developing a model that describes measured observables. Such a theoretical model should serve as an effective description of system behaviours based on well justified assumptions, so that the theory remains comprehensive without unnecessary complexity. At the same time, the theory should also not suffer from oversimplification to yet capture the essential nature of the object of the study. In pursuit of this, we formulate a Hamiltonian that accounts for the interactions in a fermionic many-body system.

### 2.1 Hartree–Fock–Bogoliubov mean-field approximation

An approximation is always needed to handle many-body problem. The choice of approach in the present thesis is the *Hartree–Fock–Bogoliubov (HFB) approximation*<sup>1</sup>, which is a mean-field approach. In the HFB theory, three interaction channels appears, namely the Hartree-, Fock-, and Bogoliubov channel. The Hartree channel accounts for the normal interaction between particles, whereas the Fock- and the Bogoliubov channel evokes the anomalous interactions and leads to the quantum many-body effect. In the context of BEC-BCS crossover studies, the Hartree and Fock channels are usually disregarded for several reasons, for example due to the presence of divergent terms at the unitary regime with contact interaction [36, 37, 38, 49] or since they are physically irrelevant energy shift in case of the homogenous system [20, 48], or they might be negligibly small and appear irrelevant in experiments [39].

Nevertheless, in a more unbiased theoretical model the Hartree and Fock channels should not be neglected ab initio. By including the all three channels we can take into account the effects of the interatomic interactions in both the normal fluid- and the superfluid phase as well as combined effects of them. Motivated by that, we include all three channels in our model to study the interacting fermions.

---

<sup>1</sup>This is also known as the *Bogoliubov–de Gennes formalism* in condensed matter physics [40, 49], and in nuclear physics it is called the Hartree–Fock–Bogoliubov theory [45]. We follow here the latter tradition.

## 2.1. HARTREE–FOCK–BOGOLIUBOV MEAN-FIELD APPROXIMATION

### 2.1.1 Model Hamiltonian

Our starting point is a Hamiltonian of the interacting fermions. In the second quantisation formalism, the Hamiltonian of the interacting particles up to two-body interactions is given by:

$$\begin{aligned} \hat{H} = & \int d^3x \sum_{\sigma=\uparrow,\downarrow} \hat{\psi}_{\sigma}^{\dagger}(\mathbf{x}) \left[ -\frac{\hbar^2}{2M} \nabla^2 - \mu_{\sigma} \right] \hat{\psi}_{\sigma}(\mathbf{x}) \\ & + \int d^3x d^3x' \hat{\psi}_{\uparrow}^{\dagger}(\mathbf{x}) \hat{\psi}_{\downarrow}^{\dagger}(\mathbf{x}') U(\mathbf{x}, \mathbf{x}') \hat{\psi}_{\downarrow}(\mathbf{x}') \hat{\psi}_{\uparrow}(\mathbf{x}). \end{aligned} \quad (2.1)$$

Here  $\hat{\psi}_{\sigma}(\mathbf{x})$  is the fermionic field operator with spin  $\sigma \in \{\uparrow, \downarrow\}$ ,  $M$  denotes the particle mass,  $\mu_{\sigma}$  is the chemical potential for the particle carrying spin  $\sigma$ , and  $U(\mathbf{x}, \mathbf{x}')$  stands for the two-body interaction potential for particles with the coordinates  $\mathbf{x}, \mathbf{x}'$ .

While it retains the information about the system within its general form, the theoretical treatment of the Hamiltonian (2.1) is problematic. As already mentioned at the beginning of the section, we avoid the difficulties by studying an approximative one instead of the original Hamiltonian, which is provided by the HFB mean-field theory. In following, we list each issue we encounter and solve them step by step towards the formulation of the HFB mean-field Hamiltonian.

### 2.1.2 Contact s-wave scattering

The first issue we have with (2.1) is the two-body interaction potential  $U(\mathbf{x}, \mathbf{x}')$ . Here, any form of two-body interaction between particles at position  $\mathbf{x}$  and  $\mathbf{x}'$  is allowed, which depends on the distance between the different species of particles:  $U(\mathbf{x}, \mathbf{x}') = U(\mathbf{x} - \mathbf{x}')$ . Calculating the interaction effects with such a general potential presents a tremendous challenge. However, for a dilute ultracold quantum gas a drastic simplification is available that eliminates the distance dependency, namely the s-wave scattering contact potential.

The s-wave scattering represents the two-body scattering in absence of the angular momentum. The s-wave scattering approximation is not only theoretically simple to describe, but also practical for modelling of experiments, since the ultracold quantum gas experiments are conducted at the temperatures where only the s-wave scattering dominates. For example, p-wave scattering between  $^6\text{Li}$  atoms freezes out below  $T \approx 6 \text{ mK}$  [60], whereas the typical temperature is in the order of 100 nK.<sup>2</sup> Moreover, an ultracold gas is usually dilute, meaning the range of the interaction potential of particles is much smaller than the average particle distances. Therefore we can approximate the interaction by a Dirac-delta distribution at point  $\mathbf{x} = \mathbf{x}'$ , i.e. contact interaction, by this we also simplify the distance dependency. Consequently, the s-wave contact simplifies the interaction between particles insofar one needs only a single parameter, namely the *s-wave scattering length*  $a_s$ . The s-wave scattering length describes both the sign (positive/repulsive or negative/attractive) and the magnitude of the interaction, but there is no preferred direction of the scattering and also there is no distance dependency.

For these reasons, we choose the s-wave contact interaction for our interaction potential:

$$U(\mathbf{x}, \mathbf{x}') = g\delta(\mathbf{x} - \mathbf{x}') \quad (2.2)$$

---

<sup>2</sup>Note that not only the scattering of atoms in the ultracold gas is a subject of this model. Also in nuclear physics, nuclei at the low energy regime have zero-angular momentum ( $l = 0$ ), and their scattering is well described by the s-wave scattering [34].

## 2.1. HARTREE–FOCK–BOGOLIUBOV MEAN-FIELD APPROXIMATION

with the interaction parameter  $g = 4\pi\hbar^2 a_s/M$  [35]. By applying (2.2) to (2.1) we obtain the Hamiltonian

$$\hat{H} = \int d^3x \left\{ \sum_{\sigma=\uparrow,\downarrow} \hat{\psi}_\sigma^\dagger(\mathbf{x}) \left[ -\frac{\hbar^2}{2M} \nabla^2 - \mu_\sigma \right] \hat{\psi}_\sigma(\mathbf{x}) + g \hat{\psi}_\uparrow^\dagger(\mathbf{x}) \hat{\psi}_\downarrow^\dagger(\mathbf{x}) \hat{\psi}_\downarrow(\mathbf{x}) \hat{\psi}_\uparrow(\mathbf{x}) \right\}, \quad (2.3)$$

where the integration over coordinate  $\mathbf{x}'$  is already performed due to the delta potential.

### 2.1.3 Hartree–Fock–Bogoliubov approximation

Even after the simplification of the interaction via the isotropic contact interaction potential, there still remains a problem. The two-body interaction term in (2.3) consists of quartic field operators terms, which can not be calculated analytically. To elude this difficulty, the interaction term might be approximated as quadratic field terms. To this end, we apply the mean-field approximation which is appropriate for our second quantised field operators. This replaces the product of two operators  $\hat{A}$  and  $\hat{B}$  by product of the operators and some c-numbers  $\langle \hat{A} \rangle$ ,  $\langle \hat{B} \rangle$  [42]:

$$\hat{A}\hat{B} \approx \langle \hat{A} \rangle \hat{B} + \langle \hat{B} \rangle \hat{A} - \langle \hat{A} \rangle \langle \hat{B} \rangle, \quad (2.4)$$

where the mean-field approximation amounts to neglecting the error

$$\hat{A}\hat{B} - \langle \hat{A} \rangle \hat{B} - \hat{A} \langle \hat{B} \rangle + \langle \hat{A} \rangle \langle \hat{B} \rangle = (\hat{A} - \langle \hat{A} \rangle) (\hat{B} - \langle \hat{B} \rangle) \approx 0. \quad (2.5)$$

Thus, it is assumed that the c-numbers approximate the operators well enough, i.e.  $\langle \hat{A} \rangle \approx \hat{A}$  and  $\langle \hat{B} \rangle \approx \hat{B}$ . Note that the expectation value  $\langle \hat{O} \rangle$  for  $\hat{O} = \hat{A}, \hat{B}$  in (2.4) is not yet defined. We will argue later how the expectation value  $\langle \hat{O} \rangle$  for  $\hat{O} = \hat{A}, \hat{B}$  has to be chosen in a self-consistent way.

The HFB quadratic field approximation divides the quartic interaction operators into products of expectation values and quadratic operators as follows [45, 46]:

$$\begin{aligned} \hat{\psi}_\uparrow^\dagger \hat{\psi}_\downarrow^\dagger \hat{\psi}_\downarrow \hat{\psi}_\uparrow &\approx + \underbrace{\langle \hat{\psi}_\uparrow^\dagger \hat{\psi}_\uparrow \rangle \hat{\psi}_\downarrow^\dagger \hat{\psi}_\downarrow + \hat{\psi}_\uparrow^\dagger \hat{\psi}_\uparrow \langle \hat{\psi}_\downarrow^\dagger \hat{\psi}_\downarrow \rangle - \langle \hat{\psi}_\uparrow^\dagger \hat{\psi}_\uparrow \rangle \langle \hat{\psi}_\downarrow^\dagger \hat{\psi}_\downarrow \rangle}_{\text{Hartree channel}} \\ &\quad - \underbrace{\langle \hat{\psi}_\uparrow^\dagger \hat{\psi}_\downarrow \rangle \hat{\psi}_\downarrow^\dagger \hat{\psi}_\uparrow - \hat{\psi}_\uparrow^\dagger \hat{\psi}_\downarrow \langle \hat{\psi}_\downarrow^\dagger \hat{\psi}_\uparrow \rangle + \langle \hat{\psi}_\uparrow^\dagger \hat{\psi}_\downarrow \rangle \langle \hat{\psi}_\downarrow^\dagger \hat{\psi}_\uparrow \rangle}_{\text{Fock channel}} \\ &\quad + \underbrace{\langle \hat{\psi}_\uparrow^\dagger \hat{\psi}_\downarrow^\dagger \rangle \hat{\psi}_\downarrow \hat{\psi}_\uparrow + \hat{\psi}_\uparrow^\dagger \hat{\psi}_\downarrow^\dagger \langle \hat{\psi}_\downarrow \hat{\psi}_\uparrow \rangle - \langle \hat{\psi}_\uparrow^\dagger \hat{\psi}_\downarrow^\dagger \rangle \langle \hat{\psi}_\downarrow \hat{\psi}_\uparrow \rangle}_{\text{Bogoliubov channel}}. \end{aligned} \quad (2.6)$$

Here the signs of the terms originate from the even- or odd numbers of permutations of the fermionic field operators. As one can see, the HFB approximation takes all six possible quadratic field operator expectation values  $\langle \hat{A} \rangle, \langle \hat{B} \rangle$  of (2.4) out of the quartic field operator. The number six of all possible quadratic fields is confirmed by the binomial coefficient:  $\binom{4}{2} = 6$ . Applying the HFB approximation (2.8) to the Hamiltonian (2.3) yields:

$$\begin{aligned} \hat{H}_{\text{HFB}} &= \int d^3x \left\{ \sum_{\sigma=\uparrow,\downarrow} \hat{\psi}_\sigma^\dagger(\mathbf{x}) \left[ -\frac{\hbar^2}{2M} \nabla^2 - \mu_\sigma \right] \hat{\psi}_\sigma(\mathbf{x}) \right. \\ &\quad + \Gamma_\downarrow^{\text{H}} \hat{\psi}_\uparrow^\dagger(\mathbf{x}) \hat{\psi}_\uparrow(\mathbf{x}) + \Gamma_\uparrow^{\text{H}} \hat{\psi}_\downarrow^\dagger(\mathbf{x}) \hat{\psi}_\downarrow(\mathbf{x}) - \frac{\Gamma_\uparrow^{\text{H}} \Gamma_\downarrow^{\text{H}}}{g} \\ &\quad - \Gamma_{\uparrow\downarrow}^{\text{F}} \hat{\psi}_\downarrow^\dagger(\mathbf{x}) \hat{\psi}_\uparrow(\mathbf{x}) - \Gamma_{\downarrow\uparrow}^{\text{F}} \hat{\psi}_\uparrow^\dagger(\mathbf{x}) \hat{\psi}_\downarrow(\mathbf{x}) + \frac{\Gamma_{\uparrow\downarrow}^{\text{F}} \Gamma_{\downarrow\uparrow}^{\text{F}}}{g} \\ &\quad \left. + \Delta^* \hat{\psi}_\downarrow(\mathbf{x}) \hat{\psi}_\uparrow(\mathbf{x}) + \Delta \hat{\psi}_\uparrow^\dagger(\mathbf{x}) \hat{\psi}_\downarrow^\dagger(\mathbf{x}) - \frac{\Delta^* \Delta}{g} \right\}. \end{aligned} \quad (2.7)$$

## 2.1. HARTREE–FOCK–BOGOLIUBOV MEAN-FIELD APPROXIMATION

In (2.7) we define the expectation values of the corresponding channels as:

$$\Gamma_{\uparrow}^{\text{H}} = g \langle \hat{\psi}_{\uparrow}^{\dagger} \hat{\psi}_{\uparrow} \rangle; \Gamma_{\downarrow}^{\text{H}} = g \langle \hat{\psi}_{\downarrow}^{\dagger} \hat{\psi}_{\downarrow} \rangle \quad (\text{Hartree channel}), \quad (2.8)$$

$$\Gamma_{\uparrow\downarrow}^{\text{F}} = g \langle \hat{\psi}_{\uparrow}^{\dagger} \hat{\psi}_{\downarrow} \rangle; \Gamma_{\downarrow\uparrow}^{\text{F}} = g \langle \hat{\psi}_{\downarrow}^{\dagger} \hat{\psi}_{\uparrow} \rangle \quad (\text{Fock channel}), \quad (2.9)$$

$$\Delta = g \langle \hat{\psi}_{\downarrow} \hat{\psi}_{\uparrow} \rangle; \Delta^* = g \langle \hat{\psi}_{\uparrow}^{\dagger} \hat{\psi}_{\downarrow}^{\dagger} \rangle \quad (\text{Bogoliubov channel}). \quad (2.10)$$

From these definitions we conclude  $(\Gamma_{\uparrow\downarrow}^{\text{F}})^* = \Gamma_{\downarrow\uparrow}^{\text{F}}$  and  $(\Delta)^* = \Delta^*$ .

### 2.1.4 Hamiltonian in momentum spectrum

As a next step, we transform the Hamiltonian (2.7) from the coordinate space to the momentum space in the finite spatial volume  $V$ . Thereby the Fourier transformations of the field operators read:

$$\begin{aligned} \hat{\psi}_{\sigma}(\mathbf{x}) &= \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{x}} \hat{a}_{\mathbf{k},\sigma}; \quad \hat{a}_{\mathbf{k},\sigma} = \frac{1}{\sqrt{V}} \int d^3x e^{-i\mathbf{k} \cdot \mathbf{x}} \hat{\psi}_{\sigma}(\mathbf{x}), \\ \hat{\psi}_{\sigma}^{\dagger}(\mathbf{x}) &= \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{x}} \hat{a}_{\mathbf{k},\sigma}^{\dagger}; \quad \hat{a}_{\mathbf{k},\sigma}^{\dagger} = \frac{1}{\sqrt{V}} \int d^3x e^{i\mathbf{k} \cdot \mathbf{x}} \hat{\psi}_{\sigma}^{\dagger}(\mathbf{x}), \end{aligned} \quad (2.11)$$

where the fermionic annihilation-/creation operators  $\hat{a}_{\mathbf{k},\sigma}, \hat{a}_{\mathbf{k},\sigma}^{\dagger}$  of the momentum  $\hbar\mathbf{k}$  and the spin  $\sigma$  are introduced, which satisfy the anti-commutator relations:

$$\begin{aligned} [\hat{a}_{\mathbf{k},\sigma}, \hat{a}_{\mathbf{k}',\sigma'}]_{+} &= [\hat{a}_{\mathbf{k},\sigma}^{\dagger}, \hat{a}_{\mathbf{k}',\sigma'}^{\dagger}]_{+} = 0, \\ [\hat{a}_{\mathbf{k},\sigma}, \hat{a}_{\mathbf{k}',\sigma'}^{\dagger}]_{+} &= \delta_{\sigma,\sigma'} \delta(\mathbf{k} - \mathbf{k}'). \end{aligned} \quad (2.12)$$

After applying the Fourier transformation, the HFB-Hamiltonian (2.7) in the momentum basis (2.11) turns out to be:

$$\begin{aligned} \hat{H}_{\text{HFB}} &= \sum_{\mathbf{k}} \left\{ (\epsilon_{\mathbf{k}} - \mu_{\uparrow} + \Gamma_{\downarrow}^{\text{H}}) \hat{a}_{\mathbf{k},\uparrow}^{\dagger} \hat{a}_{\mathbf{k},\uparrow} + (\epsilon_{\mathbf{k}} - \mu_{\downarrow} + \Gamma_{\uparrow}^{\text{H}}) \hat{a}_{\mathbf{k},\downarrow}^{\dagger} \hat{a}_{\mathbf{k},\downarrow} \right. \\ &\quad \left. - \Gamma_{\uparrow\downarrow}^{\text{F}} \hat{a}_{\mathbf{k},\downarrow}^{\dagger} \hat{a}_{\mathbf{k},\uparrow} - \Gamma_{\downarrow\uparrow}^{\text{F}} \hat{a}_{\mathbf{k},\uparrow}^{\dagger} \hat{a}_{\mathbf{k},\downarrow} + \Delta^* \hat{a}_{-\mathbf{k},\downarrow} \hat{a}_{\mathbf{k},\uparrow} + \Delta \hat{a}_{\mathbf{k},\uparrow}^{\dagger} \hat{a}_{-\mathbf{k},\downarrow}^{\dagger} \right\} \\ &\quad - V \frac{\Gamma_{\uparrow}^{\text{H}} \Gamma_{\downarrow}^{\text{H}}}{g} + V \frac{|\Gamma_{\uparrow\downarrow}^{\text{F}}|^2}{g} - V \frac{|\Delta|^2}{g}, \end{aligned} \quad (2.13)$$

where  $\epsilon_{\mathbf{k}} = \hbar^2 \mathbf{k}^2 / (2M)$  stands for the kinetic energy of the particle with the momentum  $\hbar\mathbf{k}$ .

We are now ready to determine the mean-field Hamiltonian by extremisation. The procedure is as follows: First, from the Hamiltonian (2.13) we construct the free energy  $\mathcal{F}_{\text{HFB}}$  as a function of at first arbitrary six mean-field parameters  $\Gamma_{\uparrow}^{\text{H}}, \Gamma_{\downarrow}^{\text{H}}, \Gamma_{\uparrow\downarrow}^{\text{F}}, \Gamma_{\downarrow\uparrow}^{\text{F}}, \Delta$ , and  $\Delta^*$ . Subsequent extremisation of this effective potential function w.r.t. all parameters results in the mean-field thermodynamic potential  $\mathcal{F}_{\text{HFB}}^{(\text{MF})}$  at the saddle point, containing the extremal values of the mean-field parameters. These extremal mean-field parameters then correspond to the mean-field expectation values.

That being said, not necessarily all three interaction channels, i.e. six mean-field parameters have to be taken. For example, vanishing Hartree–Fock contributions  $\Gamma_{\sigma}^{\text{H}} = \Gamma_{\sigma\sigma'}^{\text{F}} = 0$  yield the BCS theory [41]. As such, the choice of the interaction channel leads to different theories. We may investigate these various mean-field theories according to the choice of the interaction channels.

## 2.2 BCS–Bogoliubov theory

When one only takes into account the Bogoliubov channel among the three interaction channels (2.8), that is, by taking  $\Gamma_\sigma^H = \Gamma_{\sigma\sigma'}^F = 0$ , the HFB theory is reduced to the *BCS–Bogoliubov (BCS) theory*<sup>3</sup>. The BCS approach was chosen for studying fermionic many-body problem in the preceding research [47]. Here we address the important results and discuss them in the context of the present work.

We begin from the Hamiltonian with the Bogoliubov channel:

$$\hat{H}_B = \sum_{\mathbf{k}} \left\{ \sum_{\sigma} (\epsilon_{\mathbf{k}} - \mu_{\sigma}) \hat{a}_{\mathbf{k},\sigma}^\dagger \hat{a}_{\mathbf{k},\sigma} + \Delta^* \hat{a}_{-\mathbf{k},\downarrow} \hat{a}_{\mathbf{k},\uparrow} + \Delta \hat{a}_{\mathbf{k},\uparrow}^\dagger \hat{a}_{-\mathbf{k},\downarrow}^\dagger \right\} - V \frac{\Delta^* \Delta}{g}. \quad (2.14)$$

The Hamiltonian (2.14) contains the complex *BCS-order parameter*, called the “*gap*”,  $\Delta$ . Since the Hamiltonian is not affected by changing the wave vector direction  $\mathbf{k} \leftrightarrow -\mathbf{k}$  in the sum, we can replace the operator  $\hat{a}_{\mathbf{k},\sigma}$  by  $\hat{a}_{-\mathbf{k},\sigma}$ . Also, in consideration of the pairing of particles with opposite spins we may exclude from our discussions on possibility of having the abundant particles with the majority spin from the Hamiltonian and set  $\mu = \mu_\uparrow = \mu_\downarrow$  for particles with equally populated spins. With this manipulation we arrive at the Hamiltonian:

$$\hat{H}_B = \sum_{\mathbf{k}} \left\{ (\epsilon_{\mathbf{k}} - \mu) \left( \hat{a}_{\mathbf{k},\uparrow}^\dagger \hat{a}_{\mathbf{k},\uparrow} + \hat{a}_{-\mathbf{k},\downarrow}^\dagger \hat{a}_{-\mathbf{k},\downarrow} \right) + \Delta^* \hat{a}_{-\mathbf{k},\downarrow} \hat{a}_{\mathbf{k},\uparrow} + \Delta \hat{a}_{\mathbf{k},\uparrow}^\dagger \hat{a}_{-\mathbf{k},\downarrow}^\dagger \right\} - V \frac{\Delta^* \Delta}{g}. \quad (2.15)$$

### 2.2.1 Bogoliubov transformation

The Hamiltonian (2.15) is diagonalised by the *Bogoliubov transformation* for the fermions:

$$\begin{bmatrix} \hat{\alpha}_{\mathbf{k}} \\ \hat{\beta}_{\mathbf{k}}^\dagger \end{bmatrix} = \underbrace{\begin{bmatrix} u_{\mathbf{k}} & v_{\mathbf{k}} \\ -v_{\mathbf{k}}^* & u_{\mathbf{k}}^* \end{bmatrix}}_{=U_B(\mathbf{k})} \begin{bmatrix} \hat{a}_{\mathbf{k},\uparrow} \\ \hat{a}_{-\mathbf{k},\downarrow}^\dagger \end{bmatrix}, \quad (2.16)$$

or:

$$\hat{\alpha}_{\mathbf{k}} = u_{\mathbf{k}} \hat{a}_{\mathbf{k},\uparrow} + v_{\mathbf{k}} \hat{a}_{-\mathbf{k},\downarrow}^\dagger, \quad (2.17a)$$

$$\hat{\beta}_{\mathbf{k}} = u_{\mathbf{k}} \hat{a}_{-\mathbf{k},\downarrow} - v_{\mathbf{k}} \hat{a}_{\mathbf{k},\uparrow}^\dagger, \quad (2.17b)$$

where the transformed Bogoliubov-quasiparticle operators  $\hat{\alpha}_{\mathbf{k}}$ ,  $\hat{\beta}_{\mathbf{k}}$  and the transformation coefficients, so-called the *Bogoliubov-quasiparticle amplitudes* [50],  $u_{\mathbf{k}}, v_{\mathbf{k}} \in \mathbb{C}$  satisfy the canonical fermionic anticommutator relationships:

$$[\hat{\alpha}_{\mathbf{k}}, \hat{\beta}_{\mathbf{k}'}]_+ = [\hat{\alpha}_{\mathbf{k}}^\dagger, \hat{\beta}_{\mathbf{k}'}^\dagger]_+ = [\hat{\alpha}_{\mathbf{k}}, \hat{\beta}_{\mathbf{k}'}^\dagger]_+ = [\hat{\alpha}_{\mathbf{k}}^\dagger, \hat{\beta}_{\mathbf{k}'}]_+ = 0, \quad (2.18a)$$

$$[\hat{\alpha}_{\mathbf{k}}, \hat{\alpha}_{\mathbf{k}'}^\dagger]_+ = [\hat{\beta}_{\mathbf{k}}, \hat{\beta}_{\mathbf{k}'}^\dagger]_+ = \delta(\mathbf{k} - \mathbf{k}'), \quad (2.18b)$$

and the normalisation:

$$\det U_B(\mathbf{k}) = 1 \quad \Leftrightarrow \quad |u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1. \quad (2.19)$$

From (2.16) and (2.19) follows unitarity of the Bogoliubov transformation:

$$U_B^{-1}(\mathbf{k}) = U_B^\dagger(\mathbf{k}) = \begin{bmatrix} u_{\mathbf{k}}^* & -v_{\mathbf{k}} \\ v_{\mathbf{k}}^* & u_{\mathbf{k}} \end{bmatrix}. \quad (2.20)$$

---

<sup>3</sup>In Leggett’s original work both the Hartree and the Fock term were deliberately excluded on the argument that in a homogeneous system they only yields a physically irrelevant constant energy shift [20].

## 2.2. BCS–BOGOLIUBOV THEORY

The Bogoliubov transformation should diagonalise the Hamiltonian. From these conditions we can determine the quasiparticle amplitudes  $u_{\mathbf{k}}, v_{\mathbf{k}}$ :

$$u_{\mathbf{k}}, v_{\mathbf{k}} = \frac{1}{\sqrt{2}} \sqrt{1 \pm \frac{\epsilon_{\mathbf{k}} - \mu}{\epsilon_{\mathbf{B}}(\mathbf{k})}} \quad (2.21)$$

with the Bogoliubov quasiparticle energy (also known as the *Bogoliubov dispersion*):

$$\epsilon_{\mathbf{B}}(\mathbf{k}) = \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + |\Delta|^2}. \quad (2.22)$$

With this, one writes the diagonalised BCS Hamiltonian in terms of the transformed operators as:

$$\hat{H}_{\mathbf{B}} = \sum_{\mathbf{k}} \epsilon_{\mathbf{B}}(\mathbf{k}) \left( \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}} + \hat{\beta}_{\mathbf{k}}^{\dagger} \hat{\beta}_{\mathbf{k}} \right) - V \frac{|\Delta|^2}{g} - \sum_{\mathbf{k}} [\epsilon_{\mathbf{B}}(\mathbf{k}) - (\epsilon_{\mathbf{k}} - \mu)]. \quad (2.23)$$

The meaning of the diagonalised annihilator and creator becomes more transparent by following calculation:

$$\begin{aligned} & \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}} + \hat{\beta}_{\mathbf{k}}^{\dagger} \hat{\beta}_{\mathbf{k}} \\ &= (|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2) \left( \hat{a}_{\mathbf{k},\uparrow}^{\dagger} \hat{a}_{\mathbf{k},\uparrow} + \hat{a}_{-\mathbf{k},\downarrow}^{\dagger} \hat{a}_{-\mathbf{k},\downarrow} \right) + 2u_{\mathbf{k}}^* v_{\mathbf{k}} \hat{a}_{\mathbf{k},\uparrow}^{\dagger} \hat{a}_{-\mathbf{k},\downarrow}^{\dagger} + 2u_{\mathbf{k}} v_{\mathbf{k}}^* \hat{a}_{-\mathbf{k},\downarrow} \hat{a}_{\mathbf{k},\uparrow} + 2|v_{\mathbf{k}}|^2, \end{aligned} \quad (2.24)$$

affirming

$$|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2 = \frac{\epsilon_{\mathbf{k}} - \mu}{\epsilon_{\mathbf{B}}(\mathbf{k})} \quad (2.25)$$

and

$$2u_{\mathbf{k}}^* v_{\mathbf{k}} = \frac{\Delta}{\epsilon_{\mathbf{B}}(\mathbf{k})}. \quad (2.26)$$

### 2.2.2 BCS–Bogoliubov equations

To determine the mean-field Hamiltonian and calculate the thermodynamical quantities of the BCS theory, we may need the thermodynamic potential of the system. The functional grand-canonical potential of the Hamiltonian (2.23) is:

$$\begin{aligned} \mathcal{F}_{\mathbf{B}}[|\Delta|] &= -\frac{1}{\beta} \log \text{Tr} e^{-\beta \hat{H}_{\mathbf{B}}} \\ &= -V \frac{|\Delta|^2}{g} - \sum_{\mathbf{k}} [\epsilon_{\mathbf{B}}(\mathbf{k}) - (\epsilon_{\mathbf{k}} - \mu)] - \frac{2}{\beta} \sum_{\mathbf{k}} \log \left( 1 + e^{-\beta \epsilon_{\mathbf{B}}(\mathbf{k})} \right), \end{aligned} \quad (2.27)$$

where the log trace of  $e^{-\beta \hat{H}}$  yields the sum of the eigenenergies of the Hamiltonian in the thermal ensemble.

The extremising condition  $\partial_{|\Delta|} \mathcal{F}_{\mathbf{B}}[|\Delta|] = 0$  is equivalent to the saddle point condition with regard to the effective action of the pairing field [30, 31]. This yields the BCS-order parameter equation (also known as the *gap equation*) [15, 87]:

#### BCS–Bogoliubov order parameter equation

$$\frac{|\Delta|}{g} = -\frac{1}{2V} \sum_{\mathbf{k}} \frac{|\Delta|}{\epsilon_{\mathbf{B}}(\mathbf{k})} \tanh \frac{\beta \epsilon_{\mathbf{B}}(\mathbf{k})}{2}, \quad (2.28)$$



## 2.2. BCS–BOGOLIUBOV THEORY

or:

$$|\Delta| = -\frac{g}{V} \sum_{\mathbf{k}} |u_{\mathbf{k}}^* v_{\mathbf{k}}| \tanh \frac{\beta \epsilon_{\mathbf{B}}(\mathbf{k})}{2}. \quad (2.29)$$

The solution  $\Delta$  of (2.28) extremises the thermodynamic potential of the system<sup>4</sup> and leads the Hamiltonian  $\hat{H}_{\mathbf{B}}(|\Delta|)$  to the mean-field BCS Hamiltonian  $\hat{H}_{\mathbf{B}}^{(\text{MF})}(|\Delta^{(\text{MF})}|)$  in the saddle point:

$$\left. \frac{\partial \mathcal{F}_{\mathbf{B}}(|\Delta|)}{\partial |\Delta|} \right|_{\Delta=\Delta^{(\text{MF})}} = 0, \quad (2.30)$$

where the expectation value  $\Delta = gV^{-1} \langle \hat{a}_{-\mathbf{k},\downarrow} \hat{a}_{\mathbf{k},\uparrow} \rangle$  becomes the mean-field expectation value:

$$\Delta^{(\text{MF})} = \frac{g}{V} \langle \hat{a}_{-\mathbf{k},\downarrow} \hat{a}_{\mathbf{k},\uparrow} \rangle^{(\text{MF})} = \frac{1}{\mathcal{Z}_{\mathbf{B}}^{(\text{MF})}} \text{Tr} \left( \frac{g}{V} \hat{a}_{-\mathbf{k},\downarrow} \hat{a}_{\mathbf{k},\uparrow} e^{-\beta \hat{H}_{\mathbf{B}}^{(\text{MF})}} \right) \quad (2.31)$$

with the mean-field BCS grand canonical partition function  $\mathcal{Z}_{\mathbf{B}}^{(\text{MF})} = \text{Tr} e^{-\beta \hat{H}_{\mathbf{B}}^{(\text{MF})}}$ . Comparing (2.29) and (2.31) yields:

$$\langle \hat{a}_{-\mathbf{k},\downarrow} \hat{a}_{\mathbf{k},\uparrow} \rangle^{(\text{MF})} = \sum_{\mathbf{k}} u_{\mathbf{k}}^* v_{\mathbf{k}} \tanh \frac{\beta \epsilon_{\mathbf{B}}(\mathbf{k})}{2} = \sum_{\mathbf{k}} \frac{\Delta^{(\text{MF})}}{2\epsilon_{\mathbf{B}}(\mathbf{k})} \tanh \frac{\beta \epsilon_{\mathbf{B}}(\mathbf{k})}{2}. \quad (2.32)$$

In the ground state the hyperbolic tangent in (2.35) is reduced to 1 and the equation reads:

$$\lim_{T \downarrow 0} \left| \langle \hat{a}_{-\mathbf{k},\downarrow} \hat{a}_{\mathbf{k},\uparrow} \rangle^{(\text{MF})} \right| = \sum_{\mathbf{k}} |u_{\mathbf{k}}^* v_{\mathbf{k}}| = \sum_{\mathbf{k}} \frac{|\Delta^{(\text{MF})}|}{2\epsilon_{\mathbf{B}}(\mathbf{k})}. \quad (2.33)$$

Hereafter, for simplicity we omit the superscript (MF) of the mean-field parameters  $\Gamma_{\sigma}^{\text{H}}, \Gamma_{\sigma\sigma'}^{\text{F}}$  and  $|\Delta|$  when the context is unambiguous.

The trivial solution for (2.28) is  $\Delta = 0$ , in which the system favours the state without Cooper pairs. For this trivial solution the system is in the normal fluid phase, and this normal fluid phase is stable state for most temperatures. However, for a given  $g$  there is a non-trivial solution  $\Delta \neq 0$  under the Cooper pairing temperature  $T_{\text{c}}(g)$ , yielding the non-trivial ground state of the system with the spontaneously broken  $U(1)$  symmetry. This is due to the implicit temperature-dependency of the order parameter: for the lower temperature particles have fewer accessible momentum states, and it is more likely to find anti-correlated particles with opposite momenta and spins in this limited number of possible energy states, so the system is condensed to the new ground state with a finite  $\Delta \neq 0$ . Here, more attractive scattering length  $a_{\text{s}} \leq 0$  leads to larger  $\Delta$  and also higher  $T_{\text{c}}$ . This attractive interaction energy between the anti-correlated particles plays a role of the pair-breaking energy of loosely bound Cooper pairs.

Another important equation in the BCS theory is the particle density equation that is to be obtained with  $N = -\partial_{\mu} \mathcal{F}_{\mathbf{B}}^{(\text{MF})}$ :

### BCS–Bogoliubov particle density equation

$$n = \frac{1}{V} \sum_{\mathbf{k}} \left\{ 1 - \frac{\epsilon_{\mathbf{k}} - \mu}{\epsilon_{\mathbf{B}}(\mathbf{k})} \tanh \frac{\beta \epsilon_{\mathbf{B}}(\mathbf{k})}{2} \right\}. \quad (2.34)$$

<sup>4</sup>The solution of the gap equation exists if there is a cutoff for the sum, or the equation is properly renormalised. For example, the former case is offered by an energy cutoff as usual in solid state physics, and the latter case is related to the renormalisation of the Lippmann–Schwinger equation.

### 2.3. HARTREE–FOCK THEORY

The density equation also can be written in terms of the Bogoliubov quasi-amplitudes:

$$n = \frac{1}{V} \sum_{\mathbf{k}} \left\{ 1 - (|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2) \tanh \frac{\beta \epsilon_{\text{B}}(\mathbf{k})}{2} \right\}. \quad (2.35)$$

Similiar to (2.33), the particle number in the ground state reads:

$$\lim_{T \downarrow 0} N = 2 \sum_{\mathbf{k}} |v_{\mathbf{k}}|^2 = \sum_{\mathbf{k}} \left[ 1 - \frac{\epsilon_{\mathbf{k}} - \mu}{\epsilon_{\text{B}}(\mathbf{k})} \right], \quad (2.36)$$

so that  $v_{\mathbf{k}}/\sqrt{V}$  represents the density amplitude at  $T = 0$ .

In the case of the vanishing gap  $\Delta = 0$  the Bogoliubov dispersion becomes the absolute value  $\epsilon_{\text{B}}|_{\Delta=0} = |\hbar^2 \mathbf{k}^2 / (2M) - \mu|$ , and (2.34) is reduced to the density equation of the ideal Fermi gas:

$$n|_{\Delta=0} = \frac{1}{V} \sum_{\mathbf{k}} \left\{ 1 - \frac{\epsilon_{\mathbf{k}} - \mu}{|\epsilon_{\mathbf{k}} - \mu|} \tanh \frac{\beta |\epsilon_{\mathbf{k}} - \mu|}{2} \right\} = \frac{2}{V} \sum_{\mathbf{k}} \frac{1}{e^{\beta(\epsilon_{\mathbf{k}} - \mu)} + 1}. \quad (2.37)$$

### 2.3 Hartree–Fock theory

While the BCS theory is obtained by choosing the Bogoliubov channel, another choice of taking the Hartree and Fock channels leads to the Hartree–Fock theory, where its Hamiltonian reads:

$$\hat{H}_{\text{HF}} = \sum_{\mathbf{k}} \sum_{\sigma \neq \sigma'} \left\{ [\epsilon_{\mathbf{k}} - \mu_{\sigma} + \Gamma_{\sigma'}^{\text{H}}] \hat{a}_{\mathbf{k},\sigma}^{\dagger} \hat{a}_{\mathbf{k},\sigma} - \Gamma_{\sigma'\sigma}^{\text{F}} \hat{a}_{\mathbf{k},\sigma}^{\dagger} \hat{a}_{\mathbf{k},\sigma'} \right\} - V \frac{\Gamma_{\uparrow\uparrow}^{\text{H}} \Gamma_{\downarrow\downarrow}^{\text{H}}}{g} + V \frac{\Gamma_{\uparrow\downarrow}^{\text{F}} \Gamma_{\downarrow\uparrow}^{\text{F}}}{g}. \quad (2.38)$$

By introducing the Nambu-spinor notation:

$$\hat{\Psi}(\mathbf{k}) = \begin{bmatrix} \hat{a}_{\mathbf{k},\uparrow} \\ \hat{a}_{\mathbf{k},\downarrow} \end{bmatrix}, \quad (2.39)$$

we can write the Hamiltonian (2.38) in the matrix form:

$$\hat{H}_{\text{HF}} = \sum_{\mathbf{k}} \hat{\Psi}^{\dagger}(\mathbf{k}) \begin{bmatrix} \epsilon_{\mathbf{k}} - \mu_{\uparrow} + \Gamma_{\downarrow}^{\text{H}} & \Gamma_{\downarrow\uparrow}^{\text{F}} \\ \Gamma_{\uparrow\downarrow}^{\text{F}} & \epsilon_{\mathbf{k}} - \mu_{\downarrow} + \Gamma_{\uparrow}^{\text{H}} \end{bmatrix} \hat{\Psi}(\mathbf{k}) - V \frac{\Gamma_{\uparrow\uparrow}^{\text{H}} \Gamma_{\downarrow\downarrow}^{\text{H}}}{g} + V \frac{\Gamma_{\uparrow\downarrow}^{\text{F}} \Gamma_{\downarrow\uparrow}^{\text{F}}}{g}, \quad (2.40)$$

and the  $2 \times 2$ -matrix has the eigenvalues:

$$\epsilon_{\gamma,\delta}(k) = \epsilon_{\mathbf{k}} - \frac{\mu_{\text{H},\uparrow} + \mu_{\text{H},\downarrow}}{2} \pm \sqrt{\left( \frac{\mu_{\text{H},\uparrow} - \mu_{\text{H},\downarrow}}{2} \right)^2 + |\Gamma^{\text{F}}|^2}, \quad (2.41)$$

where we have introduced the Hartree-shifted chemical potential  $\mu_{\text{H},\uparrow} = \mu_{\uparrow} - \Gamma_{\downarrow}^{\text{H}}$ ,  $\mu_{\text{H},\downarrow} = \mu_{\downarrow} - \Gamma_{\uparrow}^{\text{H}}$  and the notation  $|\Gamma^{\text{F}}|^2 = \Gamma_{\uparrow\downarrow}^{\text{F}} \Gamma_{\downarrow\uparrow}^{\text{F}}$  using the hermiticity of the Hamiltonian (2.38).

#### 2.3.1 Hartree–Fock transformation

The Hamiltonian (2.38) consists of off-diagonal terms. To diagonalise the Hamiltonian, we perform an unitary transformation with the transformation matrix  $U_{\text{HF}} \in \mathbb{C}^{2 \times 2}$ :

$$\begin{bmatrix} \hat{\gamma}_{\mathbf{k}} \\ \hat{\delta}_{\mathbf{k}} \end{bmatrix} = \underbrace{\begin{bmatrix} p & -q \\ q^* & p^* \end{bmatrix}}_{=U_{\text{HF}}} \begin{bmatrix} \hat{a}_{\mathbf{k},\uparrow} \\ \hat{a}_{\mathbf{k},\downarrow} \end{bmatrix} \quad (2.42)$$

### 2.3. HARTREE-FOCK THEORY

with the normalisation condition:

$$\det U_{\text{HF}} = |p|^2 + |q|^2 = 1. \quad (2.43)$$

Due to the inverse transformation, (2.43) reads:

$$U_{\text{HF}}^{-1} = U_{\text{HF}}^\dagger = \begin{bmatrix} p^* & q \\ -q^* & p \end{bmatrix}, \quad (2.44)$$

so that follows:

$$\hat{a}_{\mathbf{k},\uparrow} = p_{\mathbf{k}}^* \hat{\gamma}_{\mathbf{k}} + q_{\mathbf{k}} \hat{\delta}_{\mathbf{k}}, \quad (2.45a)$$

$$\hat{a}_{\mathbf{k},\downarrow} = -q_{\mathbf{k}}^* \hat{\gamma}_{\mathbf{k}} + p_{\mathbf{k}} \hat{\delta}_{\mathbf{k}}. \quad (2.45b)$$

The *Hartree-Fock (HF) transformation* (2.42) as we may call it, transforms the particles  $\hat{a}_\uparrow$  and  $\hat{a}_\downarrow$  with spin  $\uparrow$  and  $\downarrow$  into the Hartree-Fock quasiparticles  $\hat{\gamma}$  and  $\hat{\delta}$  eliminating the spin-degrees of freedom. They satisfy the anti-commutator relationship similar to (2.12) and therefore are fermions.

From (2.38) and (2.45a), (2.45b) we obtain the Hamiltonian in the HF-transformed basis:

$$\begin{aligned} \hat{H}_{\text{HF}} = \sum_{\mathbf{k}} \bigg\{ & [\epsilon_{\mathbf{k}} - \mu_{\text{H},\uparrow} |p|^2 - \mu_{\text{H},\downarrow} |q|^2 + \Gamma_{\downarrow\uparrow}^{\text{F}} p q^* + \Gamma_{\uparrow\downarrow}^{\text{F}} p^* q] \hat{\gamma}_{\mathbf{k}}^\dagger \hat{\gamma}_{\mathbf{k}} \\ & + [\epsilon_{\mathbf{k}} - \mu_{\text{H},\uparrow} |q|^2 - \mu_{\text{H},\downarrow} |p|^2 - \Gamma_{\downarrow\uparrow}^{\text{F}} p q^* - \Gamma_{\uparrow\downarrow}^{\text{F}} p^* q] \hat{\delta}_{\mathbf{k}}^\dagger \hat{\delta}_{\mathbf{k}} \\ & + [(\mu_{\text{H},\uparrow} - \mu_{\text{H},\downarrow}) p q - \Gamma_{\downarrow\uparrow}^{\text{F}} p^2 + \Gamma_{\uparrow\downarrow}^{\text{F}} q^2] \hat{\gamma}_{\mathbf{k}}^\dagger \hat{\delta}_{\mathbf{k}} \\ & + [(\mu_{\text{H},\uparrow} - \mu_{\text{H},\downarrow}) p^* q^* + \Gamma_{\downarrow\uparrow}^{\text{F}} q^{*2} - \Gamma_{\uparrow\downarrow}^{\text{F}} p^{*2}] \hat{\delta}_{\mathbf{k}}^\dagger \hat{\gamma}_{\mathbf{k}} \bigg\} \\ & - V \frac{\Gamma_{\downarrow\uparrow}^{\text{H}} \Gamma_{\uparrow\downarrow}^{\text{H}}}{g} + V \frac{\Gamma_{\downarrow\uparrow}^{\text{F}} \Gamma_{\uparrow\downarrow}^{\text{F}}}{g}. \end{aligned} \quad (2.46)$$

As the eigenvalues (2.41) are real-valued and only depends on the absolute value of  $|\Gamma^{\text{F}}|$ , we can take real-valued  $p, q \in \mathbb{R}$  without loss of generality. Now, we require that the HF-transformation (2.42) is a diagonalising transformation. Then (2.46) implies then the diagonalisation conditions:

$$(\mu_{\text{H},\uparrow} - \mu_{\text{H},\downarrow}) p q - \Gamma_{\downarrow\uparrow}^{\text{F}} p^2 + \Gamma_{\uparrow\downarrow}^{\text{F}} q^2 = 0, \quad (2.47a)$$

$$(\mu_{\text{H},\uparrow} - \mu_{\text{H},\downarrow}) p q + \Gamma_{\downarrow\uparrow}^{\text{F}} q^2 - \Gamma_{\uparrow\downarrow}^{\text{F}} p^2 = 0. \quad (2.47b)$$

Since (2.47a) and (2.47b) are equal, it follows:

$$(\mu_{\text{H},\uparrow} - \mu_{\text{H},\downarrow}) p q - \Gamma_{\downarrow\uparrow}^{\text{F}} p^2 + \Gamma_{\uparrow\downarrow}^{\text{F}} q^2 = (\mu_{\text{H},\uparrow} - \mu_{\text{H},\downarrow}) p q + \Gamma_{\downarrow\uparrow}^{\text{F}} q^2 - \Gamma_{\uparrow\downarrow}^{\text{F}} p^2, \quad (2.48)$$

that is,  $\Gamma_{\uparrow\downarrow}^{\text{F}} = \Gamma_{\downarrow\uparrow}^{\text{F}} \in \mathbb{R}$ . It is a consequence of taking real-valued  $p$  and  $q$ , and we simply write the real Fock energy  $\Gamma^{\text{F}} \in \mathbb{R}$ . Now with  $\Gamma_{\uparrow\downarrow}^{\text{F}} = \Gamma_{\downarrow\uparrow}^{\text{F}}$ , we can proceed with the sum of (2.47a) and (2.47b):

$$(\mu_{\text{H},\uparrow} - \mu_{\text{H},\downarrow}) p q + \Gamma^{\text{F}} (q^2 - p^2) = 0. \quad (2.49)$$

With the property (2.43) in the form of  $q^2 = 1 - p^2$ , (2.49) is connected to a quadratic equation of  $p^2$ :

$$\left[ (\mu_{\text{H},\uparrow} - \mu_{\text{H},\downarrow})^2 + (2\Gamma^{\text{F}})^2 \right] p^4 - \left[ (\mu_{\text{H},\uparrow} - \mu_{\text{H},\downarrow})^2 + (2\Gamma^{\text{F}})^2 \right] p^2 + (\Gamma^{\text{F}})^2 = 0. \quad (2.50)$$

### 2.3. HARTREE-FOCK THEORY

From the solution of the quadratic equation (2.50) we determine the coefficients of the HF-transformation:

$$p, q = \frac{1}{\sqrt{2}} \sqrt{1 \pm \frac{\frac{\mu_{H,\uparrow} - \mu_{H,\downarrow}}{2}}{\sqrt{\left(\frac{\mu_{H,\uparrow} - \mu_{H,\downarrow}}{2}\right)^2 + (\Gamma^F)^2}}} \quad (2.51)$$

for  $[(\mu_{H,\uparrow} - \mu_{H,\downarrow})/2]^2 + (\Gamma^F)^2 \neq 0$ . Yet, there is a caveat: if the Fock term is vanishing and we have spin-balanced gas at the same time, we end up with a mathematically ill-defined expression “0/0” in (2.51). Therefore, in case of  $\mu_{\uparrow} = \mu_{\downarrow}$  the HF-transformation is only well-defined for  $\Gamma^F \neq 0$ . But if  $\mu_{\uparrow} = \mu_{\downarrow}$  and  $\Gamma^F = 0$  are valid at the same time, there is no transformation from the beginning, because the Hartree terms are already diagonal entries.

Bringing these intermediate results together, the diagonalised HF-Hamiltonian turns out to be:

$$\hat{H}_{\text{HF}} = \sum_{\mathbf{k}} \left\{ \epsilon_{\gamma}(\mathbf{k}) \hat{\gamma}_{\mathbf{k}}^{\dagger} \hat{\gamma}_{\mathbf{k}} + \epsilon_{\delta}(\mathbf{k}) \hat{\delta}_{\mathbf{k}}^{\dagger} \hat{\delta}_{\mathbf{k}} \right\} - V \frac{\Gamma_{\downarrow}^H \Gamma_{\uparrow}^H}{g} + V \frac{(\Gamma^F)^2}{g}, \quad (2.52)$$

where the eigenenergies of the  $\gamma$ - and  $\delta$ - Hartree-Fock quasiparticles are:

$$\epsilon_{\gamma,\delta}(\mathbf{k}) = \epsilon_k - \frac{1}{2} \left[ 1 \pm \frac{(\mu_{H,\uparrow} - \mu_{H,\downarrow})/2}{\Delta_{\text{HF}}} \right] \mu_{H,\uparrow} - \frac{1}{2} \left[ 1 \mp \frac{(\mu_{H,\uparrow} - \mu_{H,\downarrow})/2}{\Delta_{\text{HF}}} \right] \mu_{H,\downarrow} \pm \frac{(\Gamma^F)^2}{\Delta_{\text{HF}}^2} \Gamma^F. \quad (2.53)$$

Here  $\Delta_{\text{HF}}$  denotes the energy:

$$\Delta_{\text{HF}} = \sqrt{\left(\frac{\mu_{H,\uparrow} - \mu_{H,\downarrow}}{2}\right)^2 + (\Gamma^F)^2}. \quad (2.54)$$

Note that for equally populated spins (2.53) reduces to:

$$\epsilon_{\gamma,\delta}(\mathbf{k}) = \epsilon_k - \mu_H \pm \Gamma^F = \epsilon_k - \mu + \Gamma^H \pm \Gamma^F. \quad (2.55)$$

#### 2.3.2 Hartree- and Fock equations

As we had the density equation and order parameter equation in the BCS theory, we need similar key equations to study the theory. We first derive the density equation. For this, the effective potential of the Hartree-Fock Hamiltonian (2.52) is needed, which reads:

$$\begin{aligned} \mathcal{F}_{\text{HF}}(\Gamma_{\uparrow}^H, \Gamma_{\downarrow}^H, \Gamma^F) &= -\frac{1}{\beta} \log \text{Tr} e^{-\beta \hat{H}_{\text{HF}}} \\ &= -V \frac{\Gamma_{\downarrow}^H \Gamma_{\uparrow}^H}{g} + V \frac{(\Gamma^F)^2}{g} - \frac{1}{\beta} \sum_{\mathbf{k}} \left[ \log \left( 1 + e^{-\beta \epsilon_{\gamma}(\mathbf{k})} \right) + \log \left( 1 + e^{-\beta \epsilon_{\delta}(\mathbf{k})} \right) \right], \end{aligned} \quad (2.56)$$

with the total number of the particles  $N = N_{\uparrow} + N_{\downarrow}$ .

We now require that the effective potential is minimally sensitive with respect to the variation of the Hartree and Fock energies. By extremising the effective potential w.r.t. the Hartree

## 2.4. HARTREE–FOCK–BOGOLIUBOV THEORY

terms, i.e.  $\partial\mathcal{F}_{\text{HF}}/\partial\Gamma_{\downarrow}^{\text{H}} = 0$  and  $\partial\mathcal{F}_{\text{HF}}/\partial\Gamma_{\uparrow}^{\text{H}} = 0$ , we find the Hartree equations:

$$\begin{aligned} \frac{\Gamma_{\uparrow}^{\text{H}}}{g} = & \frac{1}{2V} \sum_{\mathbf{k}} \left\{ \left( \frac{1}{e^{\beta\epsilon_{\gamma}(\mathbf{k})} + 1} + \frac{1}{e^{\beta\epsilon_{\delta}(\mathbf{k})} + 1} \right) \right. \\ & \left. + \frac{1}{2} \left[ \frac{|\Delta\mu|}{\Delta_{\text{HF}}} + (\text{sgn}\Delta\mu - \text{sgn}\Gamma^{\text{F}}) \frac{\Delta\mu (\Gamma^{\text{F}})^2}{\Delta_{\text{HF}}^3} \right] \left( \frac{1}{e^{\beta\epsilon_{\gamma}(\mathbf{k})} + 1} - \frac{1}{e^{\beta\epsilon_{\delta}(\mathbf{k})} + 1} \right) \right\} \end{aligned} \quad (2.57)$$

and

$$\begin{aligned} \frac{\Gamma_{\downarrow}^{\text{H}}}{g} = & \frac{1}{2V} \sum_{\mathbf{k}} \left\{ \left( \frac{1}{e^{\beta\epsilon_{\gamma}(\mathbf{k})} + 1} + \frac{1}{e^{\beta\epsilon_{\delta}(\mathbf{k})} + 1} \right) \right. \\ & \left. - \frac{1}{2} \left[ \frac{|\Delta\mu|}{\Delta_{\text{HF}}} + (\text{sgn}\Delta\mu - \text{sgn}\Gamma^{\text{F}}) \frac{\Delta\mu (\Gamma^{\text{F}})^2}{\Delta_{\text{HF}}^3} \right] \left( \frac{1}{e^{\beta\epsilon_{\gamma}(\mathbf{k})} + 1} - \frac{1}{e^{\beta\epsilon_{\delta}(\mathbf{k})} + 1} \right) \right\} \end{aligned} \quad (2.58)$$

with the shorthand notation  $\mu_{\text{H},\uparrow} - \mu_{\text{H},\downarrow} = \Delta\mu$ .

Following to that, we also extremalise the effective potential with respect to the Fock term, that is,  $\partial\mathcal{F}_{\text{HF}}/\partial\Gamma^{\text{F}} = 0$ , where the condition leads to the Fock equation:

$$\frac{\Gamma^{\text{F}}}{g} = \frac{1}{2V} (\text{sgn}\Delta\mu - \text{sgn}\Gamma^{\text{F}}) \frac{(\Delta\mu/2)^2 \Gamma^{\text{F}}}{\Delta_{\text{HF}}^3} \sum_{\mathbf{k}} \left( \frac{1}{e^{\beta\epsilon_{\gamma}(\mathbf{k})} + 1} - \frac{1}{e^{\beta\epsilon_{\delta}(\mathbf{k})} + 1} \right). \quad (2.59)$$

Note that the Fock equation (2.59) for contact interaction also has the trivial solution  $\Gamma^{\text{F}} = 0$ . If we restrict ourself to the equal spin-population case, i.e.,  $\mu_{\text{H},\uparrow} = \mu_{\text{H},\downarrow} = \mu_{\text{H}}$ , then with (2.55) the Fock equation (2.59) reads instead:

$$|\Gamma^{\text{F}}| = \frac{g}{2V} \sum_{\mathbf{k}} \left( \frac{1}{e^{\beta(\epsilon_{\mathbf{k}} - \mu_{\text{H}} - |\Gamma^{\text{F}}|)} + 1} - \frac{1}{e^{\beta(\epsilon_{\mathbf{k}} - \mu_{\text{H}} + |\Gamma^{\text{F}}|)} + 1} \right). \quad (2.60)$$

Thus, for an attractive interaction  $g < 0$  the equation (2.60) allows only the solution  $\Gamma^{\text{F}} = 0$ , therefore the Fock-energy vanishes for the attractively interacting spin-balanced Fermi gas. The Hartree–Fock theory without spin polarisation is thus identical to the Hartree theory with the vanishing Fock term.

In this case, we can reduce the Hartree–Fock Hamiltonian to the Hartree-Hamiltonian:

$$\hat{H}_{\text{H}} = \sum_{\mathbf{k}} \sum_{\sigma} [\epsilon_{\mathbf{k}} - \mu + \Gamma] \hat{a}_{\mathbf{k},\sigma}^{\dagger} \hat{a}_{\mathbf{k},\sigma} - V \frac{\Gamma^2}{g}, \quad (2.61)$$

where  $\Gamma = \Gamma_{\uparrow}^{\text{H}} = \Gamma_{\downarrow}^{\text{H}}$ . Finally from the saddle point extremisation  $\partial\mathcal{F}_{\text{H}}/\partial\Gamma = 0$  we obtain the mean-field Hartree Hamiltonian  $\hat{H}_{\text{H}}^{(\text{MF})}$  with the solution  $\Gamma = \Gamma^{\text{H(MF)}}$  of the Hartree-equation:

$$\frac{\Gamma}{g} = \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{e^{\beta(\epsilon_{\mathbf{k}} - \mu + \Gamma)} + 1}. \quad (2.62)$$

## 2.4 Hartree–Fock–Bogoliubov theory

After we have examined the theories with Hartree–Fock and Bogoliubov channels independently, we finally consider the theory for all three interaction channels in HFB-Hamiltonian (2.13) without arbitrary constraints.

## 2.4. HARTREE-FOCK-BOGOLIUBOV THEORY

### 2.4.1 Hartree-Fock-Bogoliubov Hamiltonian

We take the Hartree and Fock channels with the Bogoliubov channel all together in the Hamiltonian and derive the HFB mean-field equations. Our initial step to this task is rewriting the Hamiltonian (2.13) using the symmetry of the direction of the wave vector  $\mathbf{k}$ :

$$\begin{aligned} \hat{H}_{\text{HFB}} = & \frac{1}{2} \sum_{\mathbf{k}} \left[ \sum_{\sigma \neq \sigma'} \left\{ [\epsilon_{\mathbf{k}} - \mu_{\sigma} + \Gamma_{\sigma'}^{\text{H}}] \left( \hat{a}_{\mathbf{k},\sigma}^{\dagger} \hat{a}_{\mathbf{k},\sigma} + \hat{a}_{-\mathbf{k},\sigma}^{\dagger} \hat{a}_{-\mathbf{k},\sigma} \right) \right. \right. \\ & \left. \left. - \Gamma_{\sigma'\sigma}^{\text{F}} \left( \hat{a}_{\mathbf{k},\sigma}^{\dagger} \hat{a}_{\mathbf{k},\sigma'} + \hat{a}_{-\mathbf{k},\sigma}^{\dagger} \hat{a}_{-\mathbf{k},\sigma'} \right) \right\} \right. \\ & \left. + \Delta^* \left( \hat{a}_{-\mathbf{k},\downarrow} \hat{a}_{\mathbf{k},\uparrow} + \hat{a}_{\mathbf{k},\downarrow} \hat{a}_{-\mathbf{k},\uparrow} \right) + \Delta \left( \hat{a}_{\mathbf{k},\uparrow}^{\dagger} \hat{a}_{-\mathbf{k},\downarrow}^{\dagger} + \hat{a}_{-\mathbf{k},\uparrow}^{\dagger} \hat{a}_{\mathbf{k},\downarrow}^{\dagger} \right) \right] \\ & - V \frac{\Gamma_{\uparrow\uparrow}^{\text{H}} \Gamma_{\downarrow\downarrow}^{\text{H}}}{g} + V \frac{\Gamma_{\uparrow\downarrow}^{\text{F}} \Gamma_{\downarrow\uparrow}^{\text{F}}}{g} - V \frac{\Delta^* \Delta}{g}. \end{aligned} \quad (2.63)$$

Consideration of the non-vanishing order parameter case  $\Delta \neq 0$  leads us to the restriction of the Hamiltonian with the equally populated spin similar to (2.15), so we substitute  $\mu_{\sigma} \rightarrow \mu$  and  $\Gamma_{\sigma}^{\text{H}} \rightarrow \Gamma^{\text{H}}$  in (2.65). To proceed further, we define a four-component Nambu-spinor:

$$\hat{\Psi}(\mathbf{k}) = \begin{bmatrix} \hat{a}_{\mathbf{k},\uparrow} \\ \hat{a}_{\mathbf{k},\downarrow} \\ \hat{a}_{-\mathbf{k},\uparrow}^{\dagger} \\ \hat{a}_{-\mathbf{k},\downarrow}^{\dagger} \end{bmatrix}, \quad (2.64)$$

and by means of it write the Hamiltonian in the matrix form:

$$\begin{aligned} \hat{H}_{\text{HFB}} &= \frac{1}{2} \sum_{\mathbf{k}} \hat{\Psi}^{\dagger}(\mathbf{k}) \begin{bmatrix} \epsilon_{\mathbf{k}} - \mu + \Gamma^{\text{H}} & -\Gamma_{\downarrow\uparrow}^{\text{F}} & 0 & \Delta \\ -\Gamma_{\uparrow\downarrow}^{\text{F}} & \epsilon_{\mathbf{k}} - \mu + \Gamma^{\text{H}} & -\Delta & 0 \\ 0 & -\Delta^* & -(\epsilon_{\mathbf{k}} - \mu + \Gamma^{\text{H}}) & \Gamma_{\uparrow\downarrow}^{\text{F}} \\ \Delta^* & 0 & \Gamma_{\downarrow\uparrow}^{\text{F}} & -(\epsilon_{\mathbf{k}} - \mu + \Gamma^{\text{H}}) \end{bmatrix} \hat{\Psi}(\mathbf{k}) \\ & - \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu + \Gamma^{\text{H}}) - V \frac{(\Gamma^{\text{H}})^2}{g} + V \frac{\Gamma_{\uparrow\downarrow}^{\text{F}} \Gamma_{\downarrow\uparrow}^{\text{F}}}{g} - V \frac{\Delta^* \Delta}{g}. \end{aligned} \quad (2.65)$$

The unitary matrix (2.65) is diagonalisable, so we look for the following diagonalised form of the matrix with the transformation  $U_{\text{HFB}} \in \mathbb{C}^{4 \times 4}$  for  $\hat{\Psi}$ :

$$\begin{aligned} & \begin{bmatrix} \epsilon_{\text{HFB}}^{(1)} & 0 & 0 & 0 \\ 0 & \epsilon_{\text{HFB}}^{(2)} & 0 & 0 \\ 0 & 0 & \epsilon_{\text{HFB}}^{(3)} & 0 \\ 0 & 0 & 0 & \epsilon_{\text{HFB}}^{(4)} \end{bmatrix} \\ &= U_{\text{HFB}}^{\dagger} \begin{bmatrix} \epsilon_{\mathbf{k}} - \mu + \Gamma^{\text{H}} & -\Gamma_{\downarrow\uparrow}^{\text{F}} & 0 & \Delta \\ -\Gamma_{\uparrow\downarrow}^{\text{F}} & \epsilon_{\mathbf{k}} - \mu + \Gamma^{\text{H}} & -\Delta & 0 \\ 0 & -\Delta^* & -(\epsilon_{\mathbf{k}} - \mu + \Gamma^{\text{H}}) & \Gamma_{\uparrow\downarrow}^{\text{F}} \\ \Delta^* & 0 & \Gamma_{\downarrow\uparrow}^{\text{F}} & -(\epsilon_{\mathbf{k}} - \mu + \Gamma^{\text{H}}) \end{bmatrix} U_{\text{HFB}}, \end{aligned} \quad (2.66)$$

## 2.4. HARTREE–FOCK–BOGOLIUBOV THEORY

and the transformed fermionic quasiparticle operators:

$$\begin{bmatrix} \hat{c}_{\mathbf{k},1} \\ \hat{c}_{\mathbf{k},2} \\ \hat{c}_{\mathbf{k},3}^\dagger \\ \hat{c}_{\mathbf{k},4}^\dagger \end{bmatrix} = U_{\text{HFB}} \hat{\Psi} \quad (2.67)$$

for the assumed eigenvalues  $\epsilon_{\text{HFB}}^{(1)} - \epsilon_{\text{HFB}}^{(4)}$ .

Without knowing the explicit transformation  $U_{\text{HFB}}$ , the diagonal matrix and its eigenvalues can be calculated symbolically for the elements  $\Gamma^{\text{H}}$ ,  $(\Gamma^{\text{F}})^{(*)}$  and  $\Delta^{(*)}$ . The calculation results in two doubly degenerate eigenenergies:

$$\epsilon_{\text{HFB}}^{(\pm)}(\mathbf{k}) = |\epsilon_{\text{HB}}(\mathbf{k}) \pm |\Gamma^{\text{F}}||, \quad (2.68)$$

where  $\epsilon_{\text{HB}}$  denotes the *Hartree–Bogoliubov dispersion*:

$$\epsilon_{\text{HB}}(\mathbf{k}) = \sqrt{(\epsilon_k - \mu + \Gamma^{\text{H}})^2 + |\Delta|^2}. \quad (2.69)$$

With (2.68) the grand canonical functional of the system reads:

$$\begin{aligned} \mathcal{F}_{\text{HFB}}[\Gamma^{\text{H}}, |\Gamma^{\text{F}}|, |\Delta|] \\ = -V \frac{(\Gamma^{\text{H}})^2}{g} + V \frac{|\Gamma^{\text{F}}|^2}{g} - V \frac{|\Delta|^2}{g} - \sum_{\mathbf{k}} \left[ \frac{\epsilon_{\text{HFB}}^{(+)}(\mathbf{k}) + \epsilon_{\text{HFB}}^{(-)}(\mathbf{k})}{2} - (\epsilon_k - \mu + \Gamma^{\text{H}}) \right] \\ - \frac{1}{\beta} \sum_{\mathbf{k}} \left[ \log \left( 1 + e^{-\beta \epsilon_{\text{HFB}}^{(+)}(\mathbf{k})} \right) + \log \left( 1 + e^{-\beta \epsilon_{\text{HFB}}^{(-)}(\mathbf{k})} \right) \right]. \end{aligned} \quad (2.70)$$

Now, the functional potential  $\mathcal{F}_{\text{HFB}}$  should be extremised by the interaction parameters. The extremisation w.r.t. the Hartree term  $\delta \mathcal{F}_{\text{HFB}} / \delta \Gamma^{\text{H}} = 0$  yields:

### Hartree–Fock–Bogoliubov Hartree equation

$$\begin{aligned} \frac{\Gamma^{\text{H}}}{g} = \frac{1}{2V} \sum_{\mathbf{k}} \left[ 1 - \frac{\epsilon_k - \mu + \Gamma^{\text{H}}}{\epsilon_{\text{HB}}(\mathbf{k})} \left\{ \frac{1 + \text{sgn}(\epsilon_{\text{HB}}(\mathbf{k}) - |\Gamma^{\text{F}}|)}{2} \right. \right. \\ \left. \left. - \frac{1}{e^{\beta \epsilon_{\text{HFB}}^{(+)}(\mathbf{k})} + 1} - \frac{\text{sgn}(\epsilon_{\text{HB}}(\mathbf{k}) - |\Gamma^{\text{F}}|)}{e^{\beta \epsilon_{\text{HFB}}^{(-)}(\mathbf{k})} + 1} \right\} \right]. \end{aligned} \quad (2.71)$$

Next we investigate the Fock term. Concerning the absolute valued Fock energy  $|\Gamma^{\text{F}}|$ , we first note the derivative of (2.68):

$$\frac{\partial \epsilon_{\text{HFB}}^{(\pm)}}{\partial |\Gamma^{\text{F}}|} = \frac{\epsilon_{\text{HB}} \pm |\Gamma^{\text{F}}|}{\epsilon_{\text{HFB}}^{(\pm)}} \frac{\partial (\pm |\Gamma^{\text{F}}|)}{\partial |\Gamma^{\text{F}}|} = \pm \text{sgn}(\epsilon_{\text{HB}} \pm |\Gamma^{\text{F}}|). \quad (2.72)$$

The function (2.70) should be extremised in the variation of the Fock term:  $\partial \mathcal{F}_{\text{HFB}} / \partial |\Gamma^{\text{F}*}| = 0$ . With (2.70) and (2.72) the extremising condition leads to the Fock equation:

**Hartree-Fock-Bogoliubov Fock equation**

$$\frac{|\Gamma^F|}{g} = \frac{1}{2V} \sum_{\mathbf{k}} \left[ \frac{1 - \operatorname{sgn}(\epsilon_{\text{HB}}(\mathbf{k}) - |\Gamma^F|)}{2} - \frac{1}{e^{\beta\epsilon_{\text{HFB}}^{(+)}(\mathbf{k})} + 1} + \frac{\operatorname{sgn}(\epsilon_{\text{HB}}(\mathbf{k}) - |\Gamma^F|)}{e^{\beta\epsilon_{\text{HFB}}^{(-)}(\mathbf{k})} + 1} \right]. \quad (2.73)$$

To control the absolute value energy  $\epsilon_{\text{HFB}}^{(\pm)}(\mathbf{k}) = |\epsilon_{\text{HB}}(\mathbf{k}) \pm |\Gamma^F||$  in the equation, we may divide the sum range according to the subset of wave vector space  $K$ :

$$M_{\text{HB}<\text{F}} = \{\mathbf{k} \in K : \epsilon_{\text{HB}}(\mathbf{k}) < |\Gamma^F|\}, \quad (2.74)$$

which helps to analyse the sign function and the absolute valued energy according to:

$$\operatorname{sgn}(\epsilon_{\text{HB}} \pm |\Gamma^F|) = \begin{cases} 1 & , \mathbf{k} \notin M_{\text{HB}<\text{F}} \\ -1 & , \mathbf{k} \in M_{\text{HB}<\text{F}} \end{cases}, \quad (2.75a)$$

$$\epsilon_{\text{HFB}}^{(-)}(\mathbf{k}) = \begin{cases} \epsilon_{\text{HB}}(\mathbf{k}) - |\Gamma^F| & , \mathbf{k} \notin M_{\text{HB}<\text{F}} \\ |\Gamma^F| - \epsilon_{\text{HB}}(\mathbf{k}) & , \mathbf{k} \in M_{\text{HB}<\text{F}} \end{cases}. \quad (2.75b)$$

From (2.73) and (2.75a-2.75b) again we derive:

$$\begin{aligned} |\Gamma^F| = \frac{g}{2V} & \left[ \sum_{\mathbf{k} \notin M_{\text{HB}<\text{F}}} \left\{ \frac{1}{e^{\beta\epsilon_{\text{HB}}(\mathbf{k}) - \beta|\Gamma^F|} + 1} - \frac{1}{e^{\beta\epsilon_{\text{HB}}(\mathbf{k}) + \beta|\Gamma^F|} + 1} \right\} \right. \\ & \left. + \sum_{\mathbf{k} \in M_{\text{HB}<\text{F}}} \left\{ 1 - \left( \frac{1}{e^{\beta|\Gamma^F| - \beta\epsilon_{\text{HB}}(\mathbf{k})} + 1} + \frac{1}{e^{\beta|\Gamma^F| + \beta\epsilon_{\text{HB}}(\mathbf{k})} + 1} \right) \right\} \right]. \end{aligned} \quad (2.76)$$

The summands in both sums are positive, since for  $\epsilon_{\text{HB}}(\mathbf{k}) < |\Gamma^F|$  holds:

$$\begin{aligned} \frac{1}{e^{\beta|\Gamma^F| + \beta\epsilon_{\text{HB}}(\mathbf{k})} + 1} + \frac{1}{e^{\beta|\Gamma^F| - \beta\epsilon_{\text{HB}}(\mathbf{k})} + 1} &= \frac{e^{\beta|\Gamma^F|} (e^{\beta\epsilon_{\text{HB}}(\mathbf{k})} + e^{-\beta\epsilon_{\text{HB}}(\mathbf{k})}) + 2}{e^{2\beta|\Gamma^F|} + e^{\beta|\Gamma^F|} (e^{\beta\epsilon_{\text{HB}}(\mathbf{k})} + e^{-\beta\epsilon_{\text{HB}}(\mathbf{k})}) + 1} \\ &= \frac{\cosh \beta\epsilon_{\text{HB}}(\mathbf{k}) + e^{-\beta|\Gamma^F|}}{\cosh \beta\epsilon_{\text{HB}}(\mathbf{k}) + \cosh \beta|\Gamma^F|} \leq 1, \end{aligned} \quad (2.77)$$

and for  $\epsilon_{\text{HB}}(\mathbf{k}) \geq |\Gamma^F|$  obviously:

$$\frac{1}{e^{\beta\epsilon_{\text{HB}}(\mathbf{k}) - \beta|\Gamma^F|} + 1} - \frac{1}{e^{\beta\epsilon_{\text{HB}}(\mathbf{k}) + \beta|\Gamma^F|} + 1} \geq 0. \quad (2.78)$$

Therefore, for  $g \leq 0$  the equation (2.73) has the unique solution  $\Gamma^F = 0$ , so the Fock energy vanishes. This is the same conclusion as from the Hartree-Fock theory in the previous section 2.3. We would ignore the case  $g > 0$  because the mean-field HFB theory with contact interaction would be invalid for the strong interaction, and for this the consideration of the mean-field Fock term is not necessary.

Furthermore, the extremisation w.r.t. the order parameter  $\delta\mathcal{F}_{\text{HFB}}/\delta|\Delta| = 0$  leads to:

**Hartree-Fock-Bogoliubov order parameter equation**

$$\frac{|\Delta|}{g} = -\frac{1}{2V} \sum_{\mathbf{k}} \frac{|\Delta|}{\epsilon_{\text{HB}}(\mathbf{k})} \left[ \frac{1 + \operatorname{sgn}(\epsilon_{\text{HB}}(\mathbf{k}) - |\Gamma^F|)}{2} - \frac{1}{e^{\beta\epsilon_{\text{HFB}}^{(+)}(\mathbf{k})} + 1} - \frac{\operatorname{sgn}(\epsilon_{\text{HB}}(\mathbf{k}) - |\Gamma^F|)}{e^{\beta\epsilon_{\text{HFB}}^{(-)}(\mathbf{k})} + 1} \right], \quad (2.79)$$



## 2.4. HARTREE–FOCK–BOGOLIUBOV THEORY

which recovers the order parameter equation of the BCS theory (2.28) with  $\Gamma^H = \Gamma^F = 0$ . After the extremisation with the saddle point equations (2.71), (2.73) and (2.79) we obtain the mean-field HFB Hamiltonian  $\hat{H}_{\text{HFB}}^{(\text{MF})}$ .

Finally, the particle density  $n = -V^{-1}\partial_\mu \mathcal{F}_{\text{HFB}}$  is given as follows:

### Hartree–Fock–Bogoliubov particle density equation

$$n = \frac{1}{V} \sum_{\mathbf{k}} \left[ 1 - \frac{\epsilon_{\mathbf{k}} - \mu + \Gamma^H}{\epsilon_{\text{HB}}(\mathbf{k})} \left\{ \frac{1 + \text{sgn}(\epsilon_{\text{HB}}(\mathbf{k}) - |\Gamma^F|)}{2} - \frac{1}{e^{\beta\epsilon_{\text{HFB}}^{(+)}(\mathbf{k})} + 1} - \frac{\text{sgn}(\epsilon_{\text{HB}}(\mathbf{k}) - |\Gamma^F|)}{e^{\beta\epsilon_{\text{HFB}}^{(-)}(\mathbf{k})} + 1} \right\} \right], \quad (2.80)$$

which together with (2.71) results  $\Gamma^H = gn/2$ .

### 2.4.2 Hartree–Bogoliubov equations

For  $g \leq 0$  the HFB Hamiltonian (2.65) is reduced to Hamiltonian of the *Hartree–Bogoliubov (HB) theory* with  $\Gamma^F = 0$ <sup>5</sup>:

$$\hat{H}_{\text{HB}}^{(\text{MF})} = \sum_{\mathbf{k}} \left\{ \sum_{\sigma} [\epsilon_{\mathbf{k}} - \mu + \Gamma] \hat{a}_{\mathbf{k},\sigma}^\dagger \hat{a}_{\mathbf{k},\sigma} + \Delta^* \hat{a}_{-\mathbf{k},\downarrow} \hat{a}_{\mathbf{k},\uparrow} + \Delta \hat{a}_{\mathbf{k},\uparrow}^\dagger \hat{a}_{-\mathbf{k},\downarrow}^\dagger \right\} - V \frac{\Gamma^2}{g} - V \frac{|\Delta|^2}{g} \quad (2.81)$$

with the solutions  $\Gamma$  and  $|\Delta|$  of the saddle point equations (2.71) and (2.79), respectively.

The diagonalisation of the Hamiltonian (2.81) can be done by the Bogoliubov transformation:

$$u_{\mathbf{k}}, v_{\mathbf{k}} = \frac{1}{\sqrt{2}} \sqrt{1 \pm \frac{\epsilon_{\mathbf{k}} - \mu + \Gamma}{\epsilon_{\text{HB}}(\mathbf{k})}}, \quad (2.82)$$

where we add the Hartree term  $\Gamma$  in the transformation. The transformation scheme with this redefined Bogoliubov-quasiparticle amplitudes is same as the ordinary Bogoliubov transformation. Consequently, its properties and the fermionic anti-commutator relations remain unchanged. The diagonalised Hamiltonian is:

$$\begin{aligned} \hat{H}_{\text{HB}}^{(\text{MF})} &= \sum_{\mathbf{k}} \epsilon_{\text{HB}}(\mathbf{k}) \left( \hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} + \hat{\beta}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}} \right) \\ &\quad - \sum_{\mathbf{k}} \{ \epsilon_{\text{HB}}(\mathbf{k}) - (\epsilon_{\mathbf{k}} - \mu + \Gamma) \} - V \frac{\Gamma^2}{g} - V \frac{|\Delta|^2}{g}, \end{aligned} \quad (2.83)$$

c.f. (2.23).

The mean-field Hamiltonian (2.83) has been determined by the mean-field expectation values satisfying the saddle point equations, which are again extremisation conditions of the thermo-

<sup>5</sup>This is the result of taking the interaction as c-numbers, i.e. mean-field approximation, which reduces the HFB theory to the HB theory [43].

## 2.4. HARTREE–FOCK–BOGOLIUBOV THEORY

dynamic functional:

$$\begin{aligned}\mathcal{F}_{\text{HB}}[\Gamma, |\Delta|] &= -\frac{1}{\beta} \log \left( \text{Tr} e^{-\beta \hat{H}_{\text{HB}}} \right) \\ &= -V \frac{\Gamma^2}{g} - V \frac{|\Delta|^2}{g} - \sum_{\mathbf{k}} [\epsilon_{\text{HB}}(\mathbf{k}) - (\epsilon_k - \mu + \Gamma)] - \frac{2}{\beta} \sum_{\mathbf{k}} \log \left( 1 + e^{-\beta \epsilon_{\text{HB}}(\mathbf{k})} \right).\end{aligned}\tag{2.84}$$

First extremisation condition  $\delta \mathcal{F}_{\text{HB}} / \delta \Gamma = 0$  gives the self-consistency equation:

**Hartree–Bogoliubov Hartree equation**

$$\frac{\Gamma}{g} = \frac{1}{2V} \sum_{\mathbf{k}} \left\{ 1 - \frac{\epsilon_k - \mu + \Gamma}{\epsilon_{\text{HB}}(\mathbf{k})} \tanh \frac{\beta \epsilon_{\text{HB}}(\mathbf{k})}{2} \right\}.\tag{2.85}$$

The order parameter equation is obtained from the minimal sensitivity condition  $\delta \mathcal{F}_{\text{HB}} / \delta |\Delta| = 0$  again:

**Hartree–Bogoliubov order parameter equation**

$$\frac{|\Delta|}{g} = -\frac{1}{2V} \sum_{\mathbf{k}} \frac{|\Delta|}{\epsilon_{\text{HB}}(\mathbf{k})} \tanh \frac{\beta \epsilon_{\text{HB}}(\mathbf{k})}{2},\tag{2.86}$$

which is in the same form as (2.28), however with the different dispersion  $\epsilon_{\text{HB}}$  (2.69).

The number equation of the HB theory is obtained by  $-\partial_{\mu} \mathcal{F}_{\text{HB}}^{(\text{MF})}$ :

**Hartree–Bogoliubov particle density equation**

$$n = \frac{1}{V} \sum_{\mathbf{k}} \left\{ 1 - \frac{\epsilon_k - \mu + \Gamma}{\epsilon_{\text{HB}}(\mathbf{k})} \tanh \frac{\beta \epsilon_{\text{HB}}(\mathbf{k})}{2} \right\}.\tag{2.87}$$

By compairing (2.87) and (2.85), again we find the relation:sm

$$\Gamma = g \frac{n}{2} = g n_{\sigma},\tag{2.88}$$

same as with the HFB theory.

In the HB theory the density equation obtained and the Hartree equation coincide, and they together yield the self-consistent density-interaction equation (2.87) that replaces the density equation (2.34) of the BCS theory. The consequence of this will discussed in following chapters.

## Chapter 3

# Uniform Fermi Gas

In the previous chapter we have been dealt with the interacting fermions in absence of inhomogeneity, i.e. without temporal and spatial dependency. Such a system is referred to as *uniform*. The uniform gas model stands as the simplest scenario, being a basic ground for studying more complicated situations such as optical lattice, temporal periodicity, and spatial disorder.

This chapter is dedicated for studying the Hartree and Bogoliubov theories independently within the uniform gas model. Our objective is to concentrate on each interaction channel, thereby providing a clearer interpretation of the contributions from each interaction channel. Once this analysis is complete, the unification of the Hartree and Bogoliubov theories becomes easily achievable by merging them into the Hartree–Bogoliubov theory.

### 3.1 Ideal Fermi gas

The non-interacting ideal Fermi gas is the starting point of our discussion. The Hamiltonian of the ideal Fermi gas is:

$$\hat{H}_{\text{ideal}} = \sum_{\mathbf{k}} [\epsilon_{\mathbf{k}} - \mu] \left( \hat{a}_{\mathbf{k},\uparrow}^\dagger \hat{a}_{\mathbf{k},\uparrow} + \hat{a}_{\mathbf{k},\downarrow}^\dagger \hat{a}_{\mathbf{k},\downarrow} \right). \quad (3.1)$$

The *Fermi energy*  $\epsilon_F = \hbar^2 k_F^2 / (2M)$  with the *Fermi wavevector*  $k_F$  is equal to the chemical potential of the ideal Fermi gas  $\mu$  at the ground state, and it is determined by the density of the ideal Fermi gas  $n$ :

$$\epsilon_F = \frac{\hbar^2}{2M} \underbrace{\lim_{T \downarrow 0} (3\pi^2 n)^{2/3}}_{=k_F^2} = \lim_{T \downarrow 0} \mu. \quad (3.2)$$

Thereby, the Fermi wavevector for two spin species, giving the degeneracy factor 2, is calculated via:

$$\lim_{T \downarrow 0} n = \lim_{T \downarrow 0} \frac{2}{V} \int \frac{d^3 k}{(2\pi)^3} \frac{1}{e^{\beta(\epsilon_{\mathbf{k}} - \mu)} + 1} = \frac{2}{V} \int_0^{k_F} dk \frac{4\pi k^2}{(2\pi)^3}, \quad (3.3)$$

which leads to the result:

$$n = \frac{k_F^3}{3\pi^2}. \quad (3.4)$$

In the calculation the continuum approximation of the discrete sum in thermodynamic limit  $N \rightarrow \infty$ :

$$\sum_{\mathbf{k}} \rightarrow V \int \frac{d^3 k}{(2\pi)^3} \quad (3.5)$$

### 3.1. IDEAL FERMI GAS

is applied. Especially, for  $\mathbf{k}$ -isotropic integrands we can reduce it to the one-dimensional integral:

$$V \int \frac{d^3k}{(2\pi)^3} = \frac{V}{2\pi^2} \int_0^\infty dk k^2 = \frac{M^{3/2}V}{\sqrt{2}\pi^2\hbar^3} \int_0^\infty d\epsilon_k \epsilon_k^{1/2} = 2\pi \frac{V}{\lambda_F^3} \int_0^\infty \frac{d\epsilon_k \epsilon_k^{1/2}}{\epsilon_F^{3/2}} \quad (3.6)$$

with the *Fermi-wavelength*  $\lambda_F = 2\pi/k_F$ .

For the finite temperature, the density of the particles is calculated as:

$$n = \frac{2}{V} \sum_{\mathbf{k}} \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1} = 2 \int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1} = \frac{\sqrt{2}M^{3/2}}{\pi^2\hbar^3} \int_0^\infty d\epsilon_k \epsilon_k^{1/2} \frac{\epsilon_k^{1/2}}{e^{\beta(\epsilon_k - \mu)} + 1}. \quad (3.7)$$

The integration (3.7) can be calculated by the Fermi–Dirac integral to polylogarithmic expression (see Appendix A.):

$$\lambda^3 n = -2\text{Li}_{3/2}(-e^{\beta\mu}), \quad (3.8)$$

where  $\lambda = \sqrt{2\pi\hbar^2\beta/M}$  denotes the *thermal de Broglie-wavelength*. In (3.8) we have introduced the dimensionless *phase-space density*  $\lambda^3 n$ :

$$\lambda^3 n = \frac{Nh^3}{VV_p} \quad (3.9)$$

with the thermal momentum-space volume:

$$V_p = \left(\frac{h}{\lambda}\right)^3 = (2\pi M k_B T)^{3/2}, \quad (3.10)$$

which is the cubic volume of the momentum of the thermal wavelength.

The phase-space density  $\lambda^3 n$  is the number of particles occupying the states in the phase space at thermodynamic ensemble, i.e. the number of particle in the phase-space volume  $V_p V$  in the unit of  $h$ . For non-interacting bosons, the BEC-transition occurs at  $\lambda_{\text{boson}}^3 n_{\text{boson}} = \zeta(3/2) \approx 2.612$  with the vanishing chemical potential  $\mu \uparrow 0$  [35].

Physical quantities in energy unit in the Fermi gas theory are usually discussed in dimensionless quantities scaled by the Fermi energy. We also scale the energy in inverse temperature in terms of the Fermi temperature  $T_F = \epsilon_F/k_B$ :

$$\beta\epsilon = \frac{\epsilon}{\epsilon_F} \bigg/ \frac{T}{T_F}. \quad (3.11)$$

Also the density  $n$  can be given in the form of dimensionless *Fermi-phase-space density*:

$$\lambda_F^3 n = \left(\frac{2\pi}{k_F}\right)^3 n. \quad (3.12)$$

In these dimensionless quantities, we write the density of ideal Fermi gas with two spin species (3.8) as:

$$\lambda_F^3 n = -2\pi^{3/2} \left(\frac{T}{T_F}\right)^{3/2} \text{Li}_{3/2}\left(-e^{\frac{\mu}{\epsilon_F} / \frac{T}{T_F}}\right). \quad (3.13)$$

## 3.2 BCS–Bogoliubov theory

In this section, we may recapitulate the properties of the uniform Fermi gas with the Bogoliubov channel which studied in the preceding research [47] and establish the connection with the present work.

### 3.2.1 Thermodynamic ensemble

In the thermodynamic limit the discrete  $\mathbf{k}$ -sum is approximated by the integration. The order parameter equation (2.28) in this continuum limit is:

$$\frac{1}{g} = -\frac{1}{2} \int \frac{d^3k}{(2\pi)^3} \frac{1}{\epsilon_B(k)} \tanh \frac{\beta \epsilon_B(k)}{2}, \quad (3.14)$$

and the particle number equation (2.34) reads:

$$n = \frac{1}{\lambda_F^3} \frac{2\pi}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \sqrt{\epsilon_k} \left\{ 1 - \frac{\epsilon_k - \mu}{\epsilon_B(k)} \tanh \frac{\beta \epsilon_B(k)}{2} \right\}. \quad (3.15)$$

Here we have a problem: there is an ultraviolet divergence in the order parameter equation (3.14). To regulate the divergence, the renormalisation of the s-wave scattering in the low energy limit is to be introduced [30]:

$$\frac{1}{g_r} = \frac{M}{4\pi\hbar^2 a_s} - \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\epsilon_k}, \quad (3.16)$$

so after the substitution  $g \rightarrow g_r$  (3.14) reads<sup>1</sup>:

$$\frac{M}{2\pi\hbar^2 a_s} = \int \frac{d^3k}{(2\pi)^3} \left\{ \frac{1}{\epsilon_k} - \frac{1}{\epsilon_B(k)} \tanh \frac{\beta \epsilon_B(k)}{2} \right\}, \quad (3.17)$$

or in the dimensionless form:

$$\frac{2\pi}{k_F a_s} = \frac{2}{\sqrt{\epsilon_F}} \int_0^\infty d\epsilon_k \epsilon_k^{1/2} \left\{ \frac{1}{\epsilon_k} - \frac{1}{\epsilon_B(k)} \tanh \frac{\beta \epsilon_B(k)}{2} \right\}. \quad (3.18)$$

For better grasp of (3.18) we perform substitutional integration of the right-hand-side:

$$\begin{aligned} \frac{2\pi}{k_F a_s} &= \frac{2}{\sqrt{\epsilon_F}} \int_0^\infty d\epsilon_k \frac{1}{\sqrt{\epsilon_k}} \left\{ 1 - \frac{\epsilon_k}{\epsilon_B(k)} \tanh \frac{\beta \epsilon_B(k)}{2} \right\} \\ &= \underbrace{\left[ 4 \frac{\sqrt{\epsilon_k}}{\sqrt{\epsilon_F}} \left\{ 1 - \frac{\epsilon_k - \mu}{\epsilon_B(k)} \tanh \frac{\beta \epsilon_B(k)}{2} \right\} \right]_0^\infty}_{=0} \\ &\quad - \frac{2}{\sqrt{\epsilon_F}} \int_0^\infty d\epsilon_k 2\sqrt{\epsilon_k} \frac{\partial}{\partial \epsilon_k} \left( -\frac{\epsilon_k - \mu}{\epsilon_B(k)} \tanh \frac{\beta \epsilon_B(k)}{2} \right) - \frac{2\mu}{\sqrt{\epsilon_F}} \int_0^\infty d\epsilon_k \frac{\tanh \frac{\beta \epsilon_B(k)}{2}}{\sqrt{\epsilon_k} \epsilon_B(k)} \\ &= \frac{4}{\sqrt{\epsilon_F}} \int_0^\infty d\epsilon_k \frac{\sqrt{\epsilon_k}}{\epsilon_B(k)} \left[ \frac{|\Delta|^2}{\epsilon_B^2(k)} \tanh \frac{\beta \epsilon_B(k)}{2} + \frac{(\epsilon_k - \mu)^2}{\epsilon_B^2(k)} \frac{\frac{\beta \epsilon_B(k)}{2}}{\cosh^2 \frac{\beta \epsilon_B(k)}{2}} \right] \\ &\quad - \frac{2\mu}{\sqrt{\epsilon_F}} \int_0^\infty d\epsilon_k \frac{\tanh \frac{\beta \epsilon_B(k)}{2}}{\sqrt{\epsilon_k} \epsilon_B(k)}. \end{aligned} \quad (3.19)$$

In the third and fourth rows of the equation, the first integral term is positive, and in a same

---

<sup>1</sup>It should be noted that the renormalisation (3.16) with  $g_r$  is not applied to Hartree term  $\Gamma_\sigma^H = g \langle \psi_\sigma^\dagger \psi_\sigma \rangle$  [57].

### 3.2. BCS–BOGOLIUBOV THEORY

form as the particle density equation up to the difference of its dimension. We observe that the sign of the second integral term is dependent on the sign of  $\mu$ . On the BCS side we have  $a_s < 0$ , and as the first term is positive, the  $\mu$ -dependent subtractive second term should be positive ( $\mu > 0$ ) and larger than the first term.

The density equation as the dimensionless Fermi-phase-space density  $\lambda_F^3 n$  is:

$$\begin{aligned} \lambda_F^3 n &= \frac{2\pi}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \sqrt{\epsilon_k} \left\{ 1 - \frac{\epsilon_k - \mu}{\epsilon_B(k)} \tanh \frac{\beta \epsilon_B(k)}{2} \right\} \\ &= \underbrace{\left[ \frac{2\pi}{\epsilon_F^{3/2}} \frac{2}{3} \epsilon_k^{3/2} \left\{ 1 - \frac{\epsilon_k - \mu}{\epsilon_B(k)} \tanh \frac{\beta \epsilon_B(k)}{2} \right\} \right]_0^\infty}_{=0} \\ &\quad - \frac{2\pi}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \frac{2}{3} \epsilon_k^{3/2} \frac{\partial}{\partial \epsilon_k} \left( -\frac{\epsilon_k - \mu}{\epsilon_B(k)} \tanh \frac{\beta \epsilon_B(k)}{2} \right) \\ &= \frac{4\pi}{3} \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{3/2}}{\epsilon_B(k)} \left[ \frac{|\Delta|^2}{\epsilon_B^2(k)} \tanh \frac{\beta \epsilon_B(k)}{2} + \frac{(\epsilon_k - \mu)^2}{\epsilon_B^2(k)} \frac{\frac{\beta \epsilon_B(k)}{2}}{\cosh^2 \frac{\beta \epsilon_B(k)}{2}} \right]. \end{aligned} \quad (3.20)$$

We remark that for  $\Delta = 0$ :

$$\lambda_F^3 n|_{\Delta=0} = \frac{2\pi}{3} \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \frac{\beta \epsilon_k^{3/2}}{\cosh^2 \frac{\beta |\epsilon_k - \mu|}{2}}. \quad (3.21)$$

At first the density  $n$  in (3.20) is a variable. This  $n$  should be fixed to find the solution  $\mu$  and  $\Delta$  of the equations (3.19) and (3.20), and the density of interacting uniform Fermi gas is defined to be same as the density of uniform ideal Fermi gas, i.e.  $\lambda_F^3 n = 8\pi/3$ .

#### 3.2.2 Phase transition

With the order parameter and density equations in the thermodynamic ensemble, we can evaluate of the phase transition temperature  $T_c$ . To this end the relevant equations are to be simplified for the case  $\Delta = 0$ , where the phase transition takes place. First, we consider the order parameter equation (3.19), whose integrand for  $\Delta = 0$  is equal to the sum of Fermi–Dirac distribution and  $\mu$ -proportional term as follows:

$$\begin{aligned} \epsilon_k^{-1/2} \left\{ 1 - \frac{\epsilon_k}{\epsilon_B} \right\} \tanh \frac{\beta \epsilon_B}{2} \Big|_{\Delta=0} &= \epsilon_k^{-1/2} \left\{ 1 - \frac{\epsilon_k - \mu + \mu}{|\epsilon_k - \mu|} \right\} \tanh \frac{\beta |\epsilon_k - \mu|}{2} \\ &= \frac{2\epsilon_k^{-1/2}}{e^{\beta(\epsilon_k - \mu)} + 1} - \mu \frac{\epsilon_k^{-1/2}}{|\epsilon_k - \mu|} \tanh \frac{\beta |\epsilon_k - \mu|}{2}. \end{aligned} \quad (3.22)$$

Due to the Fermi–Dirac integral (A.18) we can write the order parameter equation in terms of the polylogarithmic function:

$$\frac{2\pi}{k_F a_s} \Big|_{\Delta=0} = -4\sqrt{\pi} \left( \frac{T}{T_F} \right)^{1/2} \text{Li}_{1/2} \left( -e^{\frac{\mu}{\epsilon_F} / \frac{T}{T_F}} \right) - 2 \frac{\mu}{\epsilon_F} \int_0^\infty dt \frac{\tanh \left( \frac{|t - \frac{\mu}{\epsilon_F}|}{2 \frac{T}{T_F}} \right)}{\sqrt{t} \left| t - \frac{\mu}{\epsilon_F} \right|}. \quad (3.23)$$

When it comes to the particle density equation (3.20), we already remarked in (2.37) that the

### 3.2. BCS–BOGOLIUBOV THEORY

BCS density equation is reduced to the Fermi–Dirac distribution with vanishing order parameter. Again by means of (A.18) and (3.13) it follows immediately:

$$\lambda_F^3 n|_{\Delta=0} = -2\pi^{3/2} \left( \frac{T}{T_F} \right)^{3/2} \text{Li}_{3/2} \left( -e^{\frac{\mu}{\epsilon_F} / \frac{T}{T_F}} \right), \quad (3.24)$$

where we identify  $\lambda_F^3 n = 8\pi/3$  for the homogeneous Fermi gas with two spin species.

For given  $(k_F a_s)^{-1}$ , we can solve (3.23) and (3.24) simultaneously for  $\mu/\epsilon_F$  and  $T/T_F$ . From the solution duplet  $(\mu, T)$  we obtain the critical chemical potential  $\mu(T_c)$  and the critical temperature  $T_c$ . Or alternatively, instead of solving two equations for two parameters we can combine those two equations to:

$$\frac{2\pi}{k_F a_s (\lambda_F^3 n)^{1/3}} \Big|_{T=T_c} = \frac{1}{a_s n^{1/3}} \Big|_{T=T_c} = \frac{-4\text{Li}_{1/2}(-e^{(\beta\mu)_c}) - \frac{2}{\sqrt{\pi}}(\beta\mu)_c \int_{-(\beta\mu)_c}^{\infty} dt \frac{\tanh \frac{t}{2}}{t\sqrt{t+(\beta\mu)_c}}}{\{-2\text{Li}_{3/2}(-e^{(\beta\mu)_c})\}^{1/3}} \quad (3.25)$$

to find the single parameter solution  $(\beta\mu)_c = \beta\mu|_{T=T_c}$ . The solution  $(\beta\mu)_c$  is then inserted into (3.24) to separate  $T_c$  and  $\mu(T_c)$  for given  $(k_F a_s)^{-1}$ . In this approach, we compare the thermal excitation  $\beta\mu$  and the dilute gas parameter  $a_s n^{1/3}$ , i.e. interaction over particle distance, at the phase transition.

In either way we can calculate  $T_c$  and  $\mu(T_c)$  at the phase transition, and with (3.24) we are able to express the critical temperature as:

#### Cooper pairing temperature of the BCS–Bogoliubov theory

$$\frac{T_c}{T_F} = \left( \frac{\lambda_F^3 n}{-2\pi^{3/2} \text{Li}_{3/2} \left( -e^{\frac{\mu(T_c)}{\epsilon_F} / \frac{T_c}{T_F}} \right)} \right)^{2/3}. \quad (3.26)$$

There is a formal similarity between (3.26) and the BEC transition temperature  $T_{\text{BEC}}$ :

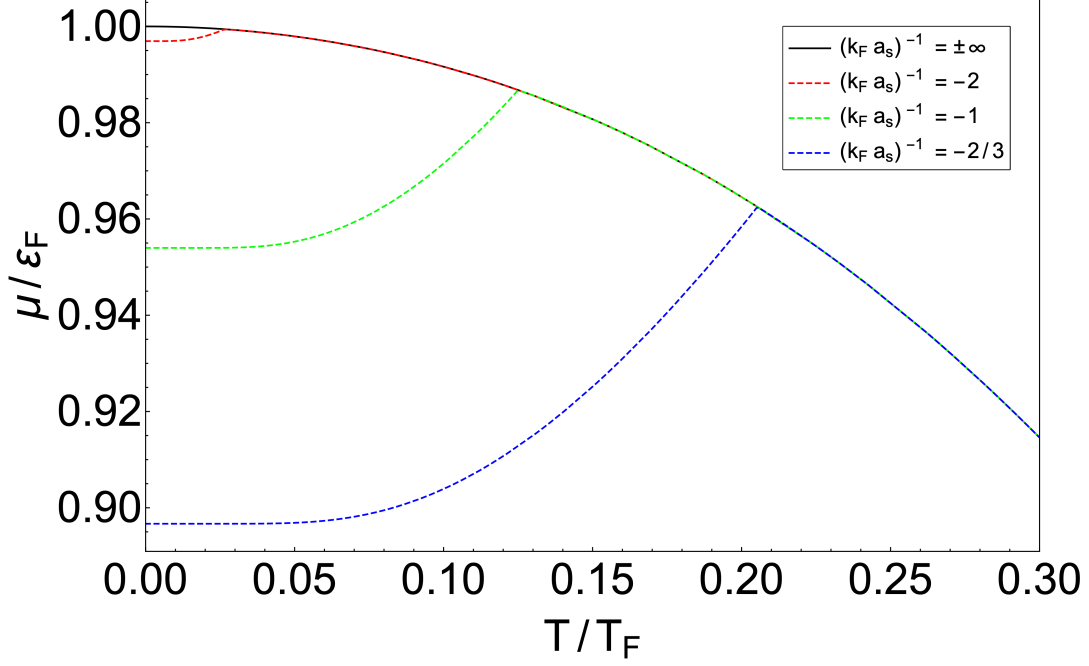
$$\frac{T_{\text{BEC}}}{T} = \left( \frac{\lambda_{\text{boson}}^3 n_{\text{boson}}}{\text{Li}_{3/2}(e^{(\beta\mu)_{\text{BEC}}})} \right)^{2/3} = \left( \frac{\lambda_{\text{boson}}^3 n_{\text{boson}}}{\zeta(3/2)} \right)^{2/3}, \quad (3.27)$$

where  $\lambda_{\text{boson}}$  and  $n_{\text{boson}}$  denote respectively the thermal wavelength and density of the bosonic particle, i.e.  $\lambda_{\text{boson}}^3 n_{\text{boson}}$  is the phase-space-density of the bosonic particles, and  $(\beta\mu)_{\text{BEC}} = 0$  as the BEC happens at  $\mu = 0$ . Similar to the Bose–Einstein condensation temperature, the BCS-phase transition temperature is also proportional to the density to the power of  $2/3$  in uniform gas. However different from the BEC which is irrelevant of interaction and  $\mu$  is arbitrarily small at the transition, finite-valued  $\mu$  at the BCS-phase transition should be calculated depending on the interaction strength using the order parameter equation.

#### 3.2.3 Condensation

Below  $T < T_c$  an interacting Fermi gas undergoes phase transition via Cooper pairing. In the BEC limit Cooper pairs are tightly bound to bosonic dimers, and the phase transition is described

### 3.2. BCS–BOGOLIUBOV THEORY



**Figure 3.1:** Chemical potential  $\mu/\epsilon_F$  of the uniform Fermi gas as a function of the temperature  $T/T_F$  at various scattering parameters  $(k_F a_s)^{-1}$  by the BCS theory.

by the Bose–Einstein condensation. However in the opposite BCS-limit and the crossover region  $|(k_F a_s)^{-1}| < 1$ , the condensation of the Cooper pairs has different meaning than BEC. In either cases, the presence of the condensation is shown by non-vanishing *off-diagonal long-range order (ODLRO)*. To calculate the ODLRO, we define the reduced single-particle density matrix element [62]:

$$\langle k_1 | \hat{\rho} | k_2 \rangle = \text{Tr} \left( \hat{a}_{k_1}^\dagger \hat{\rho} \hat{a}_{k_2} \right) \quad (3.28)$$

between  $k_1$  and  $k_2$  states. The single-particle density matrix in thermal ensemble can be written as:

$$\langle k | \hat{\rho} | k' \rangle = \delta_{k,k'} n_k, \quad (3.29)$$

where  $n_k = [e^{\beta(\epsilon_k - \mu)} \mp 1]^{-1}$  is the average occupation number of the single particle in state  $k$  for bosons or fermions. In the coordinate space we Fourier-transform (3.29) to:

$$\langle \mathbf{x} | \hat{\rho} | \mathbf{x}' \rangle = \frac{1}{V} \sum_{\mathbf{k}} n_k e^{-i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')}, \quad (3.30)$$

and for spinless bosons it is:

$$\langle \mathbf{x} | \hat{\rho} | \mathbf{x}' \rangle_{\text{boson}} = \frac{N_0(T)}{V} + \frac{1}{V} \sum_{\mathbf{k} \neq 0} n_k e^{-i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')} = \frac{N_0(T)}{V} + \int_{\mathbb{R} \setminus \{0\}} \frac{d^3 k}{(2\pi)^3} \frac{1}{e^{\beta(\epsilon_k - \mu)} - 1} e^{-i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')} \quad (3.31)$$

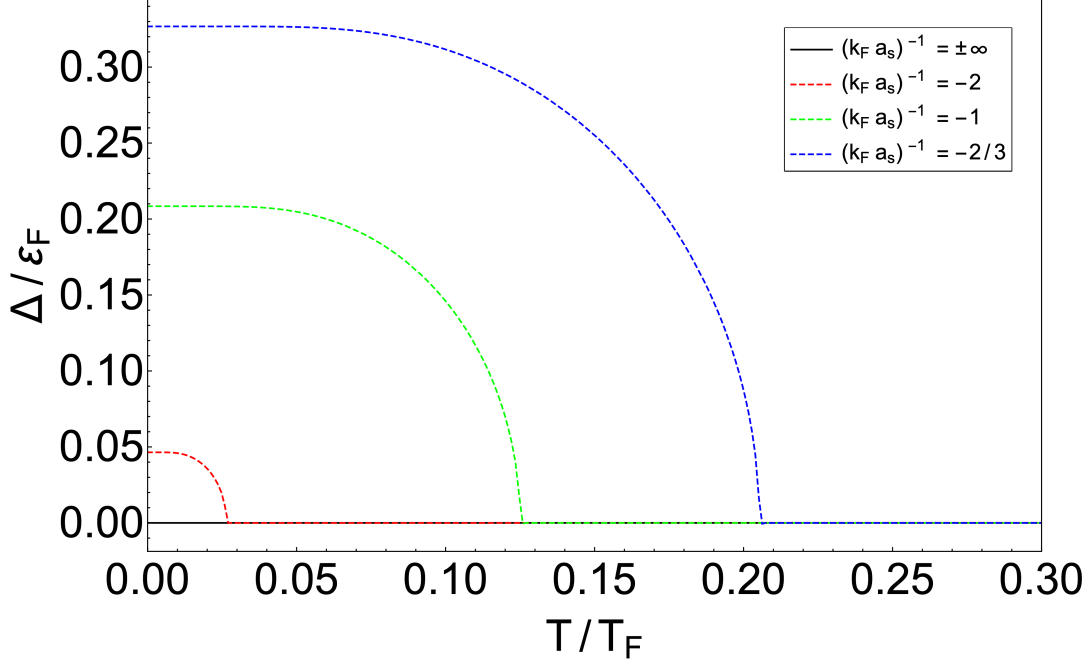
in thermodynamic limit. The second integral term can be calculated to:

$$\int_{\mathbb{R} \setminus \{0\}} \frac{d^3 k}{(2\pi)^3} \frac{1}{e^{\beta(\epsilon_k - \mu)} - 1} e^{-i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')} = \frac{1}{2\pi^2} \int_{\mathbb{R}_{>0}} dk \frac{k^2}{e^{\beta(\epsilon_k - \mu)} - 1} \frac{\sin k|\mathbf{x} - \mathbf{x}'|}{k|\mathbf{x} - \mathbf{x}'|}, \quad (3.32)$$

and in the long-range limit  $|\mathbf{x} - \mathbf{x}'| \rightarrow \infty$  the integrand becomes zero for  $k \neq 0$ , yielding vanishing long-range correlation of thermally excited particles. However the particles with ground state



### 3.2. BCS–BOGOLIUBOV THEORY



**Figure 3.2:** Order parameter  $\Delta/\epsilon_F$  of the uniform Fermi gas as a function of the temperature  $T/T_F$  at various scattering parameters  $(k_F a_s)^{-1}$  by the BCS theory.

survives at the long range because:

$$\lim_{r \rightarrow \infty} \lim_{k \rightarrow 0} \frac{k^2}{e^{k^2} - 1} \frac{\sin kr}{kr} = 1. \quad (3.33)$$

Consequently, ODLRO of spinless bosons is given by:

$$\lim_{|\mathbf{x} - \mathbf{x}'| \rightarrow \infty} \langle \mathbf{x} | \hat{\rho} | \mathbf{x}' \rangle_{\text{boson}} = \begin{cases} n_0(T) & , T < T_{\text{BEC}} \\ 0 & , T \geq T_{\text{BEC}} \end{cases} \quad (3.34)$$

with the BEC transition temperature  $T_{\text{BEC}}$ , exhibiting the non-vanishing macroscopic ground state occupation at  $T < T_{\text{BEC}}$  represented by the *condensate density*  $n_0 = N_0/V$ .

For fermions, the single-body ODLRO is simply:

$$\lim_{|\mathbf{x} - \mathbf{x}'| \rightarrow \infty} \langle \mathbf{x} | \hat{\rho} | \mathbf{x}' \rangle_{\text{fermion}} = 0, \quad (3.35)$$

because the Fermi–Dirac function always vanishes in the long-range limit as a consequence of the Pauli principle. However, a fermionic condensation in terms of ODLRO can be found in the two-body matrix element:

$$\langle k_1, k_2 | \hat{\rho} | k_3, k_4 \rangle = \text{Tr} \left( \hat{a}_{k_1}^\dagger \hat{a}_{k_2}^\dagger \hat{\rho} \hat{a}_{k_3} \hat{a}_{k_4} \right) \quad (3.36)$$

among the operators with  $k_1$ – $k_4$  states. It is shown that ODLRO of fermions is non-vanishing, provided that the Cooper pairs are occupied [62]. The fermionic condensate density  $n_0$  is given by [93]:

$$\lambda_F^3 n_0 = \pi \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \epsilon_k^{1/2} \frac{|\Delta|^2}{\epsilon_B^2(\epsilon_k)} \tanh^2 \frac{\beta \epsilon_B(\epsilon_k)}{2}. \quad (3.37)$$

### 3.2. BCS–BOGOLIUBOV THEORY

In Fig. 3.1 the chemical potential  $\mu/\epsilon_F$  as a function of temperature  $T/T_F$  at various interaction parameter  $(k_F a_s)^{-1}$  is shown.  $\mu$  is same to the ideal Fermi gas  $\mu$  above  $T_c(k_F a_s)$ , and below  $T_c$  it decreases as the temperature drops. Furthermore, the order parameter  $\Delta/\epsilon_F$  as a function of temperature  $T/T_F$  with the various scattering parameters is shown in Fig. 3.2.

#### 3.2.4 Superfluidity

The superfluid density  $n_{\text{sf}}$  is defined in the Landau two-fluid model as the density part that exhibiting different dispersion than the particle-like dispersion  $\epsilon(\mathbf{k}) = \hbar^2 k^2 / (2M)$  in its elementary excitations [96, 29]. To quantify this density, we consider the thermodynamic potential  $\mathcal{F}(\mathbf{u})$  with the Galilean transformation by the velocity  $\mathbf{u}$ :

$$\mathcal{F}(\mathbf{u}) = \mathcal{F} - \mathbf{p} \cdot \mathbf{u}, \quad (3.38)$$

which allows us to calculate the momentum  $\mathbf{p}$  of the system moving with the velocity  $\mathbf{u}$  as:

$$\mathbf{p} = -\frac{\partial \mathcal{F}(\mathbf{u})}{\partial \mathbf{u}} = MV (n_{\text{nf}} \mathbf{v}_{\text{nf}} + n_{\text{sf}} \mathbf{v}_{\text{sf}}), \quad (3.39)$$

where we divide the particle density current  $n\mathbf{v} = n_{\text{nf}} \mathbf{v}_{\text{nf}} + n_{\text{sf}} \mathbf{v}_{\text{sf}}$  with the normal fluid and the superfluid density  $n_{\text{nf}}, n_{\text{sf}}$ , as well as the normal fluid and the superfluid velocity  $\mathbf{v}_{\text{nf}}, \mathbf{v}_{\text{sf}}$ , respectively.

To this end, we apply the translation velocity  $\mathbf{u}$  to the Hamiltonian (2.15) to get:

$$\begin{aligned} \hat{H}_B^{(\text{MF})}(\mathbf{u}) &= \hat{H}_B^{(\text{MF})} + \sum_{\mathbf{k}} \left( \hbar \mathbf{k} \cdot \mathbf{u} \hat{a}_{\mathbf{k},\uparrow}^\dagger \hat{a}_{\mathbf{k},\uparrow} - \hbar \mathbf{k} \cdot \mathbf{u} \hat{a}_{-\mathbf{k},\downarrow}^\dagger \hat{a}_{-\mathbf{k},\downarrow} \right) \\ &= \sum_{\mathbf{k}} \left\{ (\epsilon_k - \mu + \hbar \mathbf{k} \cdot \mathbf{u}) \hat{a}_{\mathbf{k},\uparrow}^\dagger \hat{a}_{\mathbf{k},\uparrow} + (\epsilon_k - \mu - \hbar \mathbf{k} \cdot \mathbf{u}) \hat{a}_{-\mathbf{k},\downarrow}^\dagger \hat{a}_{-\mathbf{k},\downarrow} \right. \\ &\quad \left. + \Delta^* \hat{a}_{-\mathbf{k},\downarrow} \hat{a}_{\mathbf{k},\uparrow} + \Delta \hat{a}_{\mathbf{k},\uparrow}^\dagger \hat{a}_{-\mathbf{k},\downarrow}^\dagger \right\} - V \frac{|\Delta|^2}{g}. \end{aligned} \quad (3.40)$$

With the Nambu-spinor notation:

$$\hat{\Psi}(\mathbf{k}) = \begin{bmatrix} \hat{a}_{\mathbf{k},\uparrow} \\ \hat{a}_{-\mathbf{k},\downarrow}^\dagger \end{bmatrix}, \quad (3.41)$$

the translated Hamiltonian (3.40) reads:

$$\begin{aligned} \hat{H}_B^{(\text{MF})}(\mathbf{u}) &= \sum_{\mathbf{k}} \hat{\Psi}^\dagger(\mathbf{k}) \begin{bmatrix} \epsilon_k - \mu + \hbar \mathbf{k} \cdot \mathbf{u} & \Delta \\ \Delta^* & -(\epsilon_k - \mu - \hbar \mathbf{k} \cdot \mathbf{u}) \end{bmatrix} \hat{\Psi}(\mathbf{k}) \\ &\quad + \sum_{\mathbf{k}} (\epsilon_k - \mu - \hbar \mathbf{k} \cdot \mathbf{u}) - V \frac{|\Delta|^2}{g}, \end{aligned} \quad (3.42)$$

and diagonalisation of the matrix yields the eigenenergies  $\epsilon_B(\mathbf{k}) \pm \hbar \mathbf{k} \cdot \mathbf{u}$ . Nonetheless, the split two eigenenergies contribute same at the end after the sum over  $\mathbf{k}$ , so we can write the resulting thermodynamic potential as:

$$\mathcal{F}_B^{(\text{MF})}(\mathbf{u}) = -V \frac{|\Delta|^2}{g} - \sum_{\mathbf{k}} \{ \epsilon_B(\mathbf{k}) - (\epsilon_k - \mu) \} - 2 \sum_{\mathbf{k}} \log \left( 1 + e^{-\beta(\epsilon_B(\mathbf{k}) + \hbar \mathbf{k} \cdot \mathbf{u})} \right). \quad (3.43)$$

Next, we calculate the momentum of the translated Hamiltonian from the frame of the superfluid at rest ( $\mathbf{v}_{\text{sf}} = \mathbf{0}$ ):

$$\mathbf{p} = -\frac{\partial \mathcal{F}_B^{(\text{MF})}(\mathbf{u})}{\partial \mathbf{u}} = 2 \sum_{\mathbf{k}} \frac{\hbar \mathbf{k}}{e^{\beta(\epsilon_B(\mathbf{k}) + \hbar \mathbf{k} \cdot \mathbf{u})} + 1}, \quad (3.44)$$

### 3.2. BCS–BOGOLIUBOV THEORY

which can be expanded by the Taylor series at  $\mathbf{u} = \mathbf{0}$ :

$$\mathbf{p}(\mathbf{u}) \approx -\frac{2}{3} \sum_{\mathbf{k}} \frac{\beta \hbar^2 k^2 e^{\beta \epsilon_{\mathbf{B}}(\mathbf{k})}}{[e^{\beta \epsilon_{\mathbf{B}}(\mathbf{k})} + 1]^2} \mathbf{u}. \quad (3.45)$$

By taking the translation velocity  $\mathbf{u}$  as a small velocity of the normal fluid  $\mathbf{v}_{\text{nf}}$  we read the momentum as a function of that velocity:  $\mathbf{p}(\mathbf{v}_{\text{nf}}) = MV n_{\text{nf}} \mathbf{v}_{\text{nf}}$ , so we find the normal fluid density:

$$n_{\text{nf}} = \frac{1}{V} \frac{2}{3} \sum_{\mathbf{k}} \frac{\beta \frac{\hbar^2 k^2}{M} e^{\beta \epsilon_{\mathbf{B}}(\mathbf{k})}}{[e^{\beta \epsilon_{\mathbf{B}}(\mathbf{k})} + 1]^2} = \frac{8\pi}{3} \frac{1}{\lambda_{\text{F}}^3} \epsilon_{\text{F}}^{-3/2} \int_0^\infty d\epsilon_k \frac{\beta \epsilon_k^{3/2} e^{\beta \epsilon_{\text{B}}(\epsilon_k)}}{[e^{\beta \epsilon_{\text{B}}(\epsilon_k)} + 1]^2}, \quad (3.46)$$

or in a dimensionless form:

$$\lambda_{\text{F}}^3 n_{\text{nf}} = \frac{2\pi}{3} \epsilon_{\text{F}}^{-3/2} \int_0^\infty d\epsilon_k \frac{\beta \epsilon_k^{3/2}}{\cosh^2 \frac{\beta \epsilon_{\text{B}}(\epsilon_k)}{2}}. \quad (3.47)$$

Finally, the superfluid density is given as the subtraction of the normal fluid density from the total density:

$$n_{\text{sf}} = n - n_{\text{nf}} \quad (3.48)$$

by means of  $n_{\text{nf}}$ . From (3.20), (3.46) and (3.48) then follows:

$$\lambda_{\text{F}}^3 n_{\text{sf}} = \frac{4\pi}{3} \frac{1}{\epsilon_{\text{F}}^{3/2}} \int_0^\infty d\epsilon_k \epsilon_k^{3/2} \frac{|\Delta|^2}{\epsilon_{\text{B}}^3(\epsilon_k)} \left[ \tanh \frac{\beta \epsilon_{\text{B}}(\epsilon_k)}{2} - \frac{\frac{\beta \epsilon_{\text{B}}(\epsilon_k)}{2}}{\cosh^2 \frac{\beta \epsilon_{\text{B}}(\epsilon_k)}{2}} \right]. \quad (3.49)$$

The normal fluid density  $\lambda_{\text{F}}^3 n_{\text{nf}}$  (3.47) is identical to the density with vanishing order parameter  $\lambda_{\text{F}}^3 n|_{\Delta=0}$  (3.21), implying vanishment of the superfluid density for  $\Delta = 0$ , thus the system becomes normal fluid from  $T \geq T_c$ . Also with (3.49) it is obvious that  $n_{\text{sf}} = 0$  at  $\Delta = 0$ . This means that, in mean-field theory, pair formation and phase coherence, i.e., superfluidity happens at the same time. However it should be reminded that the coincidence of the Cooper pair breaking temperature  $T_c$  with the superfluidity critical temperature is not generally true: for instance, when the fluctuation is taken into account, in the BEC regime it is possible that the pairs are robust but the superfluidity is destroyed by phase fluctuations. Moreover, due to  $\lim_{T \downarrow 0} n_{\text{nf}}(T) = 0$  it is  $n = n_{\text{sf}}$  at  $T = 0$ . Due to these observations, in mean-field theories, the parameter regime below  $T_c$  in the phase diagram can be called as superfluid phase.

#### 3.2.5 Ground state

We consider the zero-temperature limit case. In the low-temperature limit, the hyperbolic functions in order parameter equation (3.19) and density equation (3.20) reduce to numerical constants, and the resulting equations are:

$$\lim_{T \downarrow 0} \frac{2\pi}{k_{\text{F}} a_{\text{s}}} = \frac{4|\Delta|^2}{\sqrt{\epsilon_{\text{F}}}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{1/2}}{[(\epsilon_k - \mu)^2 + |\Delta|^2]^{3/2}} - \frac{2\mu}{\sqrt{\epsilon_{\text{F}}}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{-1/2}}{[(\epsilon_k - \mu)^2 + |\Delta|^2]^{1/2}} \quad (3.50)$$

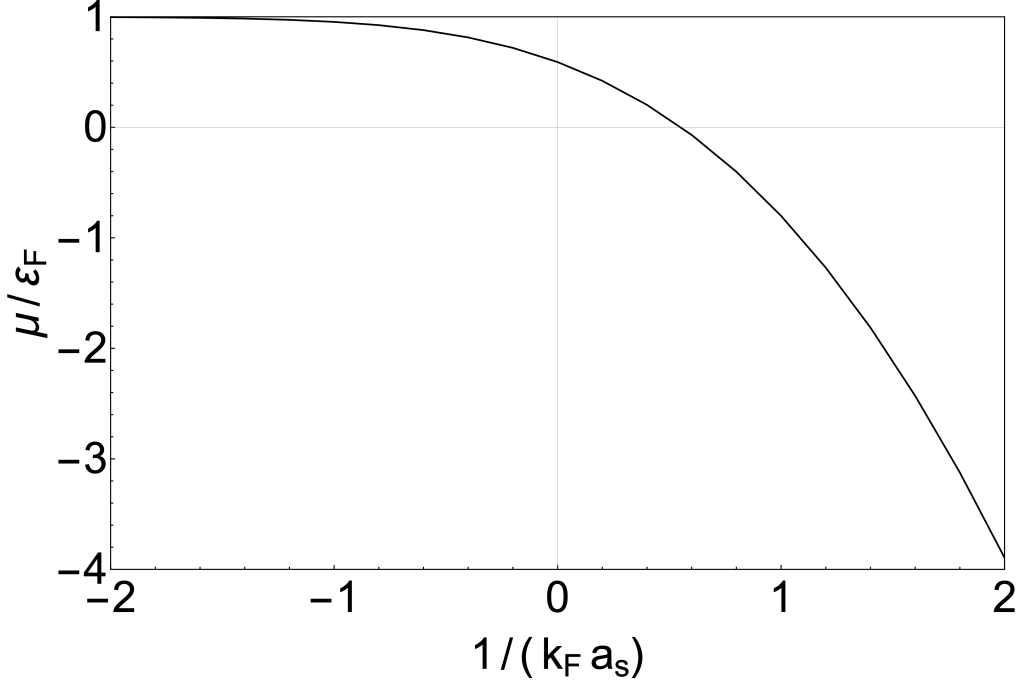
and

$$\lim_{T \downarrow 0} \lambda_{\text{F}}^3 n = \frac{4\pi |\Delta|^2}{3\epsilon_{\text{F}}^{3/2}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{3/2}}{[(\epsilon_k - \mu)^2 + |\Delta|^2]^{3/2}}. \quad (3.51)$$

Observing the common form of the above equations, we are now interested in the parametric integral:

$$I_{p,q}(\mu, \Delta) = \epsilon_{\text{F}}^{-1-p+2q} \int_0^\infty d\epsilon_k \frac{\epsilon_k^p}{[(\epsilon_k - \mu)^2 + |\Delta|^2]^q} \quad (3.52)$$

### 3.2. BCS–BOGOLIUBOV THEORY



**Figure 3.3:** Chemical potential  $\mu/\epsilon_F$  of the uniform Fermi gas as a function of the scattering parameter  $(k_F a_s)^{-1}$  at the ground state by the BCS–Bogoliubov theory, calculated with (3.54) and (3.55).

for  $p, q \in \mathbb{Q} \setminus \{0\}$ . The value of the integration (3.52) can be given in the form of known function. By means of (B.35), we can write its solution as:

$$I_{p,q}(\mu, \Delta) = \frac{B(1+p, -1-p+2q)}{\left[ \sqrt{\left(\frac{\mu}{\epsilon_F}\right)^2 + \left(\frac{|\Delta|}{\epsilon_F}\right)^2} \right]^{-1-p+2q}} {}_2F_1 \left( 1+p, -1-p+2q; \frac{1}{2}+q; \frac{1}{2} \left[ 1 + \frac{\mu}{\sqrt{\mu^2 + |\Delta|^2}} \right] \right) \quad (3.53)$$

for  $0 < \text{Re}(p+1) < 2 \text{Re}(q)$ . Here we have introduced two functions:  $B(w_1, w_2)$  is the Euler-beta function, and  ${}_2F_1(a, b; c; z)$  stands for the hypergeometric function, see Appendix B. Note that the variable  $(1 + \mu[\mu^2 + |\Delta|^2]^{-1/2})/2$  takes value between 0 and 1 where  $|\Delta| > 0$  at the BCS-ground state, which is in the convergence radius of the Gauss series (B.3).

With (3.53) the order parameter and density equations are expressed as:

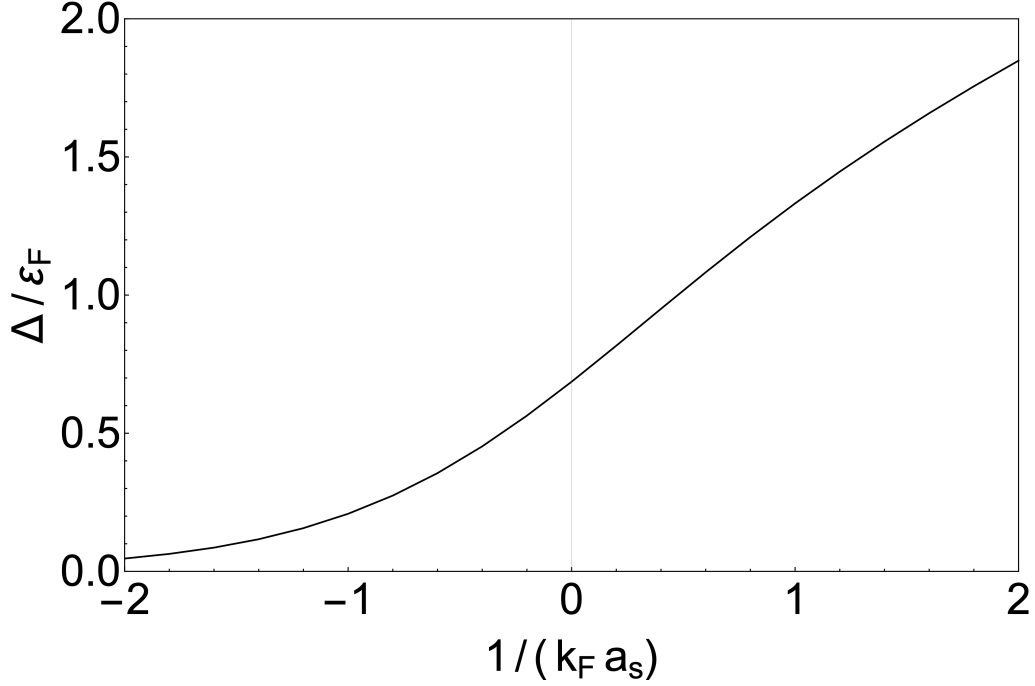
$$\begin{aligned} \lim_{T \downarrow 0} \frac{2\pi}{k_F a_s} &= \frac{\pi}{2} \left( \frac{|\Delta|}{\epsilon_F} \right)^{1/2} \left( \frac{|\Delta|}{\sqrt{\mu^2 + |\Delta|^2}} \right)^{3/2} {}_2F_1 \left( \frac{3}{2}, \frac{3}{2}; 2; \frac{1}{2} \left[ 1 + \frac{\mu}{\sqrt{\mu^2 + |\Delta|^2}} \right] \right) \\ &\quad - 2\pi \left( \frac{\mu}{\epsilon_F} \right)^{1/2} \left( \frac{\mu}{\sqrt{\mu^2 + |\Delta|^2}} \right)^{1/2} {}_2F_1 \left( \frac{1}{2}, \frac{1}{2}; 1; \frac{1}{2} \left[ 1 + \frac{\mu}{\sqrt{\mu^2 + |\Delta|^2}} \right] \right) \end{aligned} \quad (3.54)$$

and

$$\lim_{T \downarrow 0} \lambda_F^3 n = \frac{\pi^2}{2} \left( \frac{|\Delta|}{\epsilon_F} \right)^{3/2} \left( \frac{|\Delta|}{\sqrt{\mu^2 + |\Delta|^2}} \right)^{1/2} {}_2F_1 \left( \frac{5}{2}, \frac{1}{2}; 2; \frac{1}{2} \left[ 1 + \frac{\mu}{\sqrt{\mu^2 + |\Delta|^2}} \right] \right). \quad (3.55)$$

As noted in subsec. 3.2.4, the density at the ground state coincides with the superfluid density.

### 3.3. HARTREE THEORY



**Figure 3.4:** Order parameter  $\Delta/\epsilon_F$  of the uniform Fermi gas as a function of the scattering parameter  $(k_F a_s)^{-1}$  at the ground state by the BCS–Bogoliubov theory, calculated with (3.54) and (3.55).

In Fig. 3.3 and Fig. 3.4 the magnitude of the chemical potential and order parameter at the ground state are shown. In the BCS-limit  $(k_F a_s)^{-1} \rightarrow -\infty$  system behaves like non-interacting fermions, i.e.,  $\Delta$  converges to an arbitrary small magnitude and  $\mu$  reaches to  $\epsilon_F$ . Into the BEC-limit  $(k_F a_s)^{-1} \rightarrow +\infty$  the theory describes a bosonic gas qualitatively, where the bound energy of tightly bound Cooper pairs is represented as a large order parameter, and chemical potential changes its sign to negative, like in a bosonic system.

### 3.3 Hartree theory

While the BCS theory explains the phase transition from the interaction of fermions, it neglects the normal interaction between them. To study this, we now turn our interest to the *Hartree theory*. Like the case of the BCS theory, we consider the equally spin-populated case:

$$n_\uparrow = n_\downarrow \quad \Leftrightarrow \quad \Gamma_\uparrow = \Gamma_\downarrow = \Gamma, \quad (3.56)$$

where the Hamiltonian becomes (2.61) and the free energy is given by:

$$\mathcal{F}_H^{(\text{MF})} = -V \frac{\Gamma^2}{g} - \frac{2}{\beta} \sum_{\mathbf{k}} \log \left[ 1 + e^{-\beta(\epsilon_{\mathbf{k}} - \mu + \Gamma)} \right]. \quad (3.57)$$

In this case, the second term of the extremising equations (2.57) and (2.58) vanishes and the Hartree energy  $\Gamma$  is proportional to the particle density:

$$\frac{\Gamma}{g} = \langle \hat{a}_{\mathbf{k},\sigma}^\dagger \hat{a}_{\mathbf{k},\sigma} \rangle = \frac{1}{2} \frac{1}{V} \left( -\frac{\partial \mathcal{F}}{\partial \mu} \right) = \frac{n}{2}, \quad (3.58)$$

where (3.58) is a self-consistency equation of the Hartree energy  $\Gamma$ . In the thermodynamical limit, the self-consistency equation reads:

$$\frac{\Gamma}{g} = \frac{n}{2} = \int \frac{d^3 k}{(2\pi)^3} \frac{1}{e^{\beta(\epsilon_{\mathbf{k}} - \mu + \Gamma)} + 1}. \quad (3.59)$$

### 3.3. HARTREE THEORY

The resulting relation  $\Gamma = gn/2$  is in agreement with [58], and also known as the Hartree shift in solid state physics [66].

#### 3.3.1 Thermodynamic ensemble

In the presence of the Hartree interaction term  $\Gamma = gn/2$ , the chemical potential should be modified to the density-dependent one:

$$\mu_H = \mu - g\frac{n}{2}, \quad (3.60)$$

which depends on the density  $n$ , the interaction parameter  $g$  and the temperature  $T$ . Different from the ideal Fermi gas, the chemical potential of interacting fermions is not equal to the Fermi energy  $\epsilon_F$  at  $T = 0$  [51]. This deviation of ground state chemical potential from  $\epsilon_F$  is also true for the BCS theory, but above the  $T_c$  the chemical potential  $\mu$  is same to the ideal Fermi gas. In contrast,  $\mu = \mu_H + gn/2$  in the Hartree theory is different from the ideal Fermi gas chemical potential throughout any temperatures and finite interaction strengths.

With the Hartree-shifted chemical potential  $\mu_H$  we rewrite the density integration:

$$n = 2 \int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta(\epsilon_k - \mu_H)} + 1} = \frac{\sqrt{2}M^{3/2}}{\pi^2\hbar^3} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{1/2}}{z_H^{-1}e^{\beta\epsilon_k} + 1}. \quad (3.61)$$

with  $z_H = e^{\beta\mu_H}$  assigning the fugacity of the interacting Fermi gas with Hartree term  $\Gamma$ . By means of the Fermi-Dirac integral (A.18) the density equation (3.61) is to be written in terms of the polylogarithmic function<sup>2</sup>:

$$\lambda^3 n = -2\text{Li}_{3/2}(-e^{\beta\mu_H}), \quad (3.62)$$

or in the Fermi-scaled physical quantities we obtain the density equation of state:

$$\lambda_F^3 n = -2\pi^{3/2} \left(\frac{T}{T_F}\right)^{3/2} \text{Li}_{3/2}\left(-e^{\left(\frac{\mu}{\epsilon_F} - k_F a_s \frac{\lambda_F^3 n}{2\pi^2}\right) \frac{T}{T_F}}\right), \quad (3.63)$$

which is a self-consistent equation for the Fermi-phase-space-density  $\lambda_F^3 n$  as a dimensionless particle density.

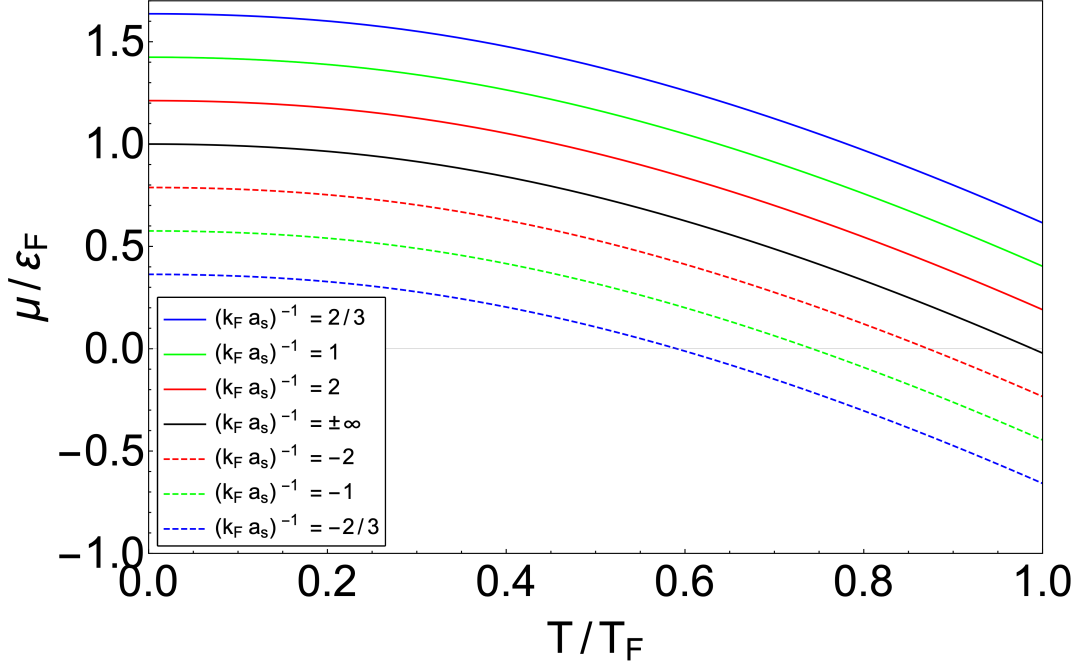
The chemical potential  $\mu$  of the ideal Fermi gas is equal to  $\epsilon_F$  at  $T = 0$ . While in the ideal Fermi gas model  $\mu$  only depends on temperature, it becomes interaction dependent by the Hartree theory. In case of a homogeneous system with the uniform constant density  $\lambda_F^3 n = 8\pi/3$ , the temperature dependence of the chemical potential appears as a constant shift to  $\mu$  of the ideal Fermi gas, as shown in the figure 3.5. This shift is called the *Hartree-shift*.

In Fig. 3.5 we read that the chemical potential becomes smaller with the increasing temperature and more attractive interaction. But in the uniform gas we do not observe the related effects, because while the density of the uniform gas is constant and only  $\mu$  varies depending  $T$  and  $k_F a_s$ , one can not directly measure the chemical potential. The thermal- and interaction effects become visible in an inhomogeneous system, as we will see in chapter 4.

---

<sup>2</sup>We remark that the density equation (3.62) also holds for bosons, whereas one uses bosonic polylogarithm  $\text{Li}_s(e^{\beta\mu})$  as in [67].

### 3.3. HARTREE THEORY



**Figure 3.5:** Chemical potential  $\mu/\epsilon_F$  of the uniform Fermi gas as a function of the temperature  $T/T_F$  at various scattering parameters  $(k_F a_s)^{-1}$  by the Hartree theory. C.f. [54], p.183.

Moreover, for the Hartree theory, also the free energy (3.57) can be given in an exact form. First, the constant energy shift is straightforward:

$$-V \frac{\Gamma^2}{g} = -\frac{V}{g} \left(g \frac{n}{2}\right)^2 = -N \frac{\Gamma}{2}. \quad (3.64)$$

The sum, i.e. the integration in the thermodynamic limit, can be integrated by parts:

$$\begin{aligned} -\frac{2}{\beta} \sum_{\mathbf{k}} \log \left(1 + e^{-\beta(\epsilon_k - \mu + \Gamma)}\right) &= -\frac{1}{\beta} \frac{4\pi}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \epsilon_k^{1/2} \log \left(1 + e^{-\beta(\epsilon_k - \mu + \Gamma)}\right) \\ &= -\frac{1}{\beta} \frac{4\pi}{\epsilon_F^{3/2}} \left[ \overbrace{\frac{2}{3} \epsilon_k^{3/2} \log \left(1 + e^{-\beta(\epsilon_k - \mu + \Gamma)}\right)}^{=0} \right]_0^\infty \\ &\quad - \int_0^\infty d\epsilon_k \frac{2}{3} \epsilon_k^{3/2} \frac{1}{e^{\beta(\epsilon_k - \mu + \Gamma)} + 1} \\ &= -\frac{1}{\beta} 2\pi^{3/2} \left(\frac{T}{T_F}\right)^{5/2} \text{Li}_{5/2} \left( -e^{\left(\frac{\mu}{\epsilon_F} - k_F a_s \frac{\lambda_F^3 n}{2\pi^2}\right) / \frac{T}{T_F}} \right), \end{aligned} \quad (3.65)$$

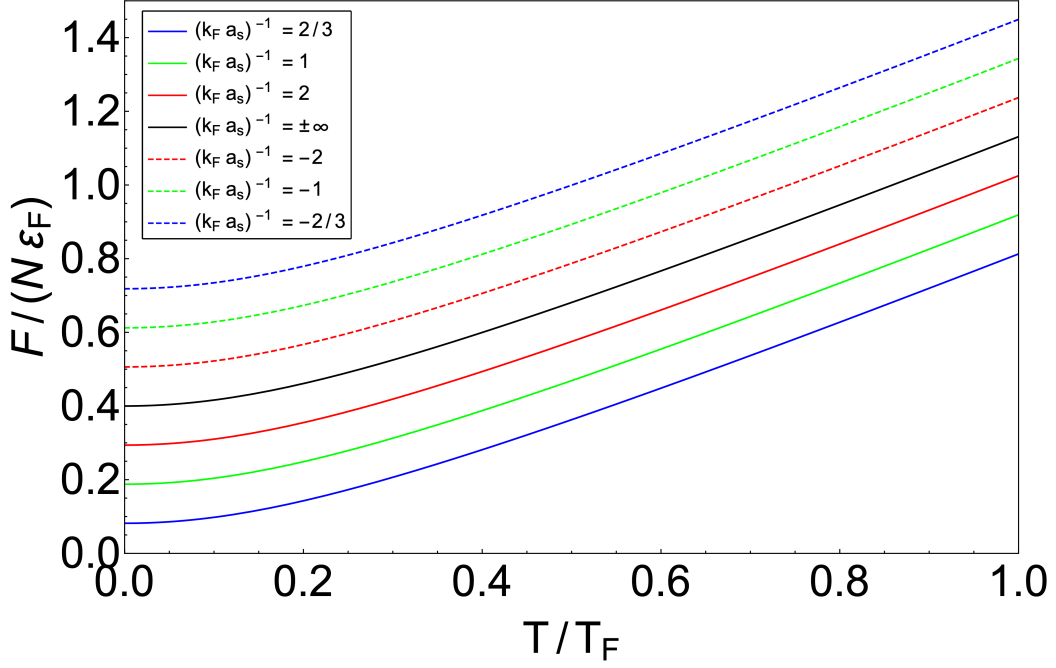
that together yield:

$$\frac{\mathcal{F}_H^{(\text{MF})}}{\epsilon_F} = -N k_F a_s \frac{\lambda_F^3 n}{4\pi^2} - 2\pi^{3/2} \left(\frac{T}{T_F}\right)^{5/2} \text{Li}_{5/2} \left( -e^{\left(\frac{\mu}{\epsilon_F} - k_F a_s \frac{\lambda_F^3 n}{2\pi^2}\right) / \frac{T}{T_F}} \right) \quad (3.66)$$

With  $N = -\partial \mathcal{F}_H^{(\text{MF})} / \partial \mu = 2\pi^{3/2} (T/T_F)^{3/2} \text{Li}_{3/2}(-e^{-\beta\mu_H})$  and  $\lambda_F^3 n = 8\pi/3$ , it is:

$$\frac{\mathcal{F}_H^{(\text{MF})}}{N \epsilon_F} = -\frac{2}{3\pi} k_F a_s + \frac{T}{T_F} \frac{\text{Li}_{5/2} \left( -e^{\left(\frac{\mu}{\epsilon_F} - \frac{4}{3\pi} k_F a_s\right) / \frac{T}{T_F}} \right)}{\text{Li}_{3/2} \left( -e^{\left(\frac{\mu}{\epsilon_F} - \frac{4}{3\pi} k_F a_s\right) / \frac{T}{T_F}} \right)}. \quad (3.67)$$

### 3.4. HARTREE–BOGOLIUBOV THEORY



**Figure 3.6:** Free energy pro particle  $\mathcal{F}/(N\epsilon_F)$  of the uniform Fermi gas as a function of the temperature  $T/T_F$  at various scattering parameters  $(k_F a_s)^{-1}$  by the Hartree theory calculated with (3.67).

The free energy of the Hartree theory is shown in Fig. 3.6.

#### 3.3.2 Ground state

The 0th order term in the approximation (A.33) corresponds to the degenerate interacting Fermi gas in the normal fluid phase. In this case, the Hartree density equation is reduced to:

$$\frac{4}{3\pi} k_F a_s \frac{\lambda_F^3 n}{8\pi/3} + \left( \frac{\lambda_F^3 n}{8\pi/3} \right)^{2/3} - \frac{\mu}{\epsilon_F} = 0. \quad (3.68)$$

For the constant uniform Fermi gas density  $\lambda_F^3 n = 8\pi/3$ , the chemical potential in terms of the scattering parameter  $k_F a_s$  reads:

$$\frac{\mu}{\epsilon_F} = 1 + \frac{4}{3\pi} k_F a_s, \quad (3.69)$$

which with  $k_F a_s = 0$  yields the ideal Fermi gas relation  $\mu = \epsilon_F$ . The linear Hartree-shift in (3.69) also holds for finite temperature, as one can read in Fig. 3.5, and agrees with the 1st order correction term in the fluctuation theory [59]. See Fig. 3.7.

### 3.4 Hartree–Bogoliubov theory

We have investigated the BCS theory and the Hartree theory in the preceding sections 3.2 and 3.3. The HB theory is generalisation of those theories, where both the normal interaction of the Hartree channel and the Cooper pairing of the Bogoliubov channel are included and the order parameter equation and the density equation are self-consistently calculated.



### 3.4. HARTREE–BOGOLIUBOV THEORY

#### 3.4.1 Thermodynamic ensemble

The renormalised order parameter equation of the HB theory in thermal ensemble can be simply obtained from the BCS theory and Hartree theory as their unification. Substitution  $\mu \rightarrow \mu_H = \mu - gn/2$  in (3.19) results directly:

$$\begin{aligned} \frac{2\pi}{k_F a_s} = & \frac{4}{\sqrt{\epsilon_F}} \int_0^\infty d\epsilon_k \frac{\sqrt{\epsilon_k}}{\epsilon_{HB}(\epsilon_k)} \left[ \frac{|\Delta|^2}{\epsilon_{HB}^2(\epsilon_k)} \tanh \frac{\beta \epsilon_{HB}(\epsilon_k)}{2} + \frac{(\epsilon_k - \mu_H)^2}{\epsilon_{HB}^2(\epsilon_k)} \frac{\frac{\beta \epsilon_{HB}(\epsilon_k)}{2}}{\cosh^2 \frac{\beta \epsilon_{HB}(\epsilon_k)}{2}} \right] \\ & - 2 \frac{\mu_H}{\sqrt{\epsilon_F}} \int_0^\infty d\epsilon_k \frac{\tanh \frac{\beta \epsilon_{HB}(\epsilon_k)}{2}}{\sqrt{\epsilon_k} \epsilon_{HB}(\epsilon_k)}, \end{aligned} \quad (3.70)$$

where the HB dispersion  $\epsilon_{HB}(\mathbf{k})$  introduced in (2.69) reads here  $\epsilon_{HB}(\epsilon_k) = [(\epsilon_k - \mu_H)^2 + |\Delta|^2]^{1/2}$ . Also the HB density equation can be derived as the same substitution  $\mu \rightarrow \mu_H$  for the BCS density equation (3.20):

$$\lambda_F^3 n = \frac{4\pi}{3} \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{3/2}}{\epsilon_{HB}(\epsilon_k)} \left[ \frac{|\Delta|^2}{\epsilon_{HB}^2(\epsilon_k)} \tanh \frac{\beta \epsilon_{HB}(\epsilon_k)}{2} + \frac{(\epsilon_k - \mu_H)^2}{\epsilon_{HB}^2(\epsilon_k)} \frac{\frac{\beta \epsilon_{HB}(\epsilon_k)}{2}}{\cosh^2 \frac{\beta \epsilon_{HB}(\epsilon_k)}{2}} \right]. \quad (3.71)$$

The order parameter equation (3.70) and the density equation (3.71) are generalised equations for determination of the order parameter  $\Delta$  and the Hartree-shifted chemical potential  $\mu_H$  for given temperature  $T/T_F$  and scattering parameter  $(k_F a_s)^{-1}$ .

Different from the BCS density equation (3.20), which only indirectly takes account the interaction via Cooper pairing below phase transition temperature, the density equation (3.71) includes explicitly the interaction parameter  $k_F a_s$  both the normal- and the superfluid phases. In normal fluid phase it is identical to the Hartree density equation (3.63), and in superfluid phase the order parameter- and the density equations together describes fermions interacting each other via normal interaction as well as anomalous pairing. Although there is no physically observable difference between BCS- and HB theory in uniform gas, behaviour of inhomogeneous system is differently predicted according to different theories.

#### 3.4.2 Phase transition

In the equations (3.70) and (3.71) we formally substituted the chemical potential  $\mu$  of the BCS theory by the Hartree-shifted chemical potential  $\mu_H = \mu - gn/2$ . This implies that the critical temperature  $T_c$  of the HB theory is same to  $T_c$  of the BCS theory. One can read this consequence as follows.

As same as the BCS theory, the critical temperature of the HB theory is to be evaluated with the order parameter equation at the vanishing  $\Delta$ :

$$\left. \frac{2\pi}{k_F a_s} \right|_{\Delta=0} = -4\sqrt{\pi} \left( \frac{T}{T_F} \right)^{1/2} \text{Li}_{1/2} \left( -e^{\frac{\mu_H}{\epsilon_F} / \frac{T}{T_F}} \right) - 2 \frac{\mu_H}{\epsilon_F} \int_0^\infty dt \frac{\tanh \left( \frac{\left| t - \frac{\mu_H}{\epsilon_F} \right|}{2 \frac{T}{T_F}} \right)}{\sqrt{t} \left| t - \frac{\mu_H}{\epsilon_F} \right|} \quad (3.72)$$

analog to (3.23), and the density equation:

$$\lambda_F^3 n|_{\Delta=0} = -2\pi^{3/2} \left( \frac{T}{T_F} \right)^{3/2} \text{Li}_{3/2} \left( -e^{\frac{\mu_H}{\epsilon_F} / \frac{T}{T_F}} \right) \quad (3.73)$$

similar to (3.24). In the equations  $\mu$  is just formally substituted by  $(\beta\mu)_c$ . However, since the equations for determination of  $T_c$  are exactly same, so are the solution,  $(T_c, \mu(T_c)) = (T_c, \mu_H(T_c))$ .

### 3.4. HARTREE–BOGOLIUBOV THEORY

This means especially that the transition temperature remains unchanged by addition of the Hartree term. The phase transition temperature  $T_c$  in uniform gas of the BCS theory as well as the HB theory, which are same, is shown as the black curve in Fig. 4.1.

While the phase transition temperature  $T_c$  in homogeneous system is a smooth curve at unitarity  $(k_F a_s) = 0$  and the BEC-regime, it is exponentially divergent into the BEC-limit. This misbehaviour is an artefact from the mean-field approximation of the Bogoliubov pairing channel, which breaks down for strong interaction beyond the weakly interacting BCS-regime.

#### 3.4.3 Ground state

Finally, we discuss about the interacting fermions at the ground state. As derived in the subsection 3.2.5, the parameters  $\mu$  and  $\Delta$  at the ground state can be calculated with the zero-temperature order parameter equation and the density equation:

$$\lim_{T \downarrow 0} \frac{2\pi}{k_F a_s} = \frac{\pi}{2} \left( \frac{|\Delta|}{\epsilon_F} \right)^{1/2} \left( \frac{|\Delta|}{\sqrt{\mu_H^2 + |\Delta|^2}} \right)^{3/2} {}_2F_1 \left( \frac{3}{2}, \frac{3}{2}; 2; \frac{1}{2} \left[ 1 + \frac{\mu_H}{\sqrt{\mu_H^2 + |\Delta|^2}} \right] \right) - 2\pi \left( \frac{\mu_H}{\epsilon_F} \right)^{1/2} \left( \frac{\mu_H}{\sqrt{\mu_H^2 + |\Delta|^2}} \right)^{1/2} {}_2F_1 \left( \frac{1}{2}, \frac{1}{2}; 1; \frac{1}{2} \left[ 1 + \frac{\mu_H}{\sqrt{\mu_H^2 + |\Delta|^2}} \right] \right), \quad (3.74)$$

$$\lim_{T \downarrow 0} \lambda_F^3 n = \frac{\pi^2}{2} \left( \frac{|\Delta|}{\epsilon_F} \right)^{3/2} \left( \frac{|\Delta|}{\sqrt{\mu_H^2 + |\Delta|^2}} \right)^{1/2} {}_2F_1 \left( \frac{5}{2}, \frac{1}{2}; 2; \frac{1}{2} \left[ 1 + \frac{\mu_H}{\sqrt{\mu_H^2 + |\Delta|^2}} \right] \right) \quad (3.75)$$

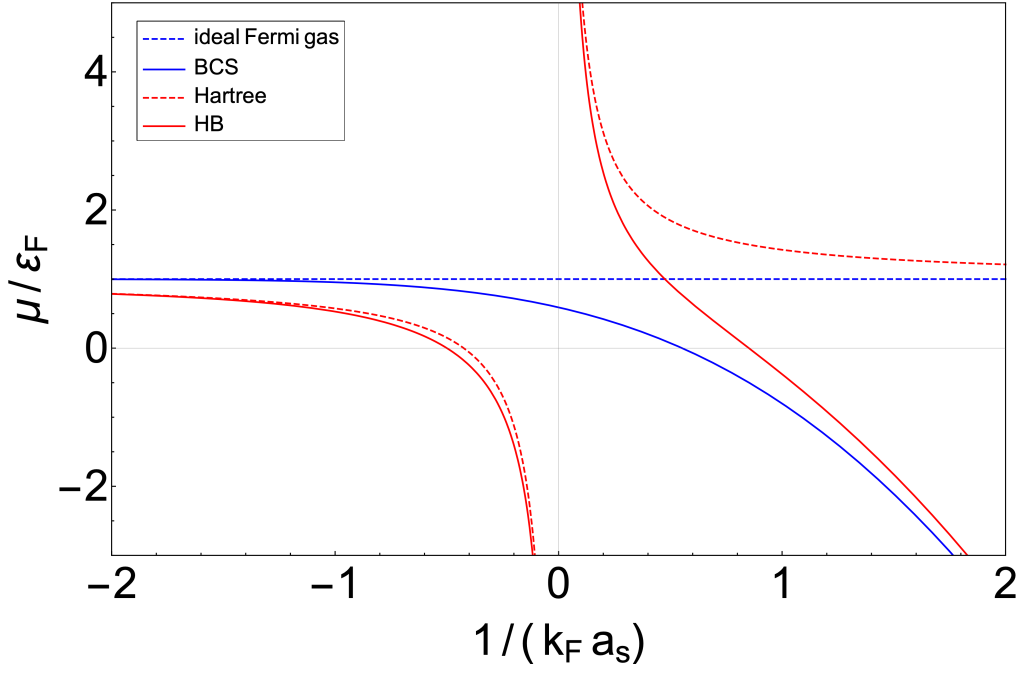
respectively, where we substitute  $\mu$  in the BCS-equations (3.54), (3.55) by  $\mu_H$  to include the Hartree shift of the HB theory.

To visualise the contributions of different interaction channels, we plot the chemical potential  $\mu$  in the absent of thermal excitations as a theoretically comparable quantity, see Fig. 3.7. We observe that in the BCS-regime the deviations from the ideal Fermi gas leading to the lower  $\mu$  from all mean-field interaction theories. In that regards the Hartree term contributes more larger than the BCS order parameter, especially for the weakly interacting regime of  $(k_F a_s)^{-1} < -1$ , Hartree contribution is dominant. And in the more strongly interacting BCS-unitary regime, of  $(k_F a_s)^{-1} \approx -1$  the order parameter contribution becomes relevant.

In the Hartree theory,  $\mu$  is convergent to the ideal Fermi gas result  $\mu = \epsilon_F$  into the BCS- and BEC limit  $(k_F a_s)^{-1} \rightarrow \pm\infty$ . This symmetric behaviour is in contrast with the BCS theory, since in the Hartree theory there is no bound Cooper molecules on the BEC-side and the both limits  $(k_F a_s)^{-1} \rightarrow \pm\infty$ , i.e.,  $k_F a_s \rightarrow \pm 0$  just represents weak repulsive- or attractive interaction between fermions without any bound states even at the ground state. At unitarity  $(k_F a_s)^{-1} = 0$ , the Hartree term introduces a singularity. As these observations show, the concepts developed in the BEC-BCS crossover can not be directly applied for the Hartree theory, since the Hartree theory completely misses the bound state of interacting fermions in three-dimensional system.

Different from the singular behaviour of the Hartree theory at unitarity, calculation with the BCS theory results a finite value, and  $\mu$  extends smoothly to the BEC limit. That being said, the seemingly innocent mean-field BCS theory also fails in the BEC-regime with its divergent behaviour to the BEC-limit  $(k_F a_s)^{-1} \rightarrow +\infty$ , and its finite results at unitarity are also quantitatively inaccurate compared to the results from Monte-Carlo calculations and experiments [59]. Therefore it is not appropriate to apply directly the mean-field theories beyond the BCS-regime,

### 3.4. HARTREE–BOGOLIUBOV THEORY



**Figure 3.7:** Chemical potential  $\mu/\epsilon_F$  of the uniform Fermi gas as a function of the scattering parameter  $(k_F a_s)^{-1}$  at the ground state by different mean-field theories: BCS–Bogoliubov (BCS) theory calculated with (3.54), (3.55), Hartree theory calculated with (3.69), and Hartree–Bogoliubov (HB) calculated with (3.74), (3.75).

regardless of the choice of interaction channels. In that respect, the singular behaviour of the mean-field Hartree and HB theory is not a real problem, as far as one sticks with the validity range of the mean-field theories, the BCS-regime.

### 3.4. HARTREE–BOGOLIUBOV THEORY

## Chapter 4

# Fermi Gas in Harmonic Trap

In laboratories, ultracold atoms experiments are usually conducted in a confining inhomogeneous potential. Especially, harmonic trap is a standard tool to trap atomic gases. From that motivated, in this chapter we investigate the system in the three-dimensional harmonic trapping potential:

$$V_{\text{HO}}(\mathbf{x}) = \frac{M}{2} \sum_{i=1}^3 \omega_i^2 x_i^2, \quad (4.1)$$

where  $\omega_i$  is the trap frequency in the direction  $x_i$ .

First of all, the addition of the harmonic trap potential (4.1) has a practical reason, namely to confine the atomic cloud during cooling and measurements. But also there are theoretical interests to study the trapping potential. It turns out that the existence of the spatial dependent external potential  $V(\mathbf{x})$  substantially alters behaviours of the system in compared to the uniform gas case. In the uniform gas case, the Hartree term only adds a physically irrelevant uniform energy shift. However in this chapter, we show that the interplay between Hartree term and a spatial inhomogeneity indeed leads to predictions of experimentally measurable quantities, e.g. modified density profile depending on interaction, which is accompanied by changes of the spatially dependent transition temperature.

Concerning literatures, there is already a publication for the harmonically trapped fermions with the Hartree term, but in the study the Bogoliubov channel was not included [56]. Also the HFB theory in a trap was studied, but the calculation was limited to the isotropic harmonic trap [57, 58]. In contrast to that, our theoretical study will offer a theoretical description for interacting Fermi gas with both Hartree and Bogoliubov channels confined by a generic form of a harmonic potential.

### 4.1 Local Density Approximation

Analog to the thermodynamic limit we have been used in the uniform gas study, which is used for approximating the sum of discrete energy state by continuous integration, the discrete energy levels introduced by the harmonic potential (4.1) can be approximated to continuous energy states by the *local-density approximation* (LDA). When a spatial background potential  $V(\mathbf{x})$  varies slowly than the relevant discrete energy levels introduced by the potential in the coordinate space, one can treat the coordinate-dependent potential as a locally uniform one at the coordinate  $\mathbf{x}$ . Accordingly, we can modify the chemical potential of the uniform fermions gas to spatial dependent chemical potential according to [51]:

$$\mu(\mathbf{x}) = \mu - V_{\text{HO}}(\mathbf{x}). \quad (4.2)$$

## 4.2. HARMONIC TRAP POTENTIAL

With the free energy  $F$  and the spatial dependent particle density  $n(\mathbf{x})$ ,  $\mu(\mathbf{x})$  is determined by the variational relation upon the grand canonical ensemble:

$$\frac{\delta \mathcal{F}}{\delta n(\mathbf{x})} = \frac{\delta(F - \mu N)}{\delta n(\mathbf{x})} = 0, \quad (4.3)$$

which yields the functional expression of density  $n(\mathbf{x})$  for the chemical potential  $\mu[n(\mathbf{x})]$  [51]. Due to the constraint of the particle confinement, the density  $n(\mathbf{x})$  should satisfy the particle number normalisation condition:

$$\int d^3x n(\mathbf{x}) = N, \quad (4.4)$$

yielding the chemical potential  $\mu$  in the trap.

LDA approximation is justified if the relevant energy varies slower than the background potential. In terms of the single-particle oscillator energy  $\hbar\omega_i$ , it means the condition:

$$|\mu| \gg \hbar\omega_i \quad \Leftrightarrow \quad \left| \frac{\mu}{\epsilon_F} \right| \gg \frac{\omega_i}{\bar{\omega}} \frac{1}{(3N)^{1/3}}. \quad (4.5)$$

Assuming that trap geometry is not extreme, i.e. provided that  $\omega_i$  and  $\bar{\omega}$  are approximately of the same order for  $i = 1, 2, 3$ , the condition (4.5) is met for large particle number of the order of  $N = 10^5$ – $10^7$ .

## 4.2 Harmonic trap potential

The harmonic trap potential  $V_{\text{HO}}(\mathbf{x})$  is minimal at the centre ( $\mathbf{x} = \mathbf{0}$ ), and it quatively grows with the distance  $|\mathbf{x}|$  from the trap centre. Aside of the intrinsic quantity  $M$ , the potential is parametrised by the oscillator frequencies  $\omega_i$ . The geometric mean of the trapping frequencies is:

$$\bar{\omega} = (\omega_1 \omega_2 \omega_3)^{1/3}, \quad (4.6)$$

which is useful for describing oscillator properties. The frequency  $\bar{\omega}$  (4.6) offers the length scale of the harmonic trapping potential:

$$\ell = \sqrt{\frac{\hbar}{M\bar{\omega}}}. \quad (4.7)$$

which is called the *oscillator length*.

On the other hand, the number of the particles  $N$  in a harmonic trap in the ground state is given by the integration over the density of states  $g(\epsilon) = \partial_\epsilon G(\epsilon)$  [35]:

$$\lim_{T \downarrow 0} N = \lim_{T \downarrow 0} \int_0^\infty d\epsilon \frac{g(\epsilon)}{e^{\beta(\epsilon - \mu)} + 1} = \int_0^{\epsilon_F} d\epsilon g(\epsilon). \quad (4.8)$$

For the ideal Fermi gas with two spin species, the number of states in a harmonic trap  $G(\epsilon)$  in continuum spectrum approximation in line with the LDA condition  $\hbar\omega_i \ll \lim_{T \downarrow 0} \mu(T) = \epsilon_F$  can be calculated as:

$$G(\epsilon) = \frac{2}{\prod_{i=1}^3 \hbar\omega_i} \int_0^\epsilon d\epsilon_1 \int_0^{\epsilon - \epsilon_1} d\epsilon_2 \int_0^{\epsilon - \epsilon_1 - \epsilon_2} d\epsilon_3 = \frac{\epsilon^3}{3\hbar^3 \omega_1 \omega_2 \omega_3}, \quad (4.9)$$

and from (4.8) and (4.9) follows:

$$\lim_{T \downarrow 0} N = \frac{\epsilon_F^3}{3\hbar^3 \omega_1 \omega_2 \omega_3}. \quad (4.10)$$

### 4.3. IDEAL FERMI GAS

Consequently, the Fermi energy of harmonically trapped particles is given in terms of the trapping frequencies (4.6) and the particle number  $N$ :

$$\epsilon_F = \hbar\bar{\omega}(3N)^{1/3}. \quad (4.11)$$

Following the above considerations, the physics of fermionic system in a harmonic trap can be described with various dimensionless units in Fermi scale. To this end, we need two physical quantities, one length scale and one velocity scale. The length scale to be introduced is the *Fermi radius* [60], [68]:

$$r_F = \sqrt{\frac{2\epsilon_F}{M\bar{\omega}^2}} = k_F\ell^2, \quad (4.12)$$

and the velocity scale we need is the *Fermi velocity*:

$$v_F = \frac{\hbar k_F}{M} = \bar{\omega}r_F. \quad (4.13)$$

We remark from (4.11)–(4.12) that the system size of harmonically trapped fermions scales with the factor:

$$2\pi\frac{r_F}{\lambda_F} = (k_F\ell)^2 = 2(3N)^{1/3}. \quad (4.14)$$

Since the trap geometry is in general not necessarily isotropic, it is convenient to introduce the isotropic dimensionless trap radii:

$$R_i = \frac{\omega_i x_i}{\bar{\omega}r_F} = \frac{\omega_i x_i}{v_F} \quad (4.15)$$

for  $i \in \{1, 2, 3\}$ . The spatial dependent harmonic trapping potential (4.1) reads then in the dimensionless unit (4.15):

$$\frac{V_{\text{HO}}(\mathbf{R}(\mathbf{x}))}{\epsilon_F} = \sum_{i=1}^3 R_i^2(x_i) = \frac{1}{v_F^2} \sum_{i=1}^3 (\omega_i x_i)^2. \quad (4.16)$$

In (4.16) we have the spherical symmetry  $V_{\text{HO}}(\mathbf{R}) = V_{\text{HO}}(R)$ . The dimensionless distance unit  $R$  is related to the harmonic potential energy scaled in Fermi energy  $\hbar\bar{\omega}/(2\epsilon_F)$ .

From the above follows a useful relation between the dimensionless parameters:

$$\frac{1}{k_F a_s} = \frac{1}{k_F \ell} \frac{\ell}{a_s} = \frac{1}{\sqrt{2 \cdot 3^{1/3}}} \left( N^{1/6} \frac{a_s}{\ell} \right)^{-1} \approx \frac{0.589}{N^{1/6}} \frac{\ell}{a_s}. \quad (4.17)$$

The parameter  $N^{1/6}a_s/\ell$  represents a measure for the interaction strength and is proportional to the scattering parameter  $k_F a_s$  in a harmonic trap [35].

### 4.3 Ideal Fermi gas

We begin our study of trapped fermions with the non-interacting ideal Fermi gas. In this case, the particle density integration (4.4) with the ideal Fermi gas density (3.13) can be analytically performed. To this end, it is convenient to integrate with variable substitution  $\mathbf{x} \rightarrow \mathbf{R}$  in accordant to (4.15):

$$\frac{1}{\lambda_F^3} \int d^3x = \frac{r_F^3}{\lambda_F^3} \int d^3R = 4\pi \frac{r_F^3}{\lambda_F^3} \int_0^\infty dR R^2, \quad (4.18)$$

### 4.3. IDEAL FERMI GAS

where we have used the isotropic property of the  $R$ -coordinates for the transformation to the spherical integration. Note the similarity between isotropic trap coordinate integration (4.18) and the isotropic thermodynamic integration (3.6), which set the analogy between the LDA and thermodynamic limit approximation.

With the substitution (4.18) for (3.13), we write (4.4) as:

$$\begin{aligned} N &= -\frac{2\pi^{3/2}}{\lambda_F^3} \left(\frac{T}{T_F}\right)^{3/2} \int d^3x \text{Li}_{3/2} \left(-e^{\beta\mu(\mathbf{x})}\right) \\ &= -8\pi^{5/2} \frac{r_F^3}{\lambda_F^3} \left(\frac{T}{T_F}\right)^{3/2} \int_0^\infty dR R^2 \text{Li}_{3/2} \left(-e^{\beta(\mu - \epsilon_F R^2)}\right). \end{aligned} \quad (4.19)$$

The integration can be performed by parts using the recursive relation  $\partial_R \text{Li}_s(-e^{a-bR^2}) = -2bR \text{Li}_{s-1}(-e^{a-bR^2})$ , where the surface term vanishes at  $R \rightarrow 0, \infty$ , that is:

$$\begin{aligned} N &= -4\pi^{5/2} \frac{r_F^3}{\lambda_F^3} \left(\frac{T}{T_F}\right)^{5/2} \int_0^\infty dR \text{Li}_{5/2} \left(-e^{\beta(\mu - \epsilon_F R^2)}\right) \\ &= -2\pi^3 \frac{r_F^3}{\lambda_F^3} \left(\frac{T}{T_F}\right)^3 \text{Li}_3(-e^{\beta\mu}), \end{aligned} \quad (4.20)$$

where we exchanged the sum of the polylogarithmic series and the  $R$ -integral to get the gaussian integral of the harmonic trap potential. By this we obtained the additional order of the polylogarithm 1/2.

Due to the proportionality  $r_F/\lambda_F \propto N^{1/3}$  of the system size factor (4.14), the particle number equation can be written in a dimensionless form as:

**Particle number equation of trapped Fermi gas by ideal Fermi gas model**

$$1 = -6 \left(\frac{T}{T_F}\right)^3 \text{Li}_3 \left(-e^{\frac{\mu}{\epsilon_F} - \frac{T}{T_F}}\right). \quad (4.21)$$

Regardless of its name, the particle number equation in harmonic trap (4.21) is independent of the number of trapped fermions  $N$  and trapping frequencies  $\omega_i$ . Because  $N$  and  $\omega_i$  are proportional to the Fermi energy  $\epsilon_F$  in a harmonic trap, and as we consider the system in the dimensionless units scaled by  $\epsilon_F$ ,  $N$  and  $\omega_i$  do not appear in the dimensionless equation. For the ideal Fermi gas it implies that the dimensionless chemical potential  $\mu/\epsilon_F$  is only a function of the dimensionless temperature  $T/T_F$ , while being independent of particle number  $N$  and trapping frequencies  $\omega_i$ . The temperature-dependent chemical potential of the ideal Fermi gas in a harmonic trap can be calculated with (4.21), and it is shown in Fig. 4.2 as the dashed blue curve.

#### 4.3.1 Density profile

Knowing the determined chemical potential  $\mu$  of the trapped gas, now the three-dimensional density of the ideal Fermi gas in harmonic trap is directly given by the LDA of the uniform gas density (3.13):

$$n(\mathbf{x}) = -\frac{2\pi^{3/2}}{\lambda_F^3} \left(\frac{T}{T_F}\right)^{3/2} \text{Li}_{3/2} \left(-e^{\left[\frac{\mu}{\epsilon_F} - \frac{\sum_{i=1}^3 (\omega_i x_i)^2}{v_F^2}\right] \frac{T}{T_F}}\right). \quad (4.22)$$



### 4.3. IDEAL FERMI GAS

However in experiments, the three-dimensional density of the gas can not be directly measured, because a measurement process requires spatial accumulation of the density in some spatial direction, like the absorption imaging is performed on the three-dimensional gas to yield a two-dimensional intensity map. In this regard, we also need to investigate spatially integrated density profiles.

The areal density is achievable by integrating the density (4.22) with respect to one of the three spatial axis. Similar for the three-dimensional integration (4.18), the one-dimensional integration in the Fermi radius scale  $\mathbf{R}(\mathbf{x})$  is given by:

$$\frac{1}{\lambda_F} \int_{-\infty}^{+\infty} dx_k = 2 \frac{\bar{\omega}}{\omega_k} \frac{r_F}{\lambda_F} \int_0^\infty dR_k. \quad (4.23)$$

Accordingly, the areal density of the ideal Fermi gas from the line-of-sight integration of (4.22) is:

$$\begin{aligned} n(x_i, x_j) &= \int_{-\infty}^{+\infty} dx_k n(\mathbf{x}) = 2 \frac{\bar{\omega}}{\omega_k} r_F \int_0^\infty dR_k n(x_i, x_j, R_k) \\ &= -\frac{\bar{\omega}}{\omega_k} \frac{2\pi^2 r_F}{\lambda_F^3} \left(\frac{T}{T_F}\right)^2 \text{Li}_2 \left( -e \left[ \frac{\mu}{\epsilon_F} - \frac{(\omega_i x_i)^2 + (\omega_j x_j)^2}{v_F^2} \right] / \frac{T}{T_F} \right). \end{aligned} \quad (4.24)$$

And for the line density, we apply the two-dimensional integration in the isotropic dimensionless coordinate  $\mathbf{R}$ :

$$\frac{1}{\lambda_F^2} \int_{-\infty}^{+\infty} dx_j dx_k = 2\pi \frac{\bar{\omega}^2}{\omega_j \omega_k} \frac{r_F^2}{\lambda_F^2} \int_0^\infty dR_{jk} R_{jk}, \quad (4.25)$$

where the cylinder-symmetric radius  $R_{jk}$  in the  $x_j$ - $x_k$ -plane is introduced as:

$$R_{jk} = \sqrt{R_j^2 + R_k^2} = \frac{\sqrt{(\omega_j x_j)^2 + (\omega_k x_k)^2}}{v_F}. \quad (4.26)$$

By means of (4.25) we calculate the one-dimensional line density in the  $x_j$ - $x_k$  plane to:

$$\begin{aligned} n(x_i) &= \int_{-\infty}^{+\infty} dx_j dx_k n(\mathbf{x}) = \frac{\bar{\omega}^2}{\omega_j \omega_k} r_F^2 2\pi \int_0^\infty dR_{jk} R_{jk} n(x_i, R_{jk}) \\ &= -\frac{\bar{\omega}^2}{\omega_j \omega_k} \frac{2\pi^{5/2} r_F^2}{\lambda_F^3} \left(\frac{T}{T_F}\right)^{5/2} \text{Li}_{5/2} \left( -e \left[ \frac{\mu}{\epsilon_F} - \frac{(\omega_i x_i)^2}{v_F^2} \right] / \frac{T}{T_F} \right). \end{aligned} \quad (4.27)$$

Following the approach of integrating the density in order to get the lower-dimensional density, also the particle number equation (4.21) can be derived in this context as a result of  $N = \int d^3x n(\mathbf{x})$ :

$$\left( \frac{(3N)^{1/3} h}{\pi r_F p_F} \right)^3 = -6 \left( \frac{T}{T_F} \right)^3 \text{Li}_3 \left( -e^{\mu/\epsilon_F} / \frac{T}{T_F} \right), \quad (4.28)$$

where  $p_F = \hbar k_F$  denotes the Fermi-momentum. Note that the left-hand-side (LHS) of (4.28) has a prefactor in form of the Fermi-phase-space density  $h/(\pi r_F p_F)$  in a harmonic trap. Here,  $[r_F p_F / h]^{1/2} = (r_F / \lambda_F)^{1/2}$  is to be interpreted as the dimensionless geometric mean Fermi radius in a harmonic trap, and  $\pi([r_F p_F / h]^{1/2})^2$  represents the circular area with this radius. Therefore the LHS of (4.28) indicates the number of oscillators trapped in the circular area of the Fermi-phase-space cell:

$$\frac{(3N)^{1/3} h}{\pi r_F p_F} = \frac{\epsilon_F / (\hbar \bar{\omega})}{\pi([r_F p_F / h]^{1/2})^2} = 1. \quad (4.29)$$

## 4.4. BCS–BOGOLIUBOV THEORY

### 4.3.2 Ground state

We further analyse the trapped ideal Fermi gas at the zero-temperature limit for a reference case. The solution of the particle number equation (4.21) in the zero-temperature limit can be given by 0-approximation of fermionic polylogarithm (A.34), which is exact in the zero-temperature limit. Here, the chemical potential  $\mu$  of trapped ideal Fermi gas at zero-temperature is equal to the Fermi energy:

$$1 = -6 \lim_{T \downarrow 0} \left( \frac{T}{T_F} \right)^3 \text{Li}_3 \left( -e^{\frac{\mu}{\epsilon_F} / \frac{T}{T_F}} \right) = \left( \frac{\mu}{\epsilon_F} \right)^3, \quad (4.30)$$

leading to the relation  $\lim_{T \downarrow 0} \mu(T) = \epsilon_F$  as same as the uniform gas case. Using this identity, we can write the zero-temperature density equation as:

$$\lim_{T \downarrow 0} n(T, \mathbf{x}) = \begin{cases} \frac{8\pi}{3} \frac{1}{\lambda_F^3} \left[ 1 - \frac{\sum_{i=1}^3 (\omega_i x_i)^2}{v_F^2} \right]^{3/2}, & \sqrt{\sum_{i=1}^3 (\omega_i x_i)^2} \leq v_F \\ 0, & \text{elsewhere} \end{cases}. \quad (4.31)$$

At the centre of the trap ( $\mathbf{x} = \mathbf{0}$ ) we get the uniform ideal Fermi gas result (3.3):

$$\lim_{T \downarrow 0} n(T, \mathbf{x} = \mathbf{0}) = \frac{8\pi}{3\lambda_F^3} = \frac{k_F^3}{3\pi^2}. \quad (4.32)$$

From (4.31) we read off that the particles with the velocity larger than the Fermi-velocity  $v_F = \bar{\omega} r_F$  have escaped the trap and the particles with energies less than the Fermi energy remain in the trap at  $T = 0$ .

The areal density profile can be obtained from the zero-temperature limit of (4.24):

$$\lim_{T \downarrow 0} n(T, x_i, x_j) = \begin{cases} \pi^2 \frac{\bar{\omega}}{\omega_k} \frac{r_F}{\lambda_F^3} \left[ 1 - \frac{(\omega_i x_i)^2 + (\omega_j x_j)^2}{v_F^2} \right]^2, & \sqrt{(\omega_i x_i)^2 + (\omega_j x_j)^2} \leq v_F \\ 0, & \text{elsewhere} \end{cases}. \quad (4.33)$$

And, correspondingly, the line density in the zero-temperature limit reads:

$$\lim_{T \downarrow 0} n(T, x_i) = \begin{cases} \frac{16\pi^2}{15} \frac{\bar{\omega}^2}{\omega_j \omega_k} \frac{r_F^2}{\lambda_F^3} \left[ 1 - \frac{(\omega_i x_i)^2}{v_F^2} \right]^{5/2}, & |\omega_i x_i| \leq v_F \\ 0, & \text{elsewhere} \end{cases}. \quad (4.34)$$

## 4.4 BCS–Bogoliubov theory

The BCS theoretical calculation for the density profile of Fermi gas in a harmonic trap with LDA proceeds similar to the ideal Fermi gas case in the previous section 4.3. The difference is the possible spatial superfluid fraction in the trap, which represents a combined effect of the BCS theory and LDA. Since the phase transition is induced by interaction, now we should take account of the interaction strength. Therefore the theory should have an additional parameter for interaction than the single parameter  $T/T_F$  of the trapped ideal Fermi gas. The interaction of the trapped fermions is again represented by the single parameter  $k_F a_s$ , like the uniform gas case, as we may see shortly.

## 4.4. BCS–BOGOLIUBOV THEORY

### 4.4.1 Phase transition

We need first to calculate the dimensionless chemical potential  $\mu/\epsilon_F$ . For a generally inhomogeneous trap geometry, this task is simplified in the isotropic trap coordinate  $\mathbf{R}$  from Eq. (4.15). The spatial integration in the dimensionless  $R$ -coordinate reads then:

$$\frac{1}{\lambda_F^3} \int d^3x = \frac{r_F^3}{\lambda_F^3} 4\pi \int_0^\infty dR R^2 = \frac{12N}{\pi^2} \int_0^\infty dR R^2, \quad (4.35)$$

provided that the integrand is correspondingly transformed into the isotropic harmonic trap coordinate  $R(\mathbf{x})$ . with that, the particle number equation reads:

$$N = \int d^3x n(\mathbf{x}) = \frac{12N}{\pi^2} \lambda_F^3 \int_0^\infty dR R^2 n(R), \quad (4.36)$$

or in the dimensionless form,

$$1 = \frac{12}{\pi^2} \lambda_F^3 \int_0^\infty dR R^2 n(R) \quad (4.37)$$

to determine the chemical potential  $\mu(k_F a_s, T)$ .

The isotropic transformation of the local density equation  $n(\mathbf{x}) \rightarrow n(R)$  follows from the particle density (3.20) with LDA in  $R$ -coordinate:

$$n(R) = \frac{4\pi}{3} \frac{1}{\lambda_F^3} \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{3/2}}{\epsilon_B(\epsilon_k, R)} \left[ \frac{|\Delta|^2(R)}{\epsilon_B^2(\epsilon_k, R)} \tanh \frac{\beta \epsilon_B(\epsilon_k, R)}{2} + \frac{(\epsilon_k - \mu(R))^2}{\epsilon_B^2(\epsilon_k, R)} \frac{\frac{\beta \epsilon_B(\epsilon_k, R)}{2}}{\cosh^2 \frac{\beta \epsilon_B(\epsilon_k, R)}{2}} \right] \quad (4.38)$$

with the LDA-Bogoliubov dispersion dependent in  $R$ :

$$\epsilon_B(\epsilon_k, R) = \sqrt{(\epsilon_k - \mu(R))^2 + |\Delta|^2(R)} \quad (4.39)$$

and the chemical potential with LDA in  $R$ -coordinate:

$$\mu(R) = \mu - \epsilon_F R^2. \quad (4.40)$$

In these terms the particle number equation is integrated over  $R$  with  $n(R)$ , where  $n(R)$  itself is constructed from the integral in momentum space (4.38), leading to:

#### Particle number equation of trapped Fermi gas by BCS–Bogoliubov theory

$$1 = \frac{16}{\pi} \int_0^\infty dR R^2 \times \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{3/2}}{\epsilon_B(\epsilon_k, R)} \left[ \frac{|\Delta|^2(R)}{\epsilon_B^2(\epsilon_k, R)} \tanh \frac{\beta \epsilon_B(\epsilon_k, R)}{2} + \frac{(\epsilon_k - \mu(R))^2}{\epsilon_B^2(\epsilon_k, R)} \frac{\frac{\beta \epsilon_B(\epsilon_k, R)}{2}}{\cosh^2 \frac{\beta \epsilon_B(\epsilon_k, R)}{2}} \right] \quad (4.41)$$

as a  $N$ -independent form. Besides of (4.41), we have the local order parameter equation:

**Order parameter equation of trapped Fermi gas by BCS–Bogoliubov theory**

$$\begin{aligned}
\frac{2\pi}{k_F a_s} = & \frac{4}{\sqrt{\epsilon_F}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{1/2}}{\epsilon_B(\epsilon_k, R)} \left[ \frac{|\Delta|^2(R)}{\epsilon_B^2(\epsilon_k, R)} \tanh \frac{\beta \epsilon_B(\epsilon_k, R)}{2} + \frac{(\epsilon_k - \mu(R))^2}{\epsilon_B^2(\epsilon_k, R)} \frac{\frac{\beta \epsilon_B(\epsilon_k, R)}{2}}{\cosh^2 \frac{\beta \epsilon_B(\epsilon_k, R)}{2}} \right] \\
& - \frac{2\mu(R)}{\sqrt{\epsilon_F}} \int_0^\infty d\epsilon_k \frac{\tanh \frac{\beta \epsilon_B(\epsilon_k, R)}{2}}{\sqrt{\epsilon_k} \epsilon_B(\epsilon_k, R)}.
\end{aligned} \tag{4.42}$$

To find the density profile  $n(R)$ , the order parameter profile  $\Delta(R)$  must be known. For this, the local order parameter equation (4.42) should be first solved for every point  $R$ , where the theory obtain the interaction dependence. And since the order parameter equation is to be solved for the scattering parameter  $k_F a_s$ , interaction effect of the BCS theory for harmonically trapped fermions is represented by the single parameter  $k_F a_s$ .

Solving afterwards the particle number normalisation equation (4.41) determines than the solution of the chemical potential value  $\mu/\epsilon_F$ . Contrary to the ideal Fermi gas case, in the BCS theory there is no analytical expression for the particle number integration in the trap due to the local order parameter equation (4.42). This means that,  $\mu$  at the given scattering parameter  $k_F a_s$  should be numerically found.

In principle we can stick with the general density expression (4.38) for the whole regime in the trap, because for vanishing  $\Delta \rightarrow 0$  the density value should become arbitrarily close to the normal fluid density. However this is not an optimal way to achieve our goal, since the calculation of the superfluid density requires much more computations than the normal fluid density. And as the order parameter becomes exponentially small towards the outer region of the trap, the numerical calculation becomes unstable and inaccurate. This is because numerical algorithms can not handle well the exponentially small quantities. To get around this problem, we might divide the superfluid- and normal fluid regions in the trap to save the computational resource and to get more accurate numerical results.

To this end, the strategy is as follows. We first choose  $T$  and  $k_F a_s$  and evaluate, whether the trapped gas is in the superfluid phase or not. We can answer this question by computing the maximal critical temperature in the trap, which corresponds to  $T_c(R = 0)$  at the centre of the trap for given  $k_F a_s$ , which is then compared with the chosen  $T$ . The maximum critical temperature  $T_c(k_F a_s, R = 0)$  in the trap can be determined in the following way. Since for  $T = T_c(R = 0)$  the system is not yet in the superfluid phase, the chemical potential is given via the ideal Fermi gas chemical potential in trap (4.21). This  $\mu$  then also satisfies the order parameter equation at  $T_c(k_F a_s, R = 0, \Delta(R = 0) = 0)$  in (4.42). By solving these two equations for both variables  $\mu$  and  $T$  at the same time, we can obtain the maximal critical temperature in the trap for given  $k_F a_s$ . The critical temperature of trapped Fermi gas is shown in the Fig. 4.1 as the blue curve. Now, by means of  $T_c(k_F a_s)$  in the trap we know whether the trapped gas has a superfluid fraction at given  $k_F a_s$  and  $T/T_F$ , where the superfluid fraction in the harmonic trap takes place in the inner regime of the trap. For  $T \geq T_c(k_F a_s, R = 0)$  we simply calculate the chemical potential of the ideal Fermi gas in the trap with (4.21). Otherwise the trapped Fermi gas has a spatial superfluid fraction. In this case, the next task is to construct a loop for a fix-point iteration at a  $m$ -th temporary numerical parameter  $\mu^{(m)}$  and the corresponding critical range  $R_c(\mu^{(m)})$ . This means, we solve the local order parameter equation (4.42) and the local density equation (4.38) together at  $\Delta(R) = 0$  for given  $k_F a_s$ ,  $T$  and numerical parameter  $\mu^{(m)}$ . This self-consistent equation for  $R$  yields the critical range  $R_c(\mu^{(m)})$  for the provisionally

#### 4.4. BCS–BOGOLIUBOV THEORY

chosen chemical potential  $\mu^{(m)}$ . These values  $\mu^{(m)}$ ,  $R_c(\mu^{(m)})$  are then fed to the particle number equation (4.41), where the density  $n(R)$  is divides the integration in the superfluid and the normal fluid regime:

$$1 = \frac{12}{\pi^2} \lambda_F^3 \int_0^\infty dR R^2 n(R),$$

$$n(R) = \begin{cases} \frac{4\pi}{3\lambda_F^3} \frac{1}{\epsilon_F^{3/2}} \int_0^\infty \frac{\epsilon_k^{3/2}}{\epsilon_B(\epsilon_k, R)} \left[ \frac{|\Delta|^2(R)}{\epsilon_B^2(\epsilon_k, R)} \tanh \frac{\beta \epsilon_B(\epsilon_k, R)}{2} + \frac{(\epsilon_k - \mu^{(m)}(R))^2}{\epsilon_B^2(\epsilon_k, R)} \frac{\frac{\beta \epsilon_B(\epsilon_k, R)}{2}}{\cosh^2 \frac{\beta \epsilon_B(\epsilon_k, R)}{2}} \right] & , R < R_c \\ -\frac{2\pi^{3/2}}{\lambda_F^3} \left( \frac{T}{T_F} \right)^{3/2} \text{Li}_{3/2} \left( -e^{\frac{\mu^{(m)}(R)}{\epsilon_F} / \frac{T}{T_F}} \right) & , R \geq R_c \end{cases} \quad (4.43)$$

with the local order parameter  $\Delta(R)$  in (4.42) for  $R < R_c$ . It describes the particle number equation at the  $m$ -th single loop, and the calculation should be repeatedly performed to the next iteration  $m + 1$  with the feedback from  $m$ -th loop, until the particle number equation (4.43) is satisfied within an enough precision. This at the same time means the the numerically convergent  $\mu^{(m)} \rightarrow \mu$  within a finite number of iterations for a desired precision, and accordingly we obtain the correct value of the critical range  $R_c(k_F a_s, T)$  and  $\mu(k_F a_s, T)$ .

##### 4.4.2 Density profile

After having found the chemical potential and the critical range, it is possible to describe the density profile in a harmonic trap by the BCS theory. The 3D density in the trap by the BCS theory reads:

##### Particle density by BCS–Bogoliubov theory

$$n(\mathbf{x}) = \begin{cases} \frac{4\pi}{3\lambda_F^3} \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{3/2}}{\epsilon_B(\epsilon_k, \mathbf{x})} \times \left[ \frac{|\Delta|^2(\mathbf{x})}{\epsilon_B^2(\epsilon_k, \mathbf{x})} \tanh \frac{\beta \epsilon_B(\epsilon_k, \mathbf{x})}{2} + \frac{(\epsilon_k - \mu(\mathbf{x}))^2}{\epsilon_B^2(\epsilon_k, \mathbf{x})} \frac{\frac{\beta \epsilon_B(\epsilon_k, \mathbf{x})}{2}}{\cosh^2 \frac{\beta \epsilon_B(\epsilon_k, \mathbf{x})}{2}} \right] & , R(\mathbf{x}) < R_c \\ -\frac{2\pi^{3/2}}{\lambda_F^3} \left( \frac{T}{T_F} \right)^{3/2} \text{Li}_{3/2} \left( -e^{\frac{\mu(\mathbf{x})}{\epsilon_F} / \frac{T}{T_F}} \right) & , R(\mathbf{x}) \geq R_c \end{cases} \quad (4.44)$$

with the spatial dependent Bogoliubov-dispersion with LDA:

$$\epsilon_B(\epsilon_k, \mathbf{x}) = \sqrt{(\epsilon_k - \mu(\mathbf{x}))^2 + \Delta^2(\mathbf{x})}, \quad (4.45)$$

where we take the substitution  $\mu(R)$  in (4.40)  $\rightarrow \mu(\mathbf{x})$  via:

$$\frac{\mu(\mathbf{x})}{\epsilon_F} = \frac{\mu}{\epsilon_F} - \frac{\sum_{i=1}^3 (\omega_i x_i)^2}{v_F^2}. \quad (4.46)$$

In the superfluid regime, i.e.  $[\sum_{i=1}^3 (\omega_i x_i)^2]^{1/2} / (v_F) < R_c$ , the particle density  $n(\mathbf{x}, \Delta(\mathbf{x}))$  should be calculated with the local order parameter  $\Delta(\mathbf{x})$  determined by the local order parameter equation (4.42). The superfluid density profile is correspondingly extended from the uniform gas case as:

$$n_{\text{sf}}(\mathbf{x}) = \begin{cases} \frac{4\pi}{3\lambda_F^3} \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{3/2}}{\epsilon_B(\epsilon_k, \mathbf{x})} \frac{|\Delta|^2(\mathbf{x})}{\epsilon_B^2(\epsilon_k, \mathbf{x})} \tanh \frac{\beta \epsilon_B(\epsilon_k, \mathbf{x})}{2} & , R(\mathbf{x}) < R_c \\ 0 & , R(\mathbf{x}) \geq R_c \end{cases} \quad (4.47)$$

#### 4.4. BCS–BOGOLIUBOV THEORY

To describe the two-dimensional areal density in the  $x_i$ – $x_j$ -plane, first we define the chemical potential with LDA:

$$\frac{\mu(x_i, x_j, R_k)}{\epsilon_F} = \frac{\mu}{\epsilon_F} - \frac{(\omega_i x_i)^2 + (\omega_j x_j)^2}{v_F^2} - R_k^2 \quad (4.48)$$

with  $R_k = \omega_k x_k / v_F$ . We perform the line-of-sight integration in  $x_k$ -direction separately in the superfluid and in the normal fluid region divided by  $R_c$ :

##### Areal particle density by BCS–Bogoliubov theory

$$n(x_i, x_j) = 2 \frac{\bar{\omega}}{\omega_k} r_F \int_0^\infty dR_k n(x_i, x_j, R_k),$$

$$n(x_i, x_j, R_k) = \begin{cases} \frac{4\pi}{3\lambda_F^3} \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{3/2}}{\epsilon_B(\epsilon_k, x_i, x_j, R_k)} \\ \quad \times \left[ \frac{|\Delta|^2(x_i, x_j, R_k)}{\epsilon_B^2(\epsilon_k, x_i, x_j, R_k)} \tanh \frac{\beta \epsilon_B(\epsilon_k, x_i, x_j, R_k)}{2} \right. \\ \quad \left. + \frac{(\epsilon_k - \mu(x_i, x_j, R_k))^2}{\epsilon_B^2(\epsilon_k, x_i, x_j, R_k)} \frac{\frac{\beta \epsilon_B(\epsilon_k, x_i, x_j, R_k)}{2}}{\cosh^2 \frac{\beta \epsilon_B(\epsilon_k, x_i, x_j, R_k)}{2}} \right], & R(x_i, x_j, R_k) < R_c \\ -\frac{2\pi^{3/2}}{\lambda_F^3} \left( \frac{T}{T_F} \right)^{3/2} \text{Li}_{3/2} \left( -e^{\frac{\mu(x_i, x_j, R_k)}{\epsilon_F} / \frac{T}{T_F}} \right), & R(x_i, x_j, R_k) \geq R_c \end{cases} \quad (4.49)$$

with the dimensionless distance  $R(x_i, x_j, R_k)$ :

$$R(x_i, x_j, R_k) = \sqrt{\frac{(\omega_i x_i)^2 + (\omega_j x_j)^2}{v_F^2} + R_k^2}. \quad (4.50)$$

In the superfluid regime, the density  $n(x_i, x_j, R_k)$  should be calculated with the local order parameter equation (4.42) with substitutions  $\mu(R)$  in (4.40)  $\rightarrow \mu(x_i, x_j, R_k)$  in (4.48).

Applying this isotropic dimensionless coordinate  $R(\mathbf{x})$  for the line density is also straightforward. We define the chemical potential first

$$\frac{\mu(x_i, R_{jk})}{\epsilon_F} = \frac{\mu}{\epsilon_F} - \frac{(\omega_i x_i)^2}{v_F^2} - R_{jk}^2, \quad (4.51)$$

and determine the line density from integrations over the  $x_j$ – $x_k$ -plane:

**Line particle density by BCS–Bogoliubov theory**

$$\begin{aligned}
n(x_i) &= 2\pi \frac{\bar{\omega}^2}{\omega_j \omega_k} r_F^2 \int_0^\infty dR_{jk} R_{jk} n(x_i, R_{jk}), \\
n(x_i, R_{jk}) &= \begin{cases} \frac{4\pi}{3\lambda_F^3} \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{3/2}}{\epsilon_B(\epsilon_k, x_i, R_{jk})} \\ \quad \times \left[ \frac{|\Delta|^2(x_i, x_j, R_k)}{\epsilon_B^2(\epsilon_k, x_i, R_{jk})} \tanh \frac{\beta \epsilon_B(\epsilon_k, x_i, R_{jk})}{2} \right. \\ \quad \left. + \frac{(\epsilon_k - \mu(x_i, R_{jk}))^2}{\epsilon_B^2(\epsilon_k, x_i, R_{jk})} \frac{\frac{\beta \epsilon_B(\epsilon_k, x_i, R_{jk})}{2}}{\cosh^2 \frac{\beta \epsilon_B(\epsilon_k, x_i, R_{jk})}{2}} \right], & R(x_i, R_{jk}) < R_c \\ -\frac{2\pi^{3/2}}{\lambda_F^3} \left( \frac{T}{T_F} \right)^{3/2} \text{Li}_{3/2} \left( -e^{\frac{\mu(x_i, R_{jk})}{\epsilon_F} / \frac{T}{T_F}} \right) & R(x_i, R_{jk}) \geq R_c \end{cases}
\end{aligned} \tag{4.52}$$

with the dimensionless distance  $R(x_i, R_{jk})$ :

$$R(x_i, R_{jk}) = \sqrt{\frac{(\omega_i x_i)^2}{v_F^2} + R_{jk}^2} \tag{4.53}$$

for its radial symmetry in the  $R_j$ – $R_k$ –plane with  $R_{jk} = [R_j^2 + R_k^2]^{1/2}$ . Again, the particle line density  $n(x_i, R_{jk}(x_j, x_k))$  in the critical range is to be calculated with the local order parameter equation (4.42) with substituting  $\mu(R)$  in (4.40)  $\rightarrow \mu(x_i, R_{jk})$  in (4.51).

## 4.5 Hartree theory

Next to the BCS theory, we consider the Hartree theory in the harmonic trap. In this case, we basically describe an interacting trapped fermions in the normal fluid phase. We show that the local Hartree interaction term alters significantly the density profile of the non-interacting Fermi gas.

### 4.5.1 Density profile

The particle number equation at equal spin-population in LDA is obtained from the self-consistency equation (3.59) with the trapping potential. Analog to (3.63), it is given by the polylogarithmic function:

$$\lambda_F^3 n(\mathbf{x}) = -2\pi^{3/2} \left( \frac{T}{T_F} \right)^{3/2} \text{Li}_{3/2} \left( -e^{\frac{\mu_H[n(\mathbf{x})]}{\epsilon_F} / \frac{T}{T_F}} \right), \tag{4.54}$$

with the Hartree-shifted chemical potential of the interacting fermions in HFA/LDA:

$$\frac{\mu_H[n(\mathbf{x})]}{\epsilon_F} = \frac{\mu}{\epsilon_F} - k_F a_s \frac{\lambda_F^3 n(\mathbf{x})}{2\pi^2} - \frac{\sum_{i=1}^3 (\omega_i x_i)^2}{v_F^2} \tag{4.55}$$

and represents a functional of the density distribution  $n(\mathbf{x})$ . Thus, (4.54) is a local self-consistent equation of  $n(\mathbf{x})$  at the position  $\mathbf{x}$ . The particle number is calculated by spatial integration over the particle density (4.55):

$$N = \int d^3x n(\mathbf{x}) = -2\pi^{3/2} \left( \frac{T}{T_F} \right)^{3/2} \frac{1}{\lambda_F^3} \int d^3x \text{Li}_{3/2} \left( -e^{\frac{\mu_H[n(\mathbf{x})]}{\epsilon_F} / \frac{T}{T_F}} \right). \tag{4.56}$$

## 4.5. HARTREE THEORY

Substitution  $\mathbf{x} \rightarrow R$  in (4.15) for (4.56) yields:

**Particle number equation of trapped Fermi gas by Hartree theory**

$$1 = -\frac{24}{\sqrt{\pi}} \left( \frac{T}{T_F} \right)^{3/2} \int_0^\infty dR R^2 \text{Li}_{3/2} \left( -e^{\frac{\mu_H(R)}{\epsilon_F} / \frac{T}{T_F}} \right) \quad (4.57)$$

with the Hartree-shifted chemical potential being a functional of the density profile  $n(R)$ :

$$\frac{\mu_H(R)}{\epsilon_F} = \frac{\mu}{\epsilon_F} - k_F a_s \frac{\lambda_F^3 n(R)}{2\pi^2} - R^2. \quad (4.58)$$

The density  $n = n(R)$  depends on the equipotential distance  $R$  in a self-consistent way. It means that the following local self-consistent equation for  $\lambda_F^3 n(R)$  should be numerically solved at the every point  $R$  while integrating (4.57):

$$\lambda_F^3 n(R) = -2\pi^{3/2} \left( \frac{T}{T_F} \right)^{3/2} \text{Li}_{3/2} \left( -e^{\frac{\mu_H(n(R))}{\epsilon_F} / \frac{T}{T_F}} \right). \quad (4.59)$$

Due to the constraints of the local self-consistent Hartree equations (4.59), we can not find an analytic form of the particle number equation (4.57) as in the ideal Fermi gas (4.21) at given  $k_F a_s$ . In the Hartree theory with a confining spatial inhomogeneity, one solves the particle number equation in a variational way along with the local Hartree self-consistent equation to infer the implicit density distribution  $n(\mathbf{x})$ . The reward of this effort is a more accurate density distribution that takes into account of the interaction and thermal effects more realistically than the simple analytical density distribution (4.22) of the ideal gas model. Moreover, the particle number equation (4.57) of the Hartree theory in the harmonic trap is again independent of the particle number  $N$ . And similar to the BCS theory, the scattering parameter  $k_F a_s$  is a single parameter that represents interaction effects in the system, this time effects from the Hartree channel.

Once the chemical potential is determined by solving (4.57) with (4.59), the three-dimensional density is given by the Hartree density equation:

**Particle density by Hartree theory**

$$n(\mathbf{x}) = -\frac{2\pi^{3/2}}{\lambda_F^3} \left( \frac{T}{T_F} \right)^{3/2} \text{Li}_{3/2} \left( -e^{\frac{\mu_H(\mathbf{x})}{\epsilon_F} / \frac{T}{T_F}} \right). \quad (4.60)$$

The density  $n(\mathbf{x})$  is given as the solution of the self-consistency equation (4.60), and here we have discarded the spatial density functional notation  $[n(\mathbf{x})]$  for the spatial dependence notation  $(\mathbf{x})$ , as we have determined  $\mu$  with the particle number equation (4.57).

Similar to (4.58), the Hartree-shifted chemical potential in the  $x_i$ - $x_j$  plane is to be written as:

$$\frac{\mu_H(x_i, x_j, R_k)}{\epsilon_F} = \frac{\mu}{\epsilon_F} - k_F a_s \frac{\lambda_F^3 n(x_i, x_j, R_k)}{2\pi^2} - \frac{(\omega_i x_i)^2 + (\omega_j x_j)^2}{v_F^2} - R_k^2 \quad (4.61)$$

for  $R_k = \omega_k x_k / v_F$ . The two-dimensional areal density is given in the integral representation of (4.60):



**Areal particle density by Hartree theory**

$$n(x_i, x_j) = -4\pi^{3/2} \frac{\bar{\omega}}{\omega_k} \frac{r_F}{\lambda_F^3} \left( \frac{T}{T_F} \right)^{3/2} \int_0^\infty dR_k \text{Li}_{3/2} \left( -e^{\frac{\mu_H(x_i, x_j, R_k)}{\epsilon_F} / \frac{T}{T_F}} \right). \quad (4.62)$$

For the one-dimensional line density we prepare the Hartree-shifted chemical potential in  $x_i$ -line:

$$\frac{\mu_H(x_i, R_{jk})}{\epsilon_F} = \frac{\mu}{\epsilon_F} - k_F a_s \frac{\lambda_F^3 n(x_i, R_{jk})}{2\pi^2} - \frac{(\omega_i x_i)^2}{v_F^2} - R_{jk}^2 \quad (4.63)$$

with  $R_{jk} = [R_j^2 + R_k^2]^{1/2}$ . In terms of the local Hartree-shifted chemical potential (4.63), line density by integration of over two directions of (4.60) is:

**Line particle density by Hartree theory**

$$n(x_i) = -4\pi^{5/2} \frac{\bar{\omega}^2}{\omega_j \omega_k} \frac{r_F^2}{\lambda_F^3} \left( \frac{T}{T_F} \right)^{3/2} \int_0^\infty dR_{jk} R_{jk} \text{Li}_{3/2} \left( -e^{\frac{\mu_H(x_i, R_{jk})}{\epsilon_F} / \frac{T}{T_F}} \right). \quad (4.64)$$

### 4.5.2 Ground state

Analogous to the ideal Fermi gas, the zero-temperature equation of state in Hartree theory in trap is given by the 0th term of the fermionic polylogarithm (A.34) like the homogeneous Hartree density equation (3.68). With  $\mu(R)$  we write:

$$\frac{4}{3\pi} k_F a_s \frac{\lambda_F^3 n(R)}{8\pi/3} + \left( \frac{\lambda_F^3 n(R)}{8\pi/3} \right)^{2/3} - \frac{\mu}{\epsilon_F} + R^2 = 0, \quad (4.65)$$

but now the density  $\lambda_F^3 n(R(\mathbf{x}))$  being a locally variant density at the spatial point  $\mathbf{x}$  instead of uniform constant one. Since the density is neither negative nor non-real,  $n(R)$  must be zero where  $R^2 = \mu/\epsilon_F$ , at  $T = 0$ . While the zero-temperature  $\mu$  is not equal to the Fermi energy in the Hartree theory, it is still the boundary of the trapped gas. And since  $\mu/\epsilon_F < 1$  for  $a_s < 0$ , attractive Hartree interaction makes the trapped gas shrinks. In that regards, at a same temperature, more negative chemical shift implies more shrinking of the trapped gas.

## 4.6 Hartree–Bogoliubov theory

As we have discussed in the previous sections 4.4 and 4.5, effects of interaction between trapped fermions are modelled by two different mean-field theories. The interaction effects in each theory are two different aspects. While one of those theories misses the interaction effect of another, a complete picture can be described by the HB theory that contains the both effects. As we have already prepared the technical parts of the BCS theory in sec. 4.4 and of the Hartree theory in sec. 4.5 separately, it is not further complicated to combine those calculations. But the resulting effect of the simple unification is significant, as we may see.

## 4.6. HARTREE–BOGOLIUBOV THEORY

### 4.6.1 Phase transition

Calculation of the spatial critical temperature profile  $T_c(k_F a_s, \mathbf{x})$  with the HB theory is similar to the BCS theory in principle, however it is more complicated. While the spatially dependent phase transition temperature  $T_c(k_F a_s, \mathbf{x})$  is calculated based on the ideal Fermi gas density  $n(T, \mathbf{x})$  (4.22) in the BCS theory, in the Hartree theory,  $T_c(k_F a_s, \mathbf{x})$  is affected by the inhomogeneous density  $n(k_F a_s, T, \mathbf{x})$  (4.60) of the interacting normal fluid. In other words, the interaction plays a double role, once affecting the density profile  $n(k_F a_s)$ , and it gives rise to the spatial dependent phase transition by local order parameter  $\Delta(k_F a_s, \mathbf{x})$  on top of the interaction-dependent density.

To add the Hartree channel in the BCS particle number equation (4.41), we substitute  $\mu(\mathbf{x})$  by  $\mu_H(\mathbf{x})$ , that leads to:

**Particle number equation of trapped Fermi gas by Hartree–Bogoliubov theory**

$$1 = \frac{16}{\pi} \int_0^\infty dR R^2 \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{3/2}}{\epsilon_{HB}(\epsilon_k, R)} \times \left[ \frac{|\Delta|^2(R)}{\epsilon_{HB}^2(\epsilon_k, R)} \tanh \frac{\beta \epsilon_{HB}(\epsilon_k, R)}{2} + \frac{(\epsilon_k - \mu_H(R))^2}{\epsilon_{HB}^2(\epsilon_k, R)} \frac{\frac{\beta \epsilon_{HB}(\epsilon_k, R)}{2}}{\cosh^2 \frac{\beta \epsilon_{HB}(\epsilon_k, R)}{2}} \right] \quad (4.66)$$

with the local self-consistent density equation and the order parameter equations to be solved:

$$\lambda_F^3 n(R) = \frac{4\pi}{3} \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{3/2}}{\epsilon_{HB}(\epsilon_k, R)} \times \left[ \frac{|\Delta|^2(R)}{\epsilon_{HB}^2(\epsilon_k, R)} \tanh \frac{\beta \epsilon_{HB}(\epsilon_k, R)}{2} + \frac{(\epsilon_k - \mu_H(R))^2}{\epsilon_{HB}^2(\epsilon_k, R)} \frac{\frac{\beta \epsilon_{HB}(\epsilon_k, R)}{2}}{\cosh^2 \frac{\beta \epsilon_{HB}(\epsilon_k, R)}{2}} \right], \quad (4.67)$$

$$\frac{2\pi}{k_F a_s} = \frac{4}{\epsilon_F^{1/2}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{1/2}}{\epsilon_{HB}(\epsilon_k, R)} \left[ \frac{|\Delta|^2(R)}{\epsilon_{HB}^2(\epsilon_k, R)} \tanh \frac{\beta \epsilon_{HB}(\epsilon_k, R)}{2} + \frac{(\epsilon_k - \mu_H(R))^2}{\epsilon_{HB}^2(\epsilon_k, R)} \frac{\frac{\beta \epsilon_{HB}(\epsilon_k, R)}{2}}{\cosh^2 \frac{\beta \epsilon_{HB}(\epsilon_k, R)}{2}} \right] - \frac{2\mu_H(R)}{\sqrt{\epsilon_F}} \int_0^\infty d\epsilon_k \frac{\tanh \frac{\beta \epsilon_{HB}(\epsilon_k, R)}{2}}{\sqrt{\epsilon_k} \epsilon_{HB}(\epsilon_k, R)}. \quad (4.68)$$

with the Hartree potential  $\mu_H(R)$  and the HB dispersion with LDA:

$$\epsilon_{HB}(\epsilon_k, R) = \sqrt{(\epsilon_k - \mu_H(R))^2 + \Delta^2(R)}. \quad (4.69)$$

The HB particle number equation should be dealt different than the BCS particle number equation. In the latter, one calculates the order parameter equation first, and then put the calculated  $\Delta(\mathbf{x})$  to the integrand  $n(\mathbf{x})$  of particle number equation. In the HB particle number equation calculation however, the local density is a subject to a self-consistent equation. Accordingly, both  $n(\mathbf{x})$  and  $\Delta(\mathbf{x})$  should be calculated simultaneously for the local density equation (4.67) and the local order parameter equation (4.68) to get the integrand  $n(\mathbf{x})$  in the particle number equation integration correctly.

Next step is calculating the critical range  $R_c$  where the order parameter vanishes. For this

#### 4.6. HARTREE–BOGOLIUBOV THEORY

purpose, we solve the order parameter equation equipped with the HB dispersion for  $\Delta(R_c) = 0$ :

$$\begin{aligned} \frac{2\pi}{k_F a_s} \Big|_{\Delta(R_c)=0} = & -4\sqrt{\pi} \left( \frac{T}{T_F} \right)^{1/2} \text{Li}_{1/2} \left( -e^{\frac{\mu_H(R)|_{R=R_c}}{\epsilon_F} / \frac{T}{T_F}} \right) \\ & - 2 \frac{\mu_H(R)|_{R=R_c}}{\epsilon_F} \int_0^\infty dt \frac{\tanh \frac{\left| t - \frac{\mu_H(R)|_{R=R_c}}{\epsilon_F} \right|}{2 \frac{T}{T_F}}}{\sqrt{t} \left| t - \frac{\mu_H(R)|_{R=R_c}}{\epsilon_F} \right|}, \end{aligned} \quad (4.70)$$

as well as the density equation at the critical range  $R_c$ :

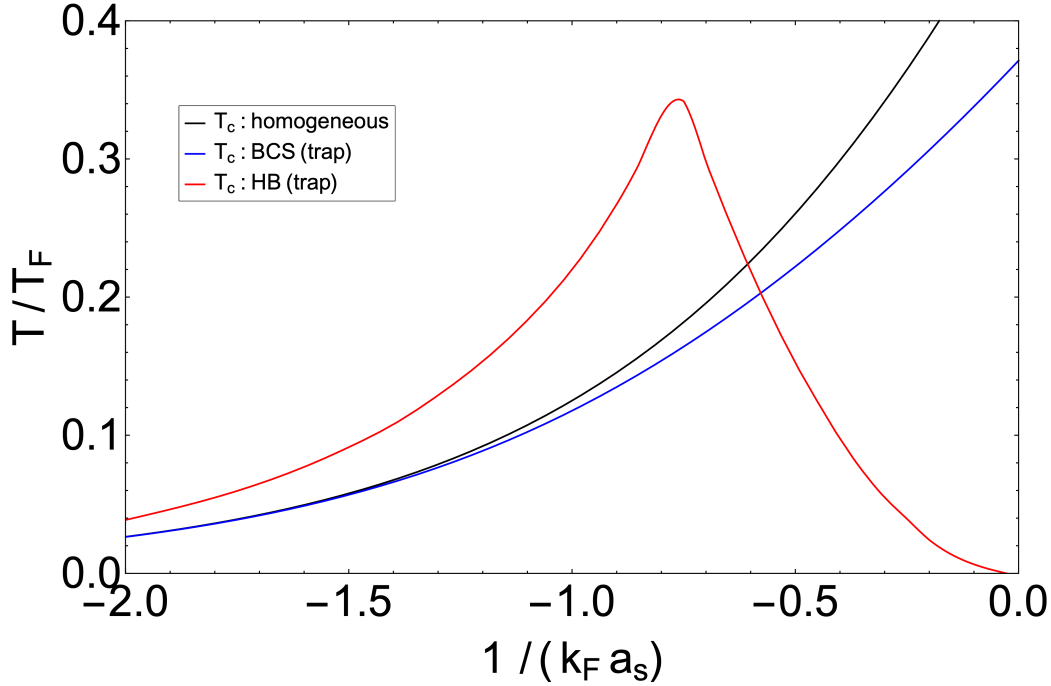
$$\lambda_F^3 n(R_c) \Big|_{\Delta(R_c)=0} = -2\pi^{3/2} \left( \frac{T}{T_F} \right)^{3/2} \text{Li}_{3/2} \left( -e^{\frac{\mu_H(R)|_{R=R_c}}{\epsilon_F} / \frac{T}{T_F}} \right). \quad (4.71)$$

Like the procedure discussed in subsec. 4.4.1,  $\mu(k_F a_s, T/T_F)$  and  $R_c(k_F a_s, T/T_F)$  of the HB theory also can be obtained by numerical calculation. Furthermore, for a given dimensionless interaction parameter  $k_F a_s$  the phase transition temperature  $T_c$  in harmonic trap can be defined. While  $T_c$  is a spatially dependent quantity, it is proportional to the density, as shown in (3.26). Since the density is largest at the centre of the trap,  $T_c(R=0)$  takes the maximum value there, and this value corresponds to the transition temperature in a harmonic trap. Therefore, at the given  $k_F a_s$ , the pair-value  $(T_c, \mu(T_c))$  can be calculated via (4.70) and (4.71) together with the particle number equation for the condition  $R_c = 0$ , where the HB particle number equation (4.66) is to be reduced to the Hartree particle number equation (4.57). The resulting  $T_c$  curves from BCS- and HB theory compared with homogeneous transition temperature are shown in Fig. 4.1.

In Fig. 4.1, BCS- $T_c$  in harmonic trap (blue) is lower than the  $T_c$  of homogeneous gas (black). This observation can be explained as follows. As the density distribution (4.31) of the trapped ideal Fermi gas at the ground state illustrates, in absence of interaction effects and thermal excitation, i.e. in the ideal Fermi gas model at the ground state, the uniform gas density  $n = 8\pi/(3\lambda_F^3)$  is realised at the trap centre, as in (4.32). Moreover, any thermal excitations in the trap give additional kinetic energies to the fermions in the trap, spreading them further from the trap centre. As the attractive interaction get stronger, corresponding pairing temperature becomes larger, however at the larger temperature the density in the trap centre decreases. Therefore  $T_c$  in trap is always lower than in the uniform gas, according to the mean-field BCS theory.

Nonetheless, this BCS-picture of the interplay between interaction and thermal excitation is yet incomplete. While particles get kinetic energies from thermal excitations and fly away to the outer region of the trap against the trapping potential, the attractive interaction, which gives a rise to the Cooper pairing, also attracts the flying away particles to the more dense region, i.e., the trap centre. This attraction effect from the Hartree channel is independent of the pair formation from the Bogoliubov channel. The Hartree- and HB theory takes this attraction into account, so for an attractive interaction the local density, especially the density at the trap centre, can be higher than the homogeneous density at finite temperatures, see Fig. 4.3. When this attractive interaction effect of the local squeezing of the density is combined with the Cooper pairing, resulting transition temperature (red in Fig. 4.1) in the BCS-regime becomes higher than  $T_c$  in the homogeneous case.

The HB theory correctly takes account of the another interaction effect which misses the BCS theory, thus should be considered as a more complete description. But this comes at a cost, as



**Figure 4.1:** Phase diagram based by BCS–Bogoliubov (BCS) theory and Hartree–Bogoliubov (HB) theory, in uniform homogeneous system and in harmonic trap based on the trap centre ( $T_c(\mathbf{x} = \mathbf{0})$ ).  $T_c$  in homogeneous Fermi gas (black) is calculated with (3.23), (3.24) or (3.72), (3.73). BCS-theoretical  $T_c$  in trapped Fermi gas (blue) is calculated with (4.21), (4.42) for  $\Delta(R=0) = 0$ . HB-theoretical  $T_c$  in trapped Fermi gas (red) is calculated with (4.67), (4.70) and (4.71) for  $\Delta(R=0) = 0$ . See [30] for mean-field transition temperature of uniform gas and [68] for the mean-field transition temperature of trapped Fermi gas.

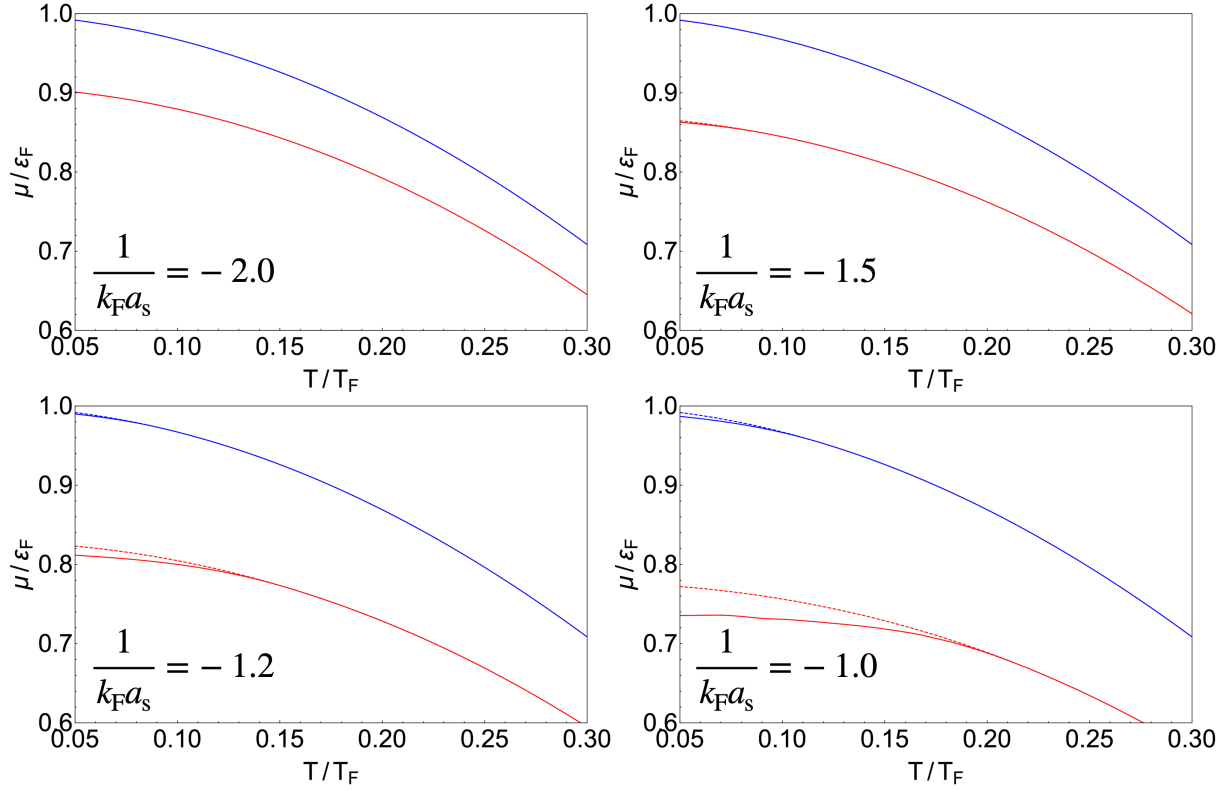
we can read from the peak of HB- $T_c$  at  $(k_F a_s)^{-1} \approx -0.8$  in Fig. 4.1. At this point the magnitude of the Hartree interaction energy  $|gn(\mathbf{x} = \mathbf{0})/2|$  is as large as the Fermi energy  $\hbar\bar{\omega}(3N)^{1/3}$ , and beyond this point  $T_c$  decreases and vanishes at unitarity, indicating the breakdown of the mean-field approximation.

#### 4.6.2 Density profile

Although one does not measure  $\mu$  directly in laboratory, as we will discuss in the next chapter 5, another observable effects like the density profile due to the interaction terms is reflected in this quantity. In other words, the effects of interaction and thermal excitation are reflected in  $\mu(k_F a_s, T/T_F)$ . In absent of interaction and thermal excitation it is  $\mu = \epsilon_F$ , and any contribution from interaction and thermal effects shifts  $\mu$  from the Fermi energy  $\epsilon_F$ . Since this chemical potential shift also differently quantified by different theories,  $\mu/\epsilon_F$  is a universal benchmark for comparison of different theories. This is most clearly to visualise at the ground state, where the boundary  $R(T=0) = r(T=0)/r_F \leq 1$  of the trapped atomic cloud is given by the square root of the chemical potential  $[\mu/\epsilon_F]^{1/2} = r/r_F$  depending of the interaction strength and theory. There, the ideal Fermi gas has the largest boundary of the Fermi radius  $r_{\text{ideal}}(T=0) = r_F$  than other interaction models due to its lack of interaction effect.

Motivated with this, we compare the chemical potential of trapped fermions by different mean-field theories at various interaction strengths and temperatures to interpret each interaction channel. Figure 4.2 compares the chemical potential  $\mu/\epsilon_F$  in harmonic trap from various mean-field theories. First, the interaction contributions of the Hartree and Bogoliubov channel are clear different in their magnitudes. In this attractive interacting BCS regime of  $(k_F a_s)^{-1} < -1$ ,

#### 4.6. HARTREE–BOGOLIUBOV THEORY



**Figure 4.2:** Chemical potential  $\mu/\epsilon_F$  of trapped Fermi as a function of temperature  $T/T_F$  at various scattering parameter  $(k_{Fa_s})^{-1}$  by various mean-field theories: ideal Fermi gas (blue dashed), BCS–Bogoliubov (blue), Hartree (red dashed) and Hartree–Bogoliubov (red).

the phase-free Hartree shift is much larger than the Bogoliubov contribution in the superfluid phase. Also, we notice that the Hartree shift in trap is no more constant as in the uniform gas, see 3.5, but becomes a temperature dependent curve. As the temperature drops, the Hartree shift becomes more significant. Although there is no phase transition temperature due to the Hartree channel, its contribution is also related to the thermal excitations, and the Hartree contribution becomes larger at lower temperature.

Now, it is possible to calculate the density profile with the determined  $\mu$ . The density distribution in the 3D coordinate space is given as follows:

##### Particle density by Hartree–Bogoliubov theory

$$n(\mathbf{x}) = \begin{cases} \frac{4\pi}{3\lambda_F^3} \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{3/2}}{\epsilon_{HB}(\epsilon_k, R)} \times \left[ \frac{|\Delta|^2(R)}{\epsilon_{HB}^2(\epsilon_k, R)} \tanh \frac{\beta \epsilon_{HB}(\epsilon_k, R)}{2} + \frac{(\epsilon_k - \mu(R))^2}{\epsilon_{HB}^2(\epsilon_k, R)} \frac{\frac{\beta \epsilon_{HB}(\epsilon_k, R)}{2}}{\cosh^2 \frac{\beta \epsilon_{HB}(\epsilon_k, R)}{2}} \right], & R(\mathbf{x}) < R_c \\ -\frac{2\pi^{3/2}}{\lambda_F^3} \left( \frac{T}{T_F} \right)^{3/2} \text{Li}_{3/2} \left( -e^{\frac{\mu_H(\mathbf{x})}{\epsilon_F} / \frac{T}{T_F}} \right), & R(\mathbf{x}) \geq R_c. \end{cases} \quad (4.72)$$

The areal density of trapped fermions by HB theory can be calculated with line-of-sight integration of (4.72) or substitution of  $\mu(x_i, x_j, R_k)$  (4.48) in the correspondent equation (4.49) of BCS theory by  $\mu_H(x_i, x_j, R_k)$  (4.61), where we read the resulting equation:

**Areal particle density by Hartree–Bogoliubov theory**

$$\begin{aligned}
n(x_i, x_j) &= 2 \frac{\bar{\omega}}{\omega_k} r_F \int_0^\infty dR_k n(x_i, x_j, R_k), \\
n(x_i, x_j, R_k) &= \begin{cases} \frac{4\pi}{3\lambda_F^3} \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{3/2}}{\epsilon_{HB}(\epsilon_k, x_i, x_j, R_k)} \\ \quad \times \left[ \frac{|\Delta|^2(x_i, x_j, R_k)}{\epsilon_{HB}^2(\epsilon_k, x_i, x_j, R_k)} \tanh \frac{\beta \epsilon_{HB}(\epsilon_k, x_i, x_j, R_k)}{2} \right. \\ \quad \left. + \frac{(\epsilon_k - \mu_H(x_i, x_j, R_k))^2}{\epsilon_{HB}^2(\epsilon_k, x_i, x_j, R_k)} \frac{\frac{\beta \epsilon_{HB}(\epsilon_k, x_i, x_j, R_k)}{2}}{\cosh^2 \frac{\beta \epsilon_{HB}(\epsilon_k, x_i, x_j, R_k)}{2}} \right], & R(x_i, x_j, R_k) < R_c \\ -\frac{2\pi^{3/2}}{\lambda_F^3} \left( \frac{T}{T_F} \right)^{3/2} \text{Li}_{3/2} \left( -e^{\frac{\mu_H(x_i, x_j, R_k)}{\epsilon_F} / \frac{T}{T_F}} \right) & , R(x_i, x_j, R_k) \geq R_c. \end{cases}
\end{aligned} \tag{4.73}$$

In a same way, the line density is obtained by spatial integration over the areal density (4.73) or substitution of the local chemical potential  $\mu(x_i, R_{jk})$  (4.51) in (4.52) by the Hartree-shifted local chemical potential (4.63), leading to the HB line density:

**Line particle density by Hartree–Bogoliubov theory**

$$\begin{aligned}
n(x_i) &= 2\pi \frac{\bar{\omega}^2}{\omega_j \omega_k} r_F^2 \int_0^\infty dR_{jk} R_{jk} n(x_i, R_{jk}), \\
n(x_i, R_{jk}) &= \begin{cases} \frac{4\pi}{3\lambda_F^3} \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \frac{\epsilon_k^{3/2}}{\epsilon_{HB}(\epsilon_k, x_i, R_{jk})} \\ \quad \times \left[ \frac{|\Delta|^2(x_i, R_{jk})}{\epsilon_{HB}^2(\epsilon_k, x_i, R_{jk})} \tanh \frac{\beta \epsilon_{HB}(\epsilon_k, x_i, R_{jk})}{2} \right. \\ \quad \left. + \frac{(\epsilon_k - \mu_H(x_i, R_{jk}))^2}{\epsilon_{HB}^2(\epsilon_k, x_i, R_{jk})} \frac{\frac{\beta \epsilon_{HB}(\epsilon_k, x_i, R_{jk})}{2}}{\cosh^2 \frac{\beta \epsilon_{HB}(\epsilon_k, x_i, R_{jk})}{2}} \right], & R(x_i, R_{jk}) < R_c \\ -\frac{2\pi^{3/2}}{\lambda_F^3} \left( \frac{T}{T_F} \right)^{3/2} \text{Li}_{3/2} \left( -e^{\frac{\mu_H(x_i, R_{jk})}{\epsilon_F} / \frac{T}{T_F}} \right) & , R(x_i, R_{jk}) \geq R_c. \end{cases}
\end{aligned} \tag{4.74}$$

We compare line densities of Fermi gas in a spherical trap at various parameters by different mean-field theories, see Fig. 4.3.

Beginning with common feature, first we note that every density profile will be more squeezed to the trap centre with decreasing temperature, meaning that the thermal excitation tends to spread out the particles towards the trap wing. This is straightforwardly to be interpreted as a consequence of the larger average kinetic energy at higher temperature. On the other hand, when there is an interaction effect, at the same given parameter  $(k_F a_s)^{-1}$  it will be more prominent at low temperatures.

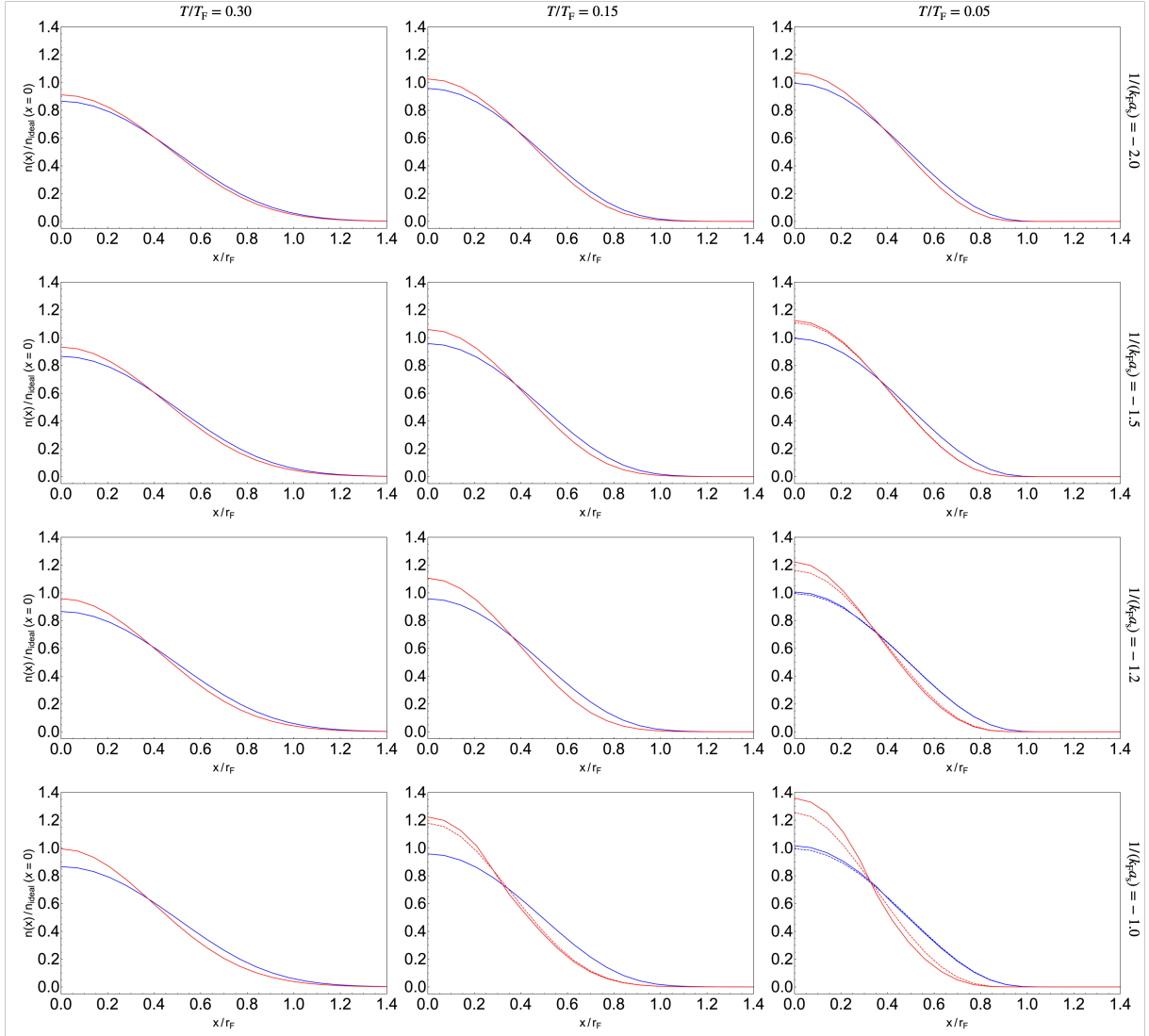
Now, we discuss the differences between theories. Ideal Fermi gas (curves in dashed blue) density only depends on temperature, however its thermal response itself is also most weak compared to the other mean-field theories with interaction. The BCS theory (curves in blue) introduces interaction effect indirectly by the Cooper pairing, which appears as a slight squeezing

#### 4.6. HARTREE–BOGOLIUBOV THEORY

in the trap centre below  $T_c$ . Due to the local phase separation (4.52), the BCS theory predicts a superfluid fraction at the trap centre surrounded by the thermal ideal Fermi gas in the trap outer regime. However, as it is already known [61], in the line density this effect appears almost invisible. Even for the strong attractive interaction of  $(k_F a_s)^{-1} = -1$  and at the extremely low temperature of  $T/T_F = 0.05$  (below right in Fig. 4.3), its density profile is barely distinguishable from the ideal Fermi gas. The Hartree theory (curves in dashed red) models interaction effect differently, namely a direct attraction between particles. Since the Hartree interaction is proportional to the density, its effect is most strong at the trap centre, where the density is largest, and becomes weak at the trap wings with decaying density. This locally varying Hartree attraction modifies the shape of density profile depending on the interaction parameter  $(k_F a_s)^{-1}$ , and in total its effect appears much larger than the BCS theory. In the Hartree theory, trapped Fermi gas become responsive to the interaction than in the BCS theory, so the Hartree theory can explain the experimentally observed shrinking of the clouds, for neither the ideal Fermi gas nor the BCS theory is able to. Although there is also similar qualitative behaviour described by the BCS theory, it turns out that the BCS theory fails to fit measured data, see ch. 5. And finally, combining the effects of both theories, the HB theory leads to the most distinguished result. Due to the higher density at the centre caused by the attractive Hartree interaction, the phase transition temperature is higher than the BCS theory, as one can read from Fig. 4.3. On the other hand, the particles in the superfluid phase do not stop to attractively interact each other. The combination of the Hartree and Bogoliubov channels enhances the order parameter  $\Delta$  compared to the BCS theory, so the superfluidity is more robust.

As the above discussion illustrates, including the Hartree term is essential for the trapped Fermi gas to be responsive of the interaction and the thermal effects. That the theoretical description of more strongly interaction and temperature dependent trapped Fermi gas by the Hartree and HB theory indeed agrees with the experiments, will be shown in the subsequent chapter 5.

## 4.6. HARTREE–BOGOLIUBOV THEORY



**Figure 4.3:** Line densities normalised by the ideal Fermi gas line density at the ground state in trap centre  $n_{\text{ideal}}(T = 0, x = 0)$  as a function of spatial coordinate normalised by the Fermi radius  $r_F$ , at various scattering parameters  $(k_F a_s)^{-1}$  and temperatures  $T/T_F$  by different mean-field theories: ideal Fermi gas (blue dashed), BCS–Bogoliubov (blue), Hartree (red dashed) and Hartree–Bogoliubov (red) theory.



## Chapter 5

# Experiment

In this chapter, we apply the theoretical model constructed in the preceding chapters for analysis of measured data from experiments on trapped interacting Fermi gas.

### 5.1 Method

In the ultracold dilute atomic gas, the s-wave scattering between  ${}^6\text{Li}$  atoms is experimentally controlled by the Feshbach resonance at the resonant frequency  $B_0 = 832.2$  G [69, 70, 71]. In the Widera research group, experiments with harmonically trapped  ${}^6\text{Li}$  atoms are conducted, where the interaction between the fermionic lithium atoms can be controlled by the Feshbach resonance technique. By taking an in-situ absorption image, we obtain the density distribution of trapped atoms as the areal density integrated over the  $x_3$ -direction. Another integration over  $x_1$  or  $x_2$  direction then yields the experimental line particle in  $x_2$  or  $x_1$  direction, respectively. The images of trapped fermionic  ${}^6\text{Li}$  atoms is prepared at two various Feshbach magnetic strength  $B = 1070$  G and  $B = 977.4$  G, where trapped gas was imaged at four various trapping parameter in each magnetic field strength, see Fig. 5.1. The total number of particle  $N$  should be experimentally measured.

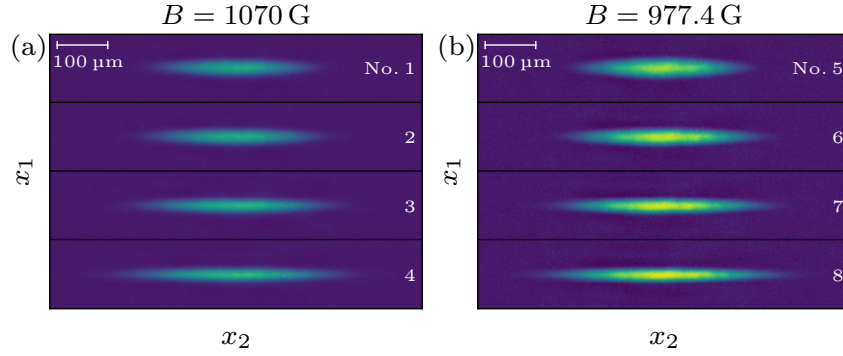
We have discussed in ch. 4 that the mean-field theories for trapped interacting fermions have only two parameters, the interaction parameter  $(k_F a_s)^{-1}$  and the temperature  $T/T_F$ . Since the parameter  $(k_F a_s)^{-1}$  is determined by the experimental setup, that is, the Feshbach magnetic field strength  $B$  which fixes the s-wave scattering length  $a_s(B)$ , the trapping frequencies  $(\omega_1, \omega_2, \omega_3)$  and the measured total number of the particle  $N$  that determine the Fermi wave vector  $k_F(\bar{\omega}, N)$ , the only remaining unknown parameter is the temperature. By means of the theoretically predicted density profile as a function of the interaction parameter  $k_F a_s$  and the temperature  $T/T_F$ , it is possible to deduce the temperature of a measured sample by fitting its density profile with mean-field theory. To this end, we evaluate the error between the theoretical line density  $n(x_i)$  and the measured line density  $n_{\text{ex}}(x_i)$  in  $x_i$ -direction:

$$\Delta n(T, x_i) = \sqrt{\frac{\sum_{m=1}^{N_j} [n^{(m)}(T, x_2) - n_{\text{ex}}^{(m)}(x_i)]^2}{N_j}} \quad (5.1)$$

where  $m$  indexes a measured point,  $N_j$  is the number of data samples in  $x_j$ -direction, where the indices  $i, j \in \{1, 2\}$  are for the spatial directions in the  $x_1$ - $x_2$  plane in Fig. 5.1, and  $i \neq j$ .

If calculation of the error (5.1) at various temperature results in a unique minimum at some finite temperature, the temperature at the minimum is identified with the temperature of the measured data. On the other hand, if there is no error minimum down to degenerate temperature given by the lowest temperature for the range of thermometry, ideally  $T = 0$ , then the

## 5.2. DATA ANALYSIS



**Figure 5.1:** in-situ absorption images of interacting  ${}^6\text{Li}$  atoms trapped in the harmonic trap with the Feshbach magnetic field (a)  $B = 1070$  G and (b)  $B = 977.4$  G. See Tab. 5.1 for the respective settings. Figure is taken from [11].

| No. | $B/\text{G}$ | $(\omega_1, \omega_2, \omega_3) / (2\pi\text{Hz})$ | $N/10^5$      | $1/(k_F a_s)$      | $T/T_F$           |
|-----|--------------|----------------------------------------------------|---------------|--------------------|-------------------|
| 1   | 1070         | (243, 26.6, 152)                                   | $4.8 \pm 0.2$ | $-1.505 \pm 0.011$ | $0.047 \pm 0.002$ |
| 2   | 1070         | (272, 26.6, 171)                                   | $5.2 \pm 0.2$ | $-1.428 \pm 0.010$ | $0.103 \pm 0.001$ |
| 3   | 1070         | (323, 26.6, 205)                                   | $5.8 \pm 0.2$ | $-1.324 \pm 0.008$ | $0.187 \pm 0.001$ |
| 4   | 1070         | (386, 26.6, 248)                                   | $6.4 \pm 0.2$ | $-1.226 \pm 0.007$ | $0.257 \pm 0.001$ |
| 5   | 977.4        | (210, 25.5, 129)                                   | $7.9 \pm 0.4$ | $-1.119 \pm 0.010$ | $0.073 \pm 0.010$ |
| 6   | 977.4        | (272, 25.5, 171)                                   | $8.4 \pm 0.5$ | $-1.010 \pm 0.009$ | $0.115 \pm 0.001$ |
| 7   | 977.4        | (323, 25.5, 205)                                   | $8.7 \pm 0.6$ | $-0.949 \pm 0.010$ | $0.182 \pm 0.002$ |
| 8   | 977.4        | (386, 25.5, 248)                                   | $9.0 \pm 0.6$ | $-0.887 \pm 0.009$ | $0.245 \pm 0.002$ |

**Table 5.1:** Experimental data and measured temperatures for the eight measured absorption images shown in Fig. 5.1. Table is taken from [11].

theory should be regarded as incapable of measuring the temperature of the sample.

The method depends on the choice of axis. Due to the experimental setup, the measurement profile has an elongated ellipsoidal shape with a short  $x_1$ -axis and a long  $x_2$ -axis. Between them, the short  $x_1$ -axis is not suited for the analysis due to its lower spatial resolution. Therefore we discard the data with the  $x_1$ -axis and choose the  $x_2$ -axis to fit the measurement data.

## 5.2 Data analysis

### 5.2.1 Feshbach magnetic field at 1070 G

At the Feshbach magnetic field strength  $B = 1070$  G,  ${}^6\text{Li}$  atoms in a dilute gas interact each other via s-wave contact scattering with the s-wave scattering length  $a_s = -3432.8 a_0$ , where  $a_0$  denotes the Bohr radius. Combination of this s-wave scattering length and the trapping frequencies, as well as the number of trapped atoms, enables experimental realisation of the inverse scattering parameter  $(k_F a_s)^{-1}$  ranging from -1.5 to -1.2. At this relatively weakly interacting BCS-regime, calculating the error at various temperatures with the mean-field Hartree theory and the HB theory offer the unique minimum for each data, see Fig. 5.2. In case of the data No.2–4, both the Hartree theory and the HB theory yield error minima at the same temperature, and therefore the correspondent measured samples must be in the normal fluid phase. For data No.1, the Hartree theory does not have an error minimum, and only the HB theory yields an error minimum for this data. Consequently, this sample is in the superfluid phase below  $T_c$  of

## 5.2. DATA ANALYSIS

the HB theory.

The ideal Fermi gas and the BCS theory do not yield the error minimum down to the degenerate temperature excepting the data No.4, where not only the Hartree theory having the error minimum at  $T = 0.257 T_F$ , but also the ideal Fermi gas theoretical calculation also yields the error minimum at  $T = 0.101 T_F$ . However we do not take the ideal Fermi gas temperature, as its error is larger than the Hartree theory and also the theory fails to offer a consistent thermometry for the lower temperature samples No.1–3 at the given  $a_s$ , see Fig. 5.2. Also in Fig 5.4, density profile of the Hartree theory agrees with the measurements better than the ideal Fermi gas. In this case, we are seeing the squeezing attractive interaction effect of the atomic cloud to the middle at higher temperature is simulated by thermal effects of confinement of thermally degenerate Fermi gas at the low temperature.

When the data sample is determined to be in the superfluid phase, besides of the particle density one can additionally evaluate the condensate density and the superfluid profile of the sample. As same as the line particle density, the line condensate density in  $x_2$ -direction is obtained by line-of-sight integration in  $x_1$  and  $x_3$  direction:

$$n_0(x_2) = \int dx_1 dx_3 n_0(\mathbf{x}) = \frac{\pi}{\lambda_F} \int dx_1 dx_3 \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \epsilon_k^{1/2} \frac{|\Delta|^2(\mathbf{x})}{\epsilon_{HB}^2(\epsilon_k, \mathbf{x})} \tanh \frac{\beta \epsilon_{HB}(\epsilon_k, \mathbf{x})}{2}. \quad (5.2)$$

Similarly, the superfluid line density can be calculated as:

$$\begin{aligned} n_{sf}(x_2) &= \int dx_1 dx_3 n_{sf}(\mathbf{x}) \\ &= \frac{4\pi}{3\lambda_F} \int dx_1 dx_3 \frac{1}{\epsilon_F^{3/2}} \int_0^\infty d\epsilon_k \epsilon_k^{3/2} \frac{|\Delta|^2(\mathbf{x})}{\epsilon_{HB}^3(\epsilon_k, \mathbf{x})} \left[ \tanh \frac{\beta \epsilon_{HB}(\epsilon_k, \mathbf{x})}{2} - \frac{\frac{\beta \epsilon_{HB}(\epsilon_k, \mathbf{x})}{2}}{\cosh^2 \frac{\beta \epsilon_{HB}(\epsilon_k, \mathbf{x})}{2}} \right]. \end{aligned} \quad (5.3)$$

The calculated line condensate density profile (5.2) and line superfluid density (5.3) as well as the density distribution are shown in Fig. 5.2 on top right in data No.1.

### 5.2.2 Feshbach magnetic field at 977.4 G

The Feshbach magnetic field strength  $B = 977.4$  G corresponds to the s-wave scattering length  $a_s = -4510.5 a_0$  for the interacting  $^6\text{Li}$  atoms. Correspondingly, experimentally realised interacting parameter regime is in the range between  $(k_F a_s)^{-1} = -1.2$  and  $(k_F a_s)^{-1} = -0.8$ , where the data No.5–8 in Fig. 5.1 are included. The thermometry on these data is shown in Fig. 5.3.

For this more strongly interacting case, the HB theory begins to exhibit unphysical behaviours. During the evaluation of error between the HB theory with data 7 and 8, the found error minima are at the temperatures slightly below  $T_c$ , so those samples are theoretically in superfluid phase, but there is no obvious difference between the Hartree theory and the HB theory. That is, while the temperature is below the transition temperature, the order parameter contributes negligibly small. Also the superfluidity effect does not help to fit the data, rather it raises deviation between the theory and the measurement. For these data No.7 and 8 at  $(k_F a_s)^{-1} > -1$ , while there are error minima with both theories, error minima with less amount of error. i.e. better fitting for experiments, are found with not the HB but the Hartree theory. The density profile of the Hartree theory lies precisely on top of the measured points, see two bottom density profiles on the right column in Fig. 5.3. Therefore, we label those data with the normal fluid samples for its smaller deviation with the Hartree theory. Also note that, when it comes to sheer thermometry issue, although two theories amount the temperature differently, the measured temperatures

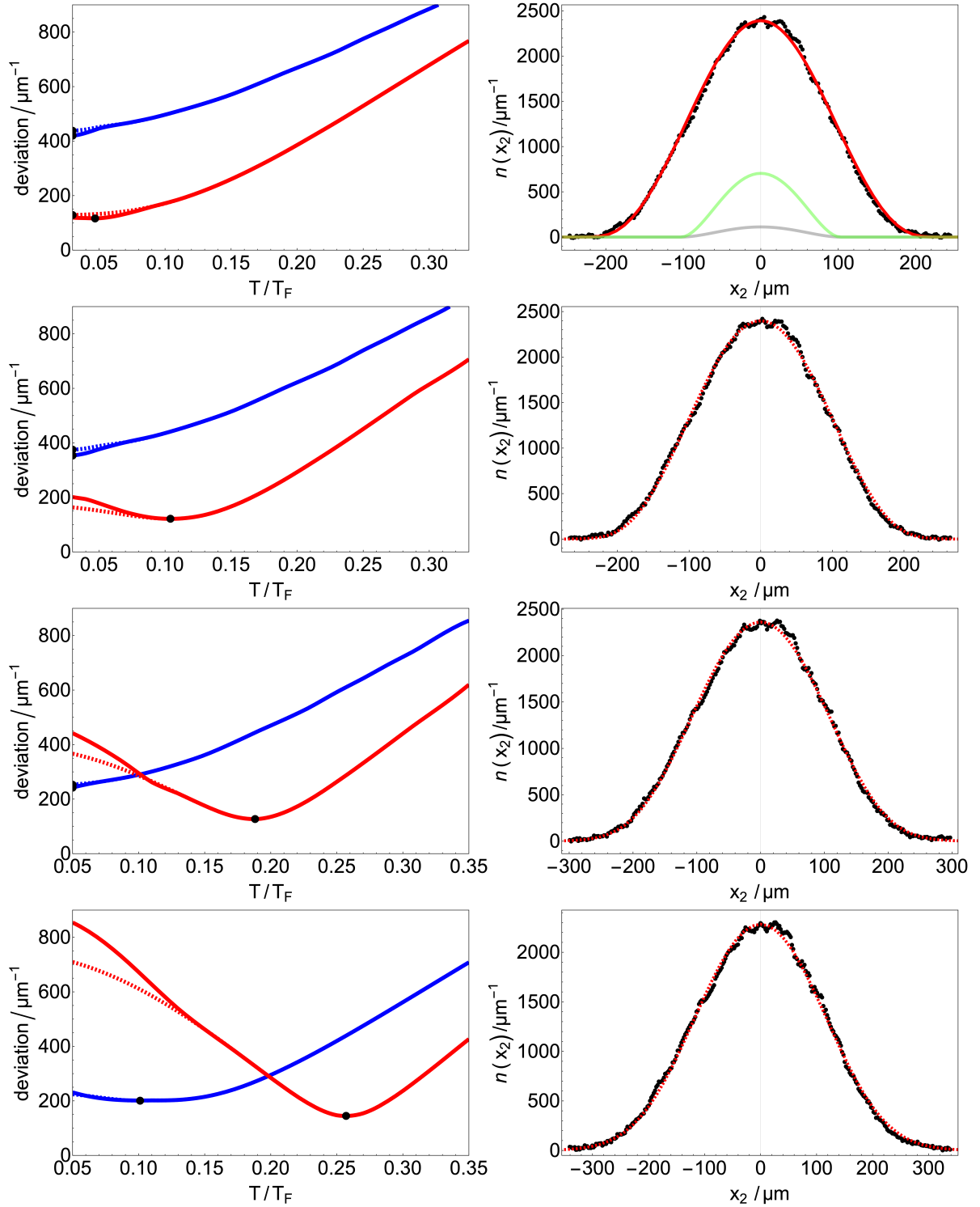
## 5.2. DATA ANALYSIS

are quite close to each other. Only problem is that, it is not clear whether the samples are in the normal fluid or in the superfluid phase. However, the thermometry problem is even more prominent with the data No.6. Non-unique error minima for this data is found at  $T = 0.115 T_F$  with the Hartree theory, and  $T = 0.162 T_F$  with the HB theory, while the Hartree theory shows smaller amount of deviation from the measurement, suggesting that the sample is in the normal fluid phase. And the density profile calculated by the Hartree theory with the temperature determined by the error minima of the Hartree theory agrees with the experiment, while the HB theoretical density profile deviates from data, see Fig. 5.5. The non-vanishing order parameter contribution is leading to a wrong direction. These observations imply the breakdown of the mean-field HB theory beyond its validity range  $(k_F a_s)^{-1} < -1$ . However, the mean-field Hartree theory still works well in this moderately strongly interacting regime, yielding the error minima for data No.6–8. Now, situation is different with the data No.5 at  $(k_F a_s)^{-1} = -1.119$ , as here the Hartree theory fails at fitting, and the unique error minimum arises from the HB theory. Also, the density profile calculated by the HB theory with non-negligible order parameter contribution overlays the measured density profile precisely. Therefore, the data is in the superfluid phase. As the data No.5 is in the validity range  $(k_F a_s)^{-1} < -1$  of the mean-field HB theory, the ambiguity with No.6–8 is again eliminated like the data No.1–4 in the former subsection 5.2.1, and its temperature and phase can be uniquely determined either by the Hartree theory or the HB theory. Its calculated condensate density as well as superfluid density is shown along with theoretical and measured particle density on top right in Fig. 5.3.

An overview of the thermometry is shown in Fig. 5.6. The data obtained in the deep BCS-regime  $(k_F a_s)^{-1} < -1.2$  with the Feshbach magnetic field  $B = 1070$  G, error minima from the Hartree and the HB theory agree each other, where only the HB theory can find the fit of the measured density profile below  $T_c$  with its distinguished density profile from the Hartree theory due to the superfluid core in the trap centre. In the strongly interacting regime  $(k_F a_s)^{-1} > -1.2$  measured at the Feshbach magnetic field  $B = 977.4$  G, some ambiguity arises concerning interpretation of the analysis with those theories as they yield different error minima. Here we should consider the magnitude of the minimum error with each theory, and error minima by the HB theory is more larger than the theory accompanied with numerical instabilities, as one reads from 5.3. It implies the different effective regime in the parameter space with different mean-field theories, where the HB theory fails for strong interactions and low temperatures.

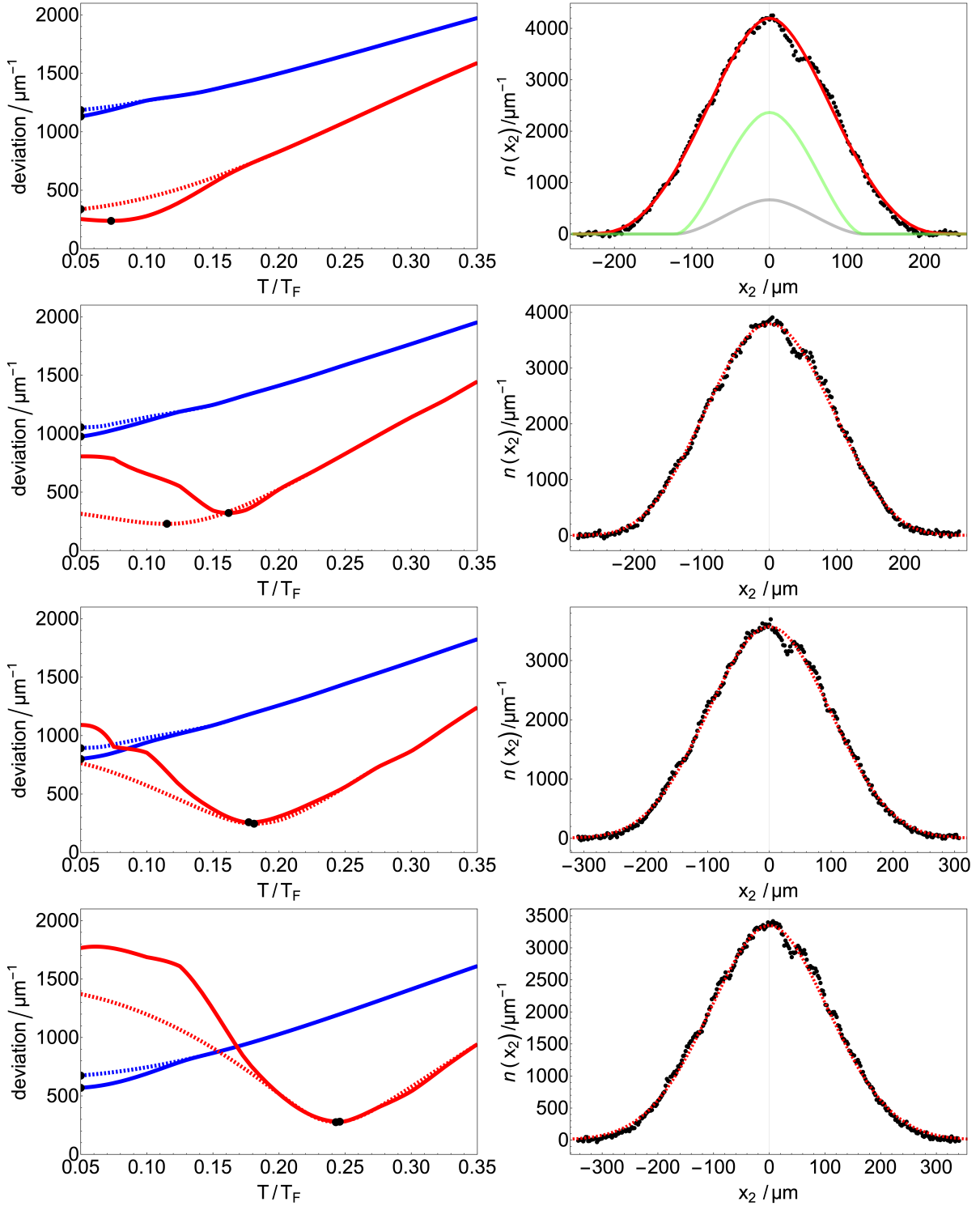
After the investigations with experimental data, we come to the conclusion that in the BCS limit the Hartree–Bogoliubov theory offers the best description among the mean-field theories studied in the thesis, including the BCS theory. With the theory it is possible to measure the temperature of the trapped interacting Fermi gas, that to our knowledge not has been available so far. Furthermore, based on the theory it is possible to infer the condensate density and the superfluid density. Thus, it is no more necessary to rely on indirect evidences like presence of vortices or formation of the bosonic condensate upon adiabatic ramping to the BEC side to find the fermionic superfluidity. Our analysis method based on the mean-field HB theory opens the possibility to measure the temperature and the superfluidity directly in the fermionic BCS regime.

## 5.2. DATA ANALYSIS

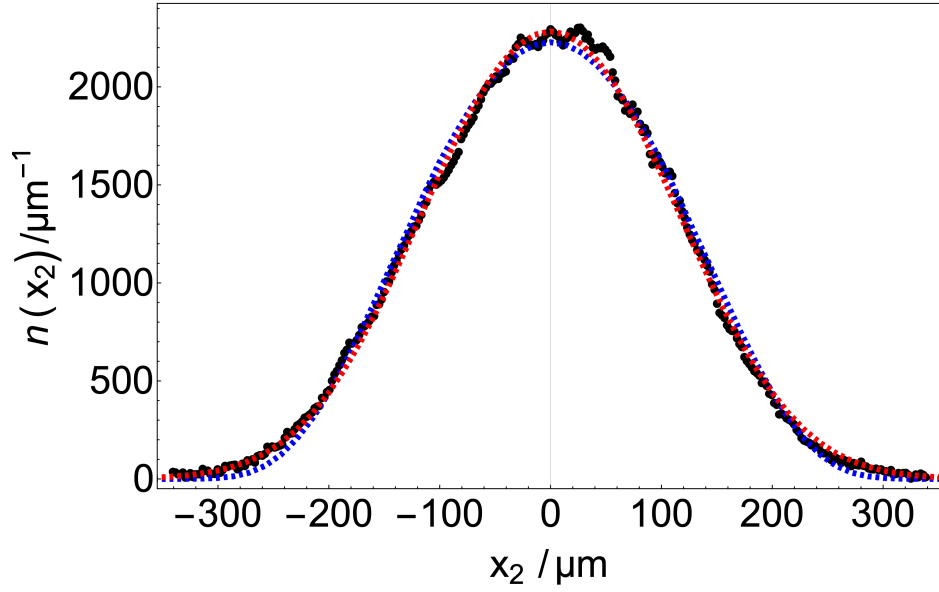


**Figure 5.2:** Data analysis of the measurement data No.1–4 in Fig. 4.3 and tab. 5.1 from top to bottom. Left column: error between the measurement and the mean-field theories: ideal Fermi gas (dashed blue), BCS–Bogoliubov (blue), Hartree (dashed red), and Hartree–Bogoliubov (red). Error Minima are marked with round points. Right column: line density from measurement (dots) and the theory at the fitted temperature with the minimal error. The line density of the data No.1 in the superfluid phase is shown with the line condensate density (grey) and the line superfluid density (green).

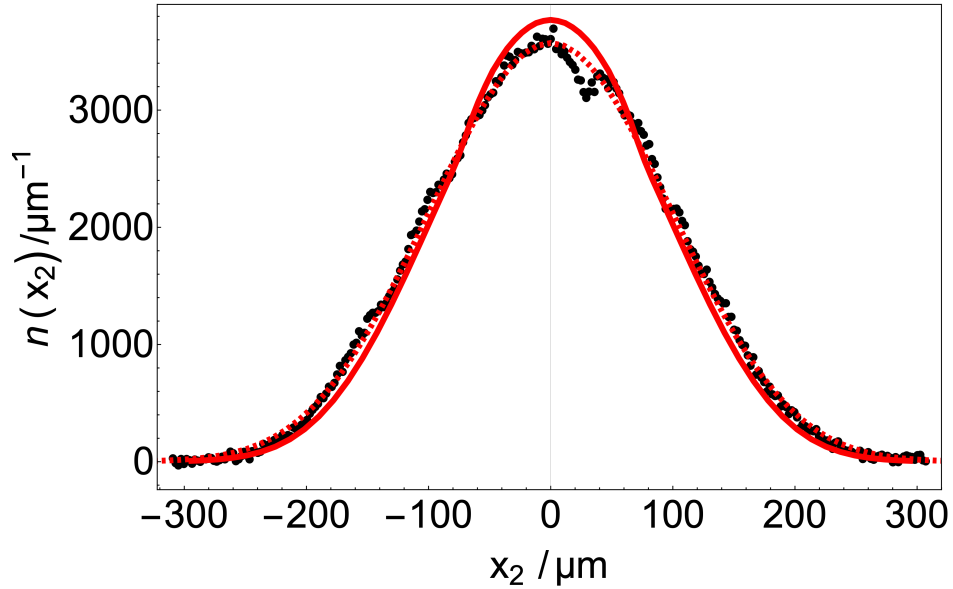
## 5.2. DATA ANALYSIS



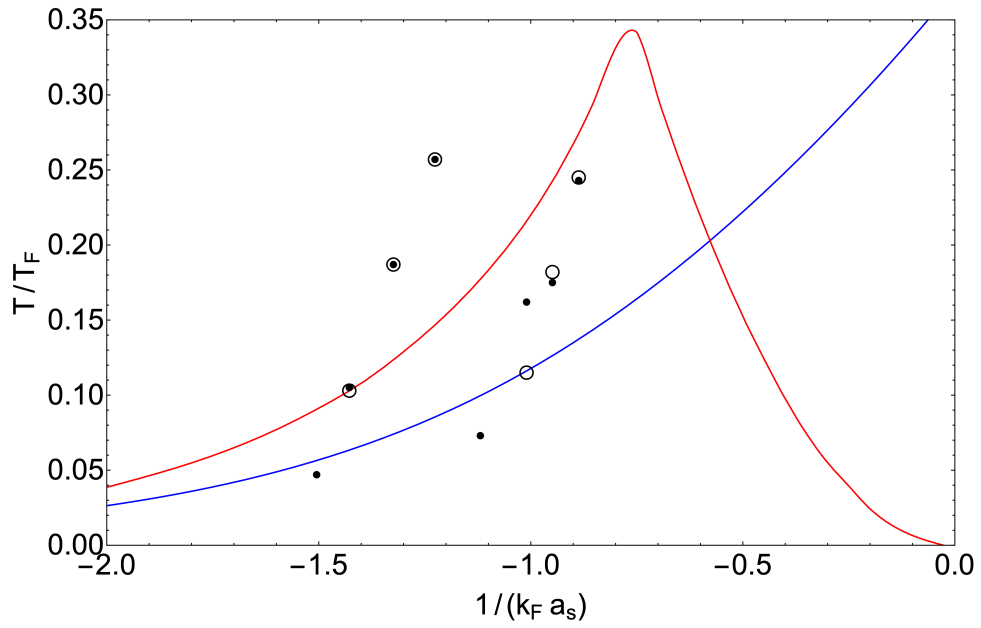
**Figure 5.3:** Data analysis of the measurement data No.5–8 in Fig. 4.3 and tab. 5.1 from top to bottom. Left column: error between the measurement and the mean-field theories: ideal Fermi gas (dashed blue), BCS–Bogoliubov (blue), Hartree (dashed red), and Hartree–Bogoliubov (red). Error Minima are marked with round points. Right column: line density from measurement (dots) and the theory at the fitted temperature with the minimal error. The line density of the data No.5 in the superfluid phase is shown with the line condensate density (grey) and the line superfluid density (green).



**Figure 5.4:** Density profiles with non-unique thermometry of the data No.4 by the ideal Fermi gas (dashed blue) at  $T = 0.101 T_F$  and by the Hartree theory (dashed red) at  $T = 0.257 T_F$ , shown with measured data (dots).



**Figure 5.5:** Density profiles with non-unique thermometry of the data No.6 by the Hartree theory (dashed red) at  $T = 0.115 T_F$  and by the Hartree-Bogoliubov theory (red) at  $T = 0.162 T_F$ , shown with measured data (dots).



**Figure 5.6:** Thermometry of the measured data No.1–8 in Fig.5.1, tab.5.1 from left to right by the Hartree theory (open circle) and the Hartree–Bogoliubov theory (point) in the phase diagram of trapped Fermi gas from the BCS theory (blue curve) and the Hartree–Bogoliubov theory (red curve).



## Chapter 6

# Conclusion

In this thesis, we have developed an extended mean-field theory for a dilute fermionic system with the Hartree–Fock–Bogoliubov (HFB) approximation. The theory categorises the possible two-body scattering processes into three channels. The Hartree channel characterises the normal interaction between particles, which is represented as an interaction energy proportional to the average density. The Fock channel describes a spin exchange process in the two-body scattering. Finally, the Bogoliubov channel corresponds to the pair creation and annihilation, and this term is responsible for the superfluidity of the fermionic system. Those mean-field interaction terms are determined by the variational approach, where their mean-field expectation values extremise the thermodynamic potential of the system. In the context of the BEC-BCS crossover, the chemical potential  $\mu$  and the order parameter  $\Delta$  of the system are calculated simultaneously as a function of the dimensionless Fermi-scaled temperature  $T/T_F$  and the dimensionless inverse scattering parameter  $(k_F a_s)^{-1}$  by means of the order parameter equation and the density equation. The phase transition temperature  $T_c/T_F$  for a given  $(k_F a_s)^{-1}$  is defined to be the temperature, where the order parameter  $\Delta(T/T_F)$  vanishes.

It is shown that the HFB mean-field theory reproduces the known mean-field theories in limiting cases, thus it is to be considered as a generalised model of interacting fermionic systems. By ignoring the Hartree and Fock terms, the theory is reduced to the BCS theory, as shown in sec. 2.2. If the order parameter is excluded, i.e., provided that the condition  $\Delta = 0$  is fulfilled, the HFB theory reduces to the Hartree–Fock theory, which is discussed in sec. 2.3. The Fock term vanishes in the spin-balanced case for an attractive contact interaction, see sec. 2.3 and 2.4, so the theory is further reduced to the Hartree theory in this case. Without any constraints, the theory turns out to be fully described by a Hartree–Bogoliubov (HB) theory, as derived in sec. 2.4.

In the HB theory, fermions are interacting via two distinguishable mechanisms, namely the normal Hartree interaction and the anomalous Cooper pairing. Above the transition temperature  $T_c$ , the fermionic many-body system is in the normal fluid phase and the theory describes directly interacting particles. Below  $T_c$  the system undergoes the phase transition due to the non-vanishing order parameter  $\Delta$ . The Cooper pairing and the phase coherence happen at the same temperature  $T_c$  simultaneously in the mean-field approximation, which is a reasonable one in the weakly interacting BCS-regime, see Fig. 1.3. Therefore below  $T_c$  the system is in the BCS-superfluid phase. According to the mean-field HB theory, particles are directly interacting with the Hartree interaction potential in both phases.

The mean-field HB theory is investigated both in the uniform and in the spatially inhomogeneous system under external harmonic trapping potential. The phase diagram is calculated in both cases, see Fig. 4.1. The attractive Hartree interaction leads to a larger density at the

trap centre and, thus, to an increased phase transition temperature. On the other hand, the Hartree interaction term is a dominating contribution in the BCS-regime, modifying the density distribution of the system. Furthermore, the additional interaction effect by the Hartree contribution cooperates with thermal excitations, emphasising the temperature dependence of the spatial density profile in the harmonic trap. Thus the fermionic system becomes more responsive to the interaction, as well as to the thermal excitation.

These theoretical predictions are reviewed by experiments of the Widera research group and are found to show remarkable agreements with their measured data, see the preprint [11]. The important finding is the effect of the interaction under spatial inhomogeneity. While there is no observable effect in the homogenous system, the local Hartree interaction term leads to measurable effects in experiments in presence of spatial inhomogeneities, like the modified density profile in a harmonic trap. The analysis of the measurement data concludes that either the Hartree term or the Bogoliubov term alone is not enough to explain the experimental results, but it is necessary to take into account both of them to be able to analyse the data. Especially, our theory offers a method for measuring the temperature of trapped Fermi gas by minimising error between theoretical calculation and measured data. To our knowledge, this is the first direct thermometry for interacting fermions, which so far has been impossible with the established BCS theory.

In conclusion, on the mean-field level, the Hartree–Bogoliubov theory is a better description than the BCS theory for interacting fermionic many-body systems. The HB theory explains the experiments more effectively than the BCS theory. Therefore, we argue that the Hartree interaction term can not be ignored, but should be integrated in the theory. Any issues caused by the Hartree term then must be handled properly with circumspection.

# Chapter 7

## Outlook

Based on the studies performed in the present thesis, we suggest the following possible goals for further researches.

### 7.1 Low-dimensional system

Physics in low-dimensional systems has been attracting considerable interest in condensed matter physics and led to many surprising predictions, a seminal example being the Berezinskii-Kosterlitz-Thouless (BKT) transition in two-dimensional (2D) system [72, 73]. The BKT transition is different from the normal to the superfluid phase transition in three-dimensional (3D) systems studied in this thesis. According to the Mermin–Wagner–Hohenberg–Coleman theorem, in a uniform 2D system there is no ODLRO at any finite temperature  $T > 0$ . However, another type of phase transition exists, namely the BKT phase transition that relies on energetically favourable states with or without proliferation and binding of vortices in a 2D gas [93].

Another important feature of low-dimensional systems is that both quantum and thermal fluctuations are generally larger than in higher dimensions. For this reason the low-dimensional systems are important, since in those systems phenomena related to quantum fluctuations, that are difficult to observe in a 3D system, can be identified.

Further complications can be added to the low-dimensional system by considering a non-trivial geometry on top of the dimensionality. A prominent example of such geometrically interesting low-dimensional systems is a bubble trap, where a gas can be confined to a spherical shell. Theoretical models of bosonic shell-shaped quantum gases for possible experiments have been suggested [75], as well as the BEC-BCS crossover in a bubble trap is theoretically studied [76]. It is expected that a quantum bubble trap for a fermionic gas can be realised in the near future.

When it comes to experiments, the preparation of a low-dimensional system is always realised via a dimensional reduction due to a manipulation of the trap geometry. In this case, the system is said to be quasi-low-dimensional, as for instance the quasi-2D uniform gas investigated in Ref. [74]. Such systems are necessarily spatially inhomogeneous, and might be subject to the Hartree term.

All these considerations raise questions regarding the meaning of the Hartree interaction in low-dimensional systems. For example, effects of the Hartree interaction on the BKT-transition in a quasi-2D system are an interesting question. Also, low-dimensional systems provide a foundation for investigating possible new effects arising from the fluctuation of the Hartree term. Finally, also studying the nature of BEC-BCS crossover on a curved manifold should benefit from insights of the Hartree–Fock–Bogoliubov theory.

## 7.2 Spin polarisation

During theoretical investigations throughout the thesis, we have restricted ourselves to the special case of a spin-balanced system. However, our formalism is open to be also extended to the spin-imbalanced case.

Around sixty years ago, shortly after the publication of the BCS theory, Fulde, Ferrell, Larkin and Ovchinnikov studied superconductivity in a spin-imbalanced system [78, 79]. They predicted the phase of Cooper pairing with a finite centre of mass momentum and a spatially oscillating order parameter that today is called the *Fulde–Ferrell–Larkin–Ovchinnikov (FFLO)* phase. Due to this spatial oscillation, the Hartree shift is usually considered even in absence of an external inhomogeneity when researching the spin-imbalanced case. In a 3D lattice, including the Hartree shift tends to enlarge the FFLO phase area in the polarisation-temperature phase diagram [80].

Furthermore, in combination with dimensionality the spin-polarisation leads to interesting observations. For instance, upon measuring the density profile of trapped spin-imbalanced fermionic atoms in a 1D array, it is found that the partially polarised core is surrounded by an either a completely paired or a fully polarised Fermi gas at proximities, which is contrasted with the superfluid core in the spin-balanced trapped 3D gas [81].

Such exotic phases in the spin-polarised Fermi gas is a viable topic suited for the HFB approach. Also, although it vanishes in the spin-balanced gas, the Fock contribution should be taken into account in the spin-polarised case, as it is related to the spin-exchange between particles.

## 7.3 Generalisation of the Hartree–Fock–Bogoliubov mean-field theory

In the Hartree–Fock–Bogoliubov mean-field approximation, each interaction channel is unbiasedly taken into account. While the theory explains experimental data in the BCS-regime quiet well, the approach is eventually unsuccessful with increasing interaction strength. In particular, the Hartree term is the source of an unphysical behaviour of the theory in the strongly interacting regime, which occurs even before reaching unitarity. This observation suggests that there might be a mechanism that suppresses the Hartree channel, depending on the parameters of the theory. Therefore, developing a systematic weighting for each interaction channel is a desirable refinement of the theory. In this respect, the Hartree–Fock–Bogoliubov theory with self-consistently weighted interaction channels is currently developed by N. Kaschweski et al., see [82].

At the end, the most natural extension of the present mean-field theory is to work out a beyond-mean-field theory. In fact, the problem is not only an issue of the Hartree term, but of the mean-field theory in general. It is also known that the mean-field BCS theory yields a diverging critical temperature curve in the BEC limit, see Fig. 1.3, and also leads to quantitatively incorrect results like the overestimated speed of sound at unitarity [59].

At unitarity and in the BEC-regime, the Hartree term is completely dominated by the fluctuations of the pairing channel, as the situation is described by the BCS beyond-mean-field theory within the functional integration approach [30]. However, when one tries to combine the Hartree and Fock channels into this approach, it is problematic to accomplish this with a Hubbard–Stratonovich transformation.

### 7.3. GENERALISATION OF THE HARTREE–FOCK–BOGOLIUBOV MEAN-FIELD THEORY

That being said, a possible Hartree–Fock–Bogoliubov beyond-mean-field theory will provide an even more accurate description along the whole crossover range [\[82\]](#).

### 7.3. GENERALISATION OF THE HARTREE-FOCK-BOGOLIUBOV MEAN-FIELD THEORY

# Appendices





## Appendix A

# Polylogarithm

The polylogarithmic function is a useful mathematical expression for description of various thermodynamic quantities. The *polylogarithm of the order  $s$*  is defined by:

$$\text{Li}_s(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^s} \quad (\text{A.1})$$

for  $s \in \mathbb{R}$  and on the disk  $z \in \mathbb{C}, |z| < 1$ . For  $|z| \geq 1$ , the function is defined by integral representation [53]:

$$\text{Li}_s(z) = \frac{z}{\Gamma(s)} \int_0^{\infty} dx \frac{x^{s-1}}{e^x - z} \quad (\text{A.2})$$

for  $\text{Re } s > 0$  and  $|\text{ph}(1 - z)| < \pi$ , or  $\text{Re } s > 1$  and  $z = 1$ .  $\Gamma(s)$  denotes the *gamma function*:

$$\Gamma(z) = \int_0^{\infty} t^{z-1} e^{-t} dt, \quad (\text{A.3})$$

having the recursive relation:

$$\Gamma(z + 1) = z\Gamma(z). \quad (\text{A.4})$$

Due to (A.4) the gamma function has poles for  $z \in \mathbb{Z}_{\leq 0}$ , since for  $z = 0$ :

$$\lim_{z \rightarrow 0} \Gamma(z) = \lim_{z \rightarrow 0} \frac{\Gamma(1)}{z} \quad (\text{A.5})$$

and so on for  $z = -1, -2, \dots$

Especially for  $s = 0$  and  $s = 1$  the polylogarithm is reduced to:

$$\text{Li}_0(z) = \frac{1}{z^{-1} - 1}, \quad (\text{A.6})$$

$$\text{Li}_1(z) = -\log(1 - z), \quad (\text{A.7})$$

as one can directly see from the definition:

$$\text{Li}_0(z) = \sum_{n=1}^{\infty} z^n = \sum_{n=0}^{\infty} z^{n+1} = \frac{z}{1 - z} = \frac{1}{z^{-1} - 1} \quad (\text{A.8})$$

and by means of the Mercator series:

$$\text{Li}_1(-z) = \sum_{n=1}^{\infty} \frac{(-1)^n z^n}{n} = - \sum_{n=1}^{\infty} \frac{(-1)^{n+1} z^n}{n} = -\log(1 + z). \quad (\text{A.9})$$

We note that (A.6) and (A.7) are related to the Bose–Einstein statistics and thermodynamic potential of a bosonic system. For fermionic systems we have:

$$-\text{Li}_0(-z) = \frac{1}{z^{-1} + 1}, \quad (\text{A.10})$$

$$-\text{Li}_1(-z) = \log(1 + z), \quad (\text{A.11})$$

correspond to the Fermi–Dirac statistics and the thermodynamic potential of a fermionic system.

There is a known relation, called the *duplication formula*, between the bosonic- and fermionic-polylogarithms for  $z \in \mathbb{R}$ :

$$\text{Li}_s(z) + \text{Li}_s(-z) = 2^{1-s} \text{Li}_s(z^2), \quad (\text{A.12})$$

which is shown by:

$$\begin{aligned} \text{Li}_s(z) + \text{Li}_s(-z) &= \sum_{n=1}^{\infty} \frac{z^n + (-1)^n z^n}{n^s} = 2 \sum_{n=1}^{\infty} \frac{z^{2n}}{(2n)^s} = 2^{1-s} \sum_{n=1}^{\infty} \frac{(z^2)^n}{n^s} \\ &= 2^{1-s} \text{Li}_s(z^2). \end{aligned} \quad (\text{A.13})$$

Especially for  $z = \pm 1$ :

$$(1 - 2^{1-s}) \underbrace{\text{Li}_s(1)}_{=\zeta(s)} = -\text{Li}_s(-1). \quad (\text{A.14})$$

(A.14) is related to the definition of the *Dirichlet-eta function* (*alternating zeta function*)  $\eta(s)$ :

$$\eta(s) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n^s} = (1 - 2^{1-s}) \zeta(s). \quad (\text{A.15})$$

The recursive relation for the derivative of polylogarithm is given by:

$$\frac{\partial}{\partial x} \text{Li}_s(f(x)) = \frac{f'(x)}{f(x)} \text{Li}_{s-1}(f(x)). \quad (\text{A.16})$$

The integration over Bose–Einstein or Fermi–Dirac distribution has a closed form in terms of the Bose–Einstein/Fermi–Dirac integrals [53]:

$$\text{Li}_{s+1}(e^x) = \frac{1}{\Gamma(s+1)} \int_0^{\infty} dt \frac{t^s}{e^{t-x} - 1}, \quad s > -1, x < 0 \text{ or } s > 0, x \leq 0, \quad (\text{A.17})$$

$$-\text{Li}_{s+1}(-e^x) = \frac{1}{\Gamma(s+1)} \int_0^{\infty} dt \frac{t^s}{e^{t-x} + 1}, \quad s > -1. \quad (\text{A.18})$$

The polylogarithmic expression (A.18) of the Fermi–Dirac integral offers great benefits for calculations of the density in the normal fluid phase and the thermal cloud of the trapped gas, and also helps finding the critical temperature, because it has a analytic form instead of the numerical integration. It also yields concise expressions of the thermodynamic quantities of the system in terms of the fugacity  $z = e^{\beta\mu}$ . Such expressions are also used for the density calculations of trapped bosons [28].

Yet there is a drawback. It turns out that the polylogarithm is cumbersome to calculate for

too large or too small quantities, making its numerical calculation unstable. This issue becomes more prominent as the temperature drops, where the inverse temperature value is large so that fugacity becomes very large or diminishing to very small quantity. It is therefore advisable to adopt an approximation for large thermal chemical potentials  $\beta\mu \rightarrow \pm\infty$ . Rough approximation for  $s > 0$  is given by [60]:

$$-\text{Li}_s(-e^x) \left\{ \begin{array}{l} \xrightarrow{x \rightarrow -\infty} e^x \\ \xrightarrow{x \rightarrow +\infty} \frac{x^s}{\Gamma(s+1)} \end{array} \right. . \quad (\text{A.19})$$

One can show the validity of the approximation as follows. For  $x \ll 0$  we find:

$$-\text{Li}_s(-e^x) = e^x - \sum_{n=2}^{\infty} \frac{(-1)^n e^{nx}}{n^s} = e^x + \mathcal{O}(e^{2x}), \quad x \ll 0 \quad (\text{A.20})$$

whereby the second alternating series term converges rapidly to zero. For the approximation in case of  $x \gg 0$  we begin with the Fermi–Dirac integral expression (A.18) of the polylogarithm:

$$-\text{Li}_s(-e^x) = \frac{1}{\Gamma(s)} \int_0^{\infty} dt \frac{t^{s-1}}{e^{t-x} + 1}. \quad (\text{A.21})$$

We note that the denominator of integrand is close to one for  $t \ll x$  and very large for  $t \gg x$ . This observation leads us to splitting of the integration range at  $t = x$  [63]:

$$\begin{aligned} -\text{Li}_s(-e^x) &= \frac{1}{\Gamma(s)} \left[ \int_0^x dt t^{s-1} - \int_0^x dt \frac{t^{s-1}}{e^{-(t-x)} + 1} + \int_x^{\infty} dt \frac{t^{s-1}}{e^{t-x} + 1} \right] \\ &= \frac{x^s}{\Gamma(s+1)} - \frac{1}{\Gamma(s)} \int_0^x dt \frac{t^{s-1}}{e^{-(t-x)} + 1} + \frac{1}{\Gamma(s)} \int_x^{\infty} dt \frac{t^{s-1}}{e^{t-x} + 1}, \end{aligned} \quad (\text{A.22})$$

where we have used the identity  $1/(x+1) = 1 - 1/(x^{-1}+1)$  at the first row and  $s\Gamma(s) = \Gamma(s+1)$  at the second row. Substituting  $u = x - t$  in second integrand and  $u = t - x$  in third integrand yields:

$$\begin{aligned} -\text{Li}_s(-e^x) &= \frac{x^s}{\Gamma(s+1)} + \frac{1}{\Gamma(s)} \int_x^0 du \frac{(x-u)^{s-1}}{e^u + 1} + \frac{1}{\Gamma(s)} \int_0^{\infty} du \frac{(x+u)^{s-1}}{e^u + 1} \\ &= \frac{x^s}{\Gamma(s+1)} + \frac{1}{\Gamma(s)} \int_0^{\infty} du \frac{(x+u)^{s-1} - (x-u)^{s-1}}{e^u + 1} + \frac{1}{\Gamma(s)} \int_x^{\infty} du \frac{(x-u)^{s-1}}{e^u + 1}. \end{aligned} \quad (\text{A.23})$$

Now we substitute again  $t = u - x$  for the last integral to get the polylogarithm:

$$\frac{1}{\Gamma(s)} \int_x^{\infty} du \frac{(x-u)^{s-1}}{e^u + 1} = \frac{(-1)^{s-1}}{\Gamma(s)} \int_0^{\infty} dt \frac{t^{s-1}}{e^{t+x} + 1} = -(-1)^{s-1} \text{Li}_s(-e^{-x}), \quad (\text{A.24})$$

so that we have:

$$-\text{Li}_s(-e^x) = \frac{x^s}{\Gamma(s+1)} + \frac{1}{\Gamma(s)} \int_0^{\infty} du \frac{(x+u)^{s-1} - (x-u)^{s-1}}{e^u + 1} - (-1)^{s-1} \text{Li}_s(-e^{-x}). \quad (\text{A.25})$$

We see that the integrand in the second integral term contributes very small amount for  $u \ll x$ . If we choose large  $x \gg 0$ , then the denominator is also very large compared to the numerator when  $u \geq x$ , so that the integrand remains small and integral converges to a very small amount.

And we have already observed that the second polylogarithm term also becomes negligible for large  $x \gg 0$ . In conclusion, for large  $x$  we can approximate:

$$-\text{Li}_s(-e^x) \approx \frac{x^s}{\Gamma(s+1)}, \quad x \gg 0. \quad (\text{A.26})$$

The rough approximation (A.19) of the fermionic polylogarithm can be interpreted as the density profile behaviour of the nearly degenerate trapped Fermi gas at low temperature. Since the three-dimensional spatial density is represented by the polylogarithm of the order  $3/2$ , for  $T \ll T_F$  the approximation (A.19) describes the fermionic density distribution  $n(\mathbf{x}) \propto (\epsilon_F - V_{\text{HO}}(\mathbf{x}))^{3/2}$  at  $T = 0$  in the central region of the trap, and the exponential vanishment  $n(\mathbf{x}) \propto T^{3/2} e^{-V_{\text{HO}}(\mathbf{x})/(k_B T)}$  at the wing. The polylogarithm interpolates between these two extreme regime. Here we see the difficulty of the thermometry of the trapped Fermi gas: the temperature dependence is only visible at the wing in the outer region [60]. And the density itself becomes very low and difficult to measure in these outer region, making the thermometry of the Fermi gas challenging.

The above approximation is computationally oriented and separately treated for each cases  $x \ll 0$  and  $x \gg 0$ . Considering physical problem, we can also find a systematical approximation of the fermionic polylogarithm by means of the *Sommerfeld expansion* for the nearly degenerate Fermi gas ( $T \ll T_F$ ), where we develop the series of the fermionic polylogarithm around the Fermi surface. The expansion is applied to integrals of the form [64]:

$$\int d\epsilon f(\epsilon) \frac{1}{e^{\frac{\epsilon-\mu}{k_B T}} + 1} \quad (\text{A.27})$$

in vicinity of  $k_B T \ll \mu$ , i.e. degenerate Fermi gas.

We first substitute  $x \rightarrow \beta\mu$  for (A.25) and write:

$$-\text{Li}_s(-e^{\beta\mu}) = \frac{(\beta\mu)^s}{\Gamma(s+1)} + \frac{1}{\Gamma(s)} \int_0^\infty du \frac{(\beta\mu + u)^{s-1} - (\beta\mu - u)^{s-1}}{e^u + 1} - (-1)^{s-1} \text{Li}_s(-e^{-\beta\mu}). \quad (\text{A.28})$$

The last polylogarithm is written in the series as:

$$-\text{Li}_s(-e^{-\beta\mu}) = \sum_{n=1}^{\infty} (-1)^{n-1} \frac{e^{-\beta\mu n}}{n^s}. \quad (\text{A.29})$$

The second integral term is to be expanded with the Newton's generalised binomial formula:

$$(x+y)^r = \sum_{n=0}^{\infty} \binom{r}{n} x^{r-n} y^n = \sum_{n=0}^{\infty} \frac{\Gamma(r+1)}{\Gamma(n+1)\Gamma(r-n+1)} x^{r-n} y^n \quad (\text{A.30})$$

for  $r \in \mathbb{R}$ . Then one applies (A.30) into (A.28):

$$\begin{aligned} \int_0^\infty dt \frac{(\beta\mu + t)^{s-1} - (\beta\mu - t)^{s-1}}{e^t + 1} &= \int_0^\infty du \frac{(\beta\mu)^{s-1}}{e^u + 1} \sum_{n=0}^{\infty} [1 - (-1)^n] \binom{s-1}{n} (\beta\mu)^{-n} u^n \\ &= 2(\beta\mu)^{s-1} \sum_{n=1}^{\infty} \underbrace{\binom{s-1}{2n-1}}_{\frac{\Gamma(s)}{\Gamma(2n)\Gamma(s-2n+1)}} (\beta\mu)^{-2n+1} \underbrace{\int_0^\infty du \frac{u^{2n-1}}{e^u + 1}}_{=-\Gamma(2n)\text{Li}_{2n}(-1)} \\ &= 2\Gamma(s) \sum_{n=1}^{\infty} \underbrace{(-\text{Li}_{2n}(-1))}_{=\eta(2n)} \frac{(\beta\mu)^{s-2n}}{\Gamma(s-2n+1)}. \end{aligned} \quad (\text{A.31})$$

Lastly, we can identify the first term in (A.28) with extended 0th term of the series above:

$$\underbrace{2\eta(0)}_{=1} \frac{(\beta\mu)^s}{\Gamma(s+1)} = \frac{(\beta\mu)^s}{\Gamma(s+1)}. \quad (\text{A.32})$$

From these follows the expanded form of the fermionic polylogarithm:

$$-\text{Li}_s(-e^{\beta\mu}) = 2 \sum_{n=0}^{\infty} \frac{\eta(2n)}{\Gamma(s-2n+1)} (\beta\mu)^{s-2n} + (-1)^{s-1} \sum_{m=1}^{\infty} (-1)^{m-1} \frac{e^{-\beta\mu m}}{m^s}. \quad (\text{A.33})$$

In the central region of the trap we can ignore the exponential term for  $T \ll T_F$ . This approximation yields the Sommerfeld expansion in  $\beta\mu \gg 0$ :

$$-\text{Li}_s(-e^{\beta\mu}) = \frac{(\beta\mu)^s}{\Gamma(s+1)} + \frac{2\eta(2)(\beta\mu)^{s-2}}{\Gamma(s-1)} + \frac{2\eta(4)(\beta\mu)^{s-4}}{\Gamma(s-3)} + \frac{2\eta(6)(\beta\mu)^{s-6}}{\Gamma(s-5)} + \dots \quad (\text{A.34})$$

The approximation (A.26) corresponds to the 0th order term of (A.34), which is usually known [60]. The 0th order approximation itself is temperature independent and exact for the degenerate Fermi gas ( $T = 0$ ), where  $\beta^s$  is canceled by the prefactor  $\beta^{-s}$  of the polylogarithm term in the equations of states<sup>1</sup>. We also note that the higher order correction terms gives small thermodynamical dependence of  $T$  which is absent in the 0th order approximation.

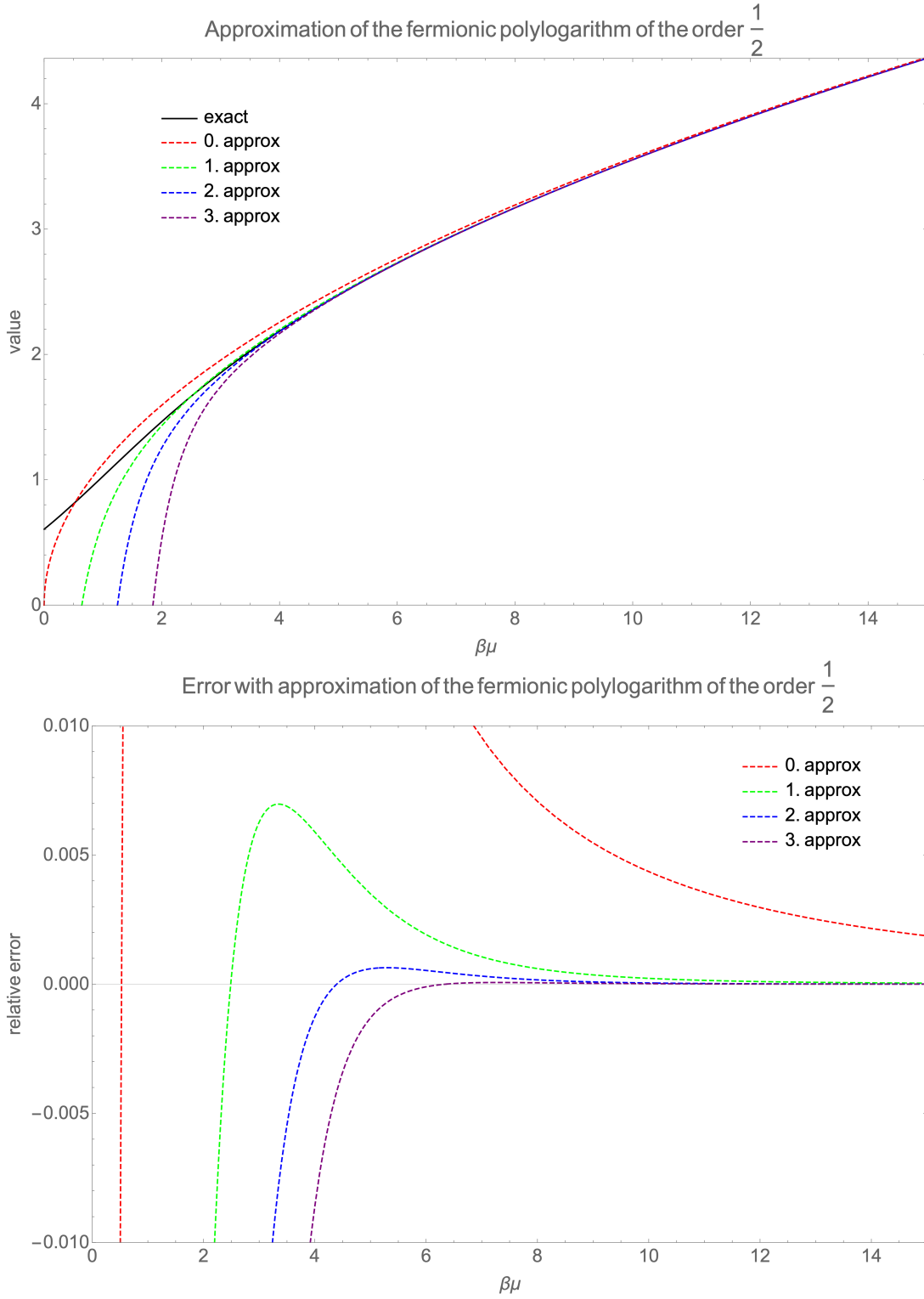
On the other hand, the series (A.34) breaks after the expansion order  $n \leq (s-1)/2$  if the polylogarithm order  $s$  is an integer. This is because the binomial series in (A.31) becomes finite for  $s \in \mathbb{Z}$  with the vanishing binomial coefficients at  $2n > s-1$ . For  $s \notin \mathbb{Z}$  the series is infinite.

For the bosonic polylogarithm  $\text{Li}_s(e^{\beta\mu})$  an analogous series expansion is known as the *Robinson formular* [97]:

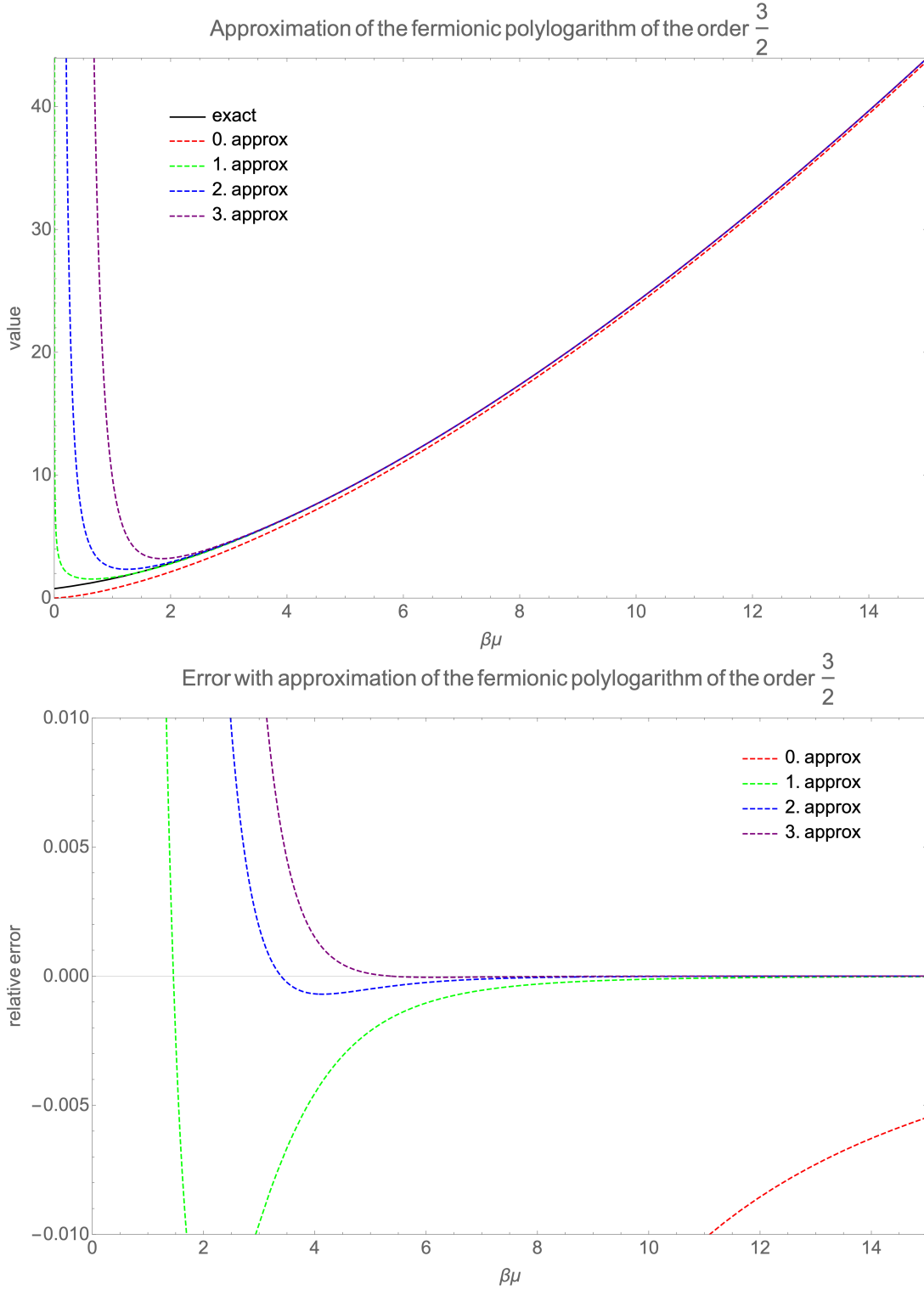
$$\text{Li}_s(e^{\beta\mu}) = \Gamma(-s+1)(-\beta\mu)^{s-1} + \sum_{n=0}^{\infty} \frac{\zeta(s-n)}{\Gamma(n+1)} (\beta\mu)^n. \quad (\text{A.35})$$

---

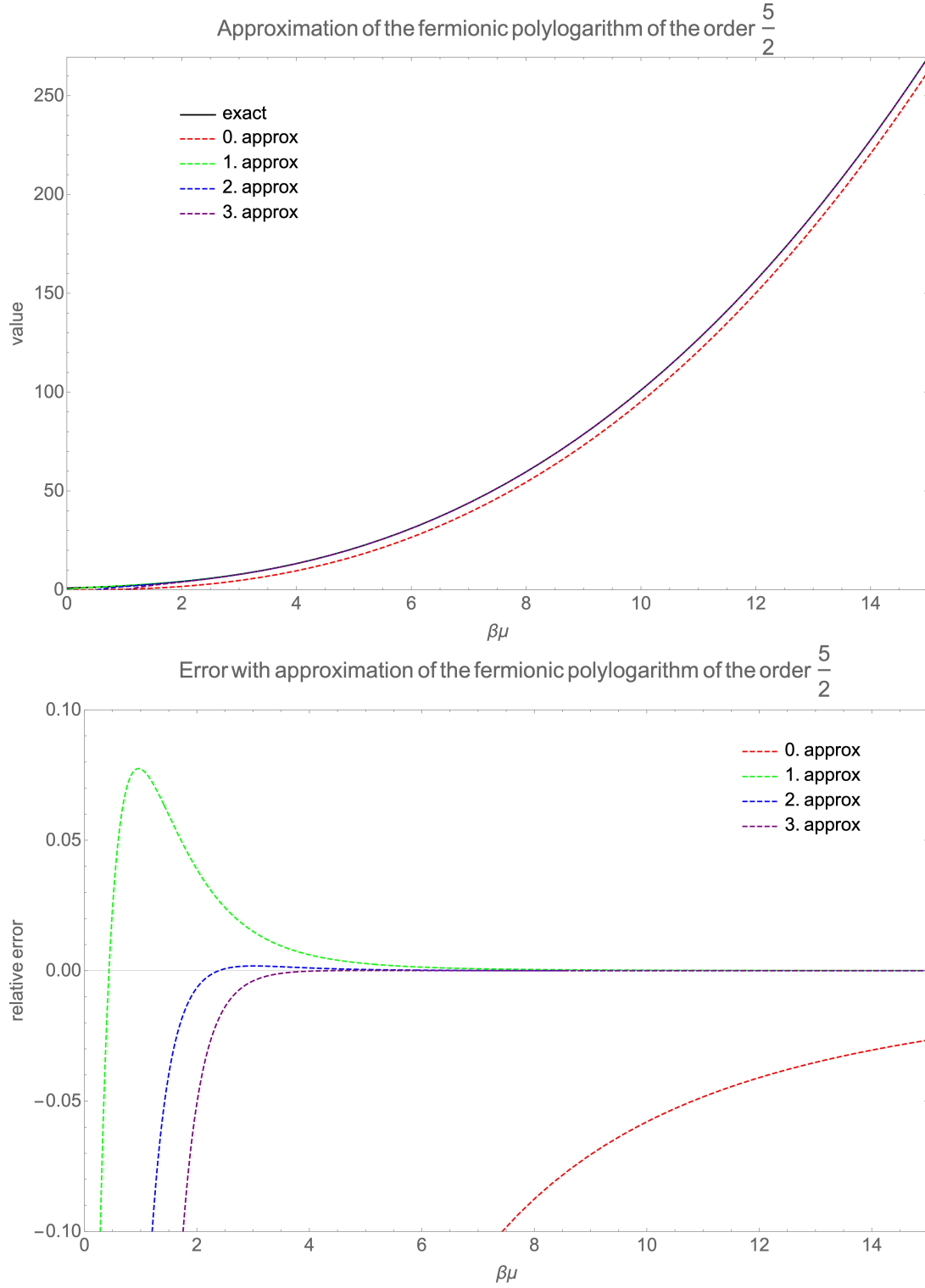
<sup>1</sup>For example, the density in the three-dimensional box is only proportional to  $\lim_{T \rightarrow 0} \mu^{3/2} = \epsilon_F^{3/2}$  at  $T = 0$ . This is well-known as the Fermi sea.



**Figure A.1:** Plot of the approximations (A.34) of the fermionic polylogarithm of the order  $1/2$  (above) and the relative error of the approximation (below). The relative error is calculated by  $(\text{approx}(x) - \text{exact}(x))/\text{exact}(x)$ .



**Figure A.2:** Plot of the approximations (A.34) of the fermionic polylogarithm of the order  $3/2$  (above) and the relative error of the approximation (below). The relative error is calculated by  $(\text{approx}(x) - \text{exact}(x))/\text{exact}(x)$ .



**Figure A.3:** Plot of the approximations (A.34) of the fermionic polylogarithm of the order  $5/2$  (above) and the relative error of the approximation (below). The relative error is calculated by  $(\text{approx}(x) - \text{exact}(x))/\text{exact}(x)$ .



## Appendix B

# Hypergeometric Function

The hypergeometric function is pervasive in many branches of mathematics thanks to its rich properties in various contexts. In physics, the function offers solutions for many problems as differential equation:

$$u''(z) + P(z)u'(z) + Q(z)u(z) = 0, \quad (\text{B.1})$$

where  $P(z)$  and  $Q(z)$  are at first arbitrary functions of  $z$ . Any linear, second order, homogeneous differential equations can be written in the form of (B.1). If the differential equation has at most three singularities—as in the most cases—, those singularities can be transformed to three points  $(0, 1, \infty)$  on the extended complex plane  $\mathbb{C} \cup \{\infty\}$  being  $\infty$  the complex infinity, whereby  $P(z)$  and  $Q(z)$  becomes rational functions of  $z$ <sup>1</sup>. Then the differential equations turns into the form of [86, 88]:

$$z(1-z)u''(z) + [c - (1+a+b)z]u'(z) - abu(z) = 0 \quad (\text{B.2})$$

with parameters  $a, b, c \in \mathbb{C}$ , called the *Gauss's hypergeometric equation* or the *differential equation of the Gauss type*. In other words, we can transform the differential equations of our interests to the single one of the Gauss type (B.2). The solution to the Gauss hypergeometric equation is the *Euler–Gauss hypergeometric function* [85], or shortly the *hypergeometric function* that is defined by the *Gauss series* [53, ?, 85]:

$$\begin{aligned} {}_2F_1(a, b; c; z) &= \sum_{n=0}^{\infty} \frac{a^{\overline{n}} b^{\overline{n}}}{c^{\overline{n}} n!} z^n = 1 + \frac{ab}{c} z + \frac{a(a+1)b(b+1)}{c(c+1)2!} z^2 + \dots \\ &= \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(b+n)}{\Gamma(c+n)\Gamma(n+1)} z^n \end{aligned} \quad (\text{B.3})$$

for  $a, b, c \in \mathbb{C}$  with exception of  $c \notin \mathbb{Z}_{\leq 0}$  and  $z \in \mathbb{C}_{|z|<1}$ . The series absolutely and uniformly convergent on the unit disk  $|z| < 1$ , and the convergence extends if  $\text{Re}(a+b-c) < 0$ .  $x^{\overline{n}}$  is the Capelli notation for the rising factorial:

$$x^{\overline{n}} = \prod_{i=0}^{n-1} (x+i) = x(x+1)(x+2)\dots(x+n-2)(x+n-1) = \frac{(x+n-1)!}{(x-1)!} \quad (\text{B.4})$$

for  $x \in \mathbb{N}$  and  $n \in \mathbb{N}$ . The Analytic continuation for  $x \in \mathbb{C}$  of the rising factorial is done by substitution of the factorial by the gamma function:

$$x^{\overline{n}} = \frac{\Gamma(x+n)}{\Gamma(x)}. \quad (\text{B.5})$$

Observe that  $x^{\overline{n}} = 0$  for  $x \in \mathbb{Z}_{\leq 0}$  and  $n > |x|$ . Therefore, for  $a \in \mathbb{Z}_{\leq 0}$  or  $b \in \mathbb{Z}_{\leq 0}$  the series

---

<sup>1</sup>Refer Ch.15 in [86] for the transformation procedure by means of the Riemann differential equation.

(B.3) breaks at finite order. In this case, for  $n \leq |x|$  the poles of the gamma function (A.5) in numerator and denominator in (B.5) cancel each other, and the hypergeometric function is reduced to a polynomial of  $z$  [86].

One of the significance of the hypergeometric function lies in its revealing power of complicated relationships among the combinatorial numbers generalising the binomial series [85]. To see this, we take an example of the Stirling numbers. First note that the binomial series for  $z \in \mathbb{R}_{|z|<1}$  and  $a \in \mathbb{R}$ :

$$(1+z)^a = \sum_{n=0}^{\infty} \binom{a}{n} z^n \quad (\text{B.6})$$

is the generating function of a binomial coefficient [85]:

$$\binom{a}{n} = \frac{a(a-1)\dots(a-n+1)}{n!} = \frac{a^n}{n!} = \frac{\Gamma(a+1)}{\Gamma(n+1)\Gamma(a-n+1)}. \quad (\text{B.7})$$

The symbol  $x^n$  denotes the falling factorial, which defined as:

$$x^n = \prod_{i=0}^{n-1} (x-i) = x(x-1)(x-2)\dots(x-n+2)(x-n+1) = \frac{x!}{(x-n)!} \quad (\text{B.8})$$

for  $x \in \mathbb{N}$  and  $n \in \mathbb{N}$ , and its analytical continuation for  $x \in \mathbb{C}$  is again given by the Gamma function:

$$x^n = \frac{\Gamma(x+1)}{\Gamma(x-n+1)}. \quad (\text{B.9})$$

The falling factorial is the generating function for the *Stirling number of the first kind*  $s(n, k) \in \mathbb{Z}$ :

$$x^n = \sum_{k=0}^n s(n, k) x^k, \quad (\text{B.10})$$

where  $s(n, k)$  can be positive or negative integer, as one reads from the definition of the falling factorial (B.8). Continuing to the first kind, the *Stirling number of the second kind*  $S(n, k) \in \mathbb{Z}_{\geq 0}$  is defined as the expansion coefficients of  $x^n$  as the series expansion of the falling factorial:

$$x^n = \sum_{k=0}^n S(n, k) x^k, \quad (\text{B.11})$$

and  $S(n, k)$  is same to the number of partitions of  $\{1, 2, \dots, n\}$  into  $k$ -nonempty subsets [53].

In this context, the rising factorial is also the generating function of the *unsigned Stirling number of the first kind*  $c(n, k) \in \mathbb{Z}_{\geq 0}$ :

$$x^{\bar{n}} = \sum_{k=0}^n c(n, k) x^k = \sum_{k=0}^n |s(n, k)| x^k, \quad (\text{B.12})$$

which is the number of permutations of  $\{1, 2, \dots, n\}$  with  $k$ -cycles [53]. Since the structure of the rising- and falling factorial only differ in the alternating sign of the sequence, the generated  $n$ -th coefficients are also only different in their signs by  $(-1)^{n-k}$ . That is, the Stirling number of the first kind is given by  $s(n, k) = (-1)^{n-k} c(n, k)$ . Between the String numbers of the first and the second kind holds the relation:

$$c(n, k) = (-1)^{n-k} s(n, k) = S(-k, -n), \quad (\text{B.13})$$

following from their definitions. Therefore the rising- and falling factorials are related by:

$$\begin{aligned} a^{\overline{n}} &= (a + n - 1)^{\overline{n}} = (-1)^n (-a)^{\underline{n}} \\ &\Leftrightarrow \\ a^{\underline{n}} &= (a - n + 1)^{\overline{n}} = (-1)^n (-a)^{\overline{n}}. \end{aligned} \quad (\text{B.14})$$

With above one finds [88]:

$$(1 - z)^a = \sum_{n=0}^{\infty} \frac{a^{\underline{n}}}{n!} (-z)^n = \sum_{n=0}^{\infty} \frac{(-1)^n \sum_{k=0}^n s(n, k) a^k}{n!} z^n = \sum_{n=0}^{\infty} \frac{(-1)^n \sum_{k=0}^n (-1)^{n-k} c(n, k) a^k}{n!} z^n \quad (\text{B.15})$$

$$= \sum_{n=0}^{\infty} \frac{(-a)^{\overline{n}}}{n!} z^n, \quad (\text{B.16})$$

which with (B.3) leads to the identity [86]:

$$(1 - z)^{-a} = \sum_{n=0}^{\infty} \left( \begin{matrix} a \\ n \end{matrix} \right) z^n = {}_2F_1(a, b; b; z), \quad (\text{B.17})$$

and it is the generating function of the multiset coefficient  $\left( \begin{matrix} a \\ n \end{matrix} \right) = (n!)^{-1} \sum_{k=0}^n c(n, k) a^k$ , i.e. the number of  $k$ -elements multisets of  $\{1, 2, \dots, n\}$ :

$$\left( \begin{matrix} a \\ n \end{matrix} \right) = \frac{a(a+1)\dots(a+n-1)}{n!} = \frac{a^{\overline{n}}}{n!} = \frac{\Gamma(a+n)}{\Gamma(n+1)\Gamma(a)}, \quad (\text{B.18})$$

c.f. (B.6) and (B.7). The binomial series and the hypergeometric functions in the special case  $b = c$  ((B.6) and (B.17)) are the generating functions of the binomial- and the multiset coefficients ((B.7) and (B.18)), where again the binomial- and multiset coefficients multiplied by  $n!$  are the generating functions of the signed- and unsigned Stirling number of the first kind ((B.10) and (B.12)), respectively.

In contrast to the binomial coefficient (B.7), whose underlying elements are distinguishable, the multiset coefficient (B.18) allows repeated elements in each subsets, meaning that the underlying elements are indistinguishable. Also from (B.17) the motivation of the naming “hypergeometric” becomes clear, as it is conceived as a generalisation of the geometric series.

|       |     | Repetition                                                         |                               |
|-------|-----|--------------------------------------------------------------------|-------------------------------|
|       |     | Yes                                                                | No                            |
| Order | Yes | sequence<br>$n^k$                                                  | permutation<br>$n!/(n-k)!$    |
|       | No  | multichoose<br>$\left( \begin{matrix} n \\ k \end{matrix} \right)$ | combination<br>$\binom{n}{k}$ |

**Table B.1:** Permutation and combination of  $n$ -elements set and  $k$ -elements subsets.

The analytic continuation of the Gauss hypergeometric function (B.3) for  $|z| \geq 1$  can be given by the integral representation [53, 88] (called the *Euler formula* for the hypergeometric function [86]):

$${}_2F_1(a, b; c; z) = \frac{1}{\text{B}(a, c-a)} \int_0^1 dt \frac{t^{b-1} (1-t)^{c-b-1}}{(1-zt)^a} \quad (\text{B.19})$$

for  $\text{Re}(c) > \text{Re}(b) > 0$ . Here, the symmetric symbol  $B(w_1, w_2) = B(w_2, w_1)$  stands for the *Euler-beta function* [94]:

$$B(w_1, w_2) = \int_0^1 dt t^{w_1-1} (1-t)^{w_2-1} = \frac{\Gamma(w_1)\Gamma(w_2)}{\Gamma(w_1+w_2)} \quad (\text{B.20})$$

with  $w_1, w_2 \in \mathbb{C} : \text{Re}(w_1), \text{Re}(w_2) > 0$ , which can be seen as a generalisation of the binomial- and multiset coefficient:

$$\frac{1}{B(w_1, w_2 + 1)} = (w_1 + w_2 + 1) \binom{w_1 + w_2}{w_2} = (w_1 + w_2) \left( \binom{w_1}{w_2} \right). \quad (\text{B.21})$$

Also note the relation [84]:

$${}_2F_1(a, b; c; z) = (1-z)^{-a} {}_2F_1\left(a, c-b; c; \frac{-z}{1-z}\right), \quad (\text{B.22})$$

which follows from (B.19).

Similar to the recursive relation for the derivative of the polylogarithm (A.16), the recursive derivative of the hypergeometric function reads:

$$\frac{\partial}{\partial x} {}_2F_1(a, b; c; f(x)) = \frac{ab}{c} f'(x) {}_2F_1(a+1, b+1; c+1; f(x)), \quad (\text{B.23})$$

which results from the derivative of the power series.

Furthermore, there are special relations between the hypergeometric functions. The following hypergeometric functions  ${}_2F_1(a \pm 1, b; c; z)$ ,  ${}_2F_1(a, b \pm 1; c; z)$ ,  ${}_2F_1(a, b; c \pm 1; z)$  are called *contiguous* to  ${}_2F_1(a, b; c; z)$ . Among them holds linear dependent relations, called the *contiguous relations*. There are 16 contiguous relations given by F. Gauss, for example [53, ?]:

$$(c-a){}_2F_1(a-1, b; c; z) + [2a-c-(a-b)z]{}_2F_1(a, b; c; z) + a(z-1){}_2F_1(a+1, b; c; z) = 0. \quad (\text{B.24})$$

By repeated application of the contiguous relations, the hypergeometric function  ${}_2F_1(a+l, b+m; c+n; z)$  can be expressed by linear combination of  ${}_2F_1(a, b; c; z)$  and its contiguous functions for  $l, m, n \in \mathbb{Z}$  [90].

An another important feature of the hypergeometric function is its generality. With the parameters  $a, b$  and  $c$ , many special functions consist of elementary functions can be represented as a special case of the hypergeometric function. For example, (A.6) and (A.10) are:

$$z \cdot {}_2F_1(1, b; b; \pm z) = \frac{z}{1 \mp z} = \pm \text{Li}_0(\pm z) \quad (\text{B.25})$$

due to (B.17), and also (A.7) and (A.11) are given by [?, 85]:

$$z \cdot {}_2F_1(1, 1; 2; \pm z) = \mp \log(1 \mp z) = \pm \text{Li}_1(\pm z). \quad (\text{B.26})$$

More generally, polylogarithm of a positive integer order  $n \in \mathbb{Z}_{>0}$  can be represented by means of the generalised hypergeometric function:

$${}_pF_q(a_1, \dots, a_p; b_1, \dots, b_q; z) = \sum_{n=0}^{\infty} \frac{\prod_{i=1}^p a_i^{\bar{n}}}{\prod_{j=1}^q b_j^{\bar{n}} n!} z^n \quad (\text{B.27})$$

as [89]:

$$\text{Li}_n(z) = z \cdot {}_{n+1}F_n(1, a_1, a_2, \dots, a_n; a_1 + 1, a_2 + 2, \dots, a_n + 1; z). \quad (\text{B.28})$$

The exponential function in terms of the hypergeometric function is obtained by setting  $a = c = 1$  and taking the limit  $b \rightarrow \infty$  [85]:

$$e^x = \lim_{b \rightarrow \infty} \left( \frac{1}{1 - \frac{x}{b}} \right)^b = \lim_{b \rightarrow \infty} {}_1F_2 \left( 1, b; 1; \frac{x}{b} \right). \quad (\text{B.29})$$

Hyperbolic functions can be expressed by limit of hypergeometric functions as well [92]:

$$\cosh z = \lim_{a, b \rightarrow \infty} {}_2F_1 \left( a, b; \frac{1}{2}; \frac{z^2}{4ab} \right) \quad (\text{B.30})$$

and

$$\sinh z = z \lim_{a, b \rightarrow \infty} {}_2F_1 \left( a, b; \frac{3}{2}; \frac{z^2}{4ab} \right). \quad (\text{B.31})$$

Also, the elliptic integrals can be defined as special case of the hypergeometric function using the integral form of the hypergeometric function [84]:

$$K(k), E(k) = \frac{\pi}{2} \cdot {}_2F_1 \left( \pm \frac{1}{2}, \frac{1}{2}; 1; k^2 \right), \quad (\text{B.32})$$

where  $K(k)$  is the *complete elliptic integral of the first kind* and  $E(k)$  is the *second kind*:

$$K(k), E(k) = \int_0^{\pi/2} d\vartheta (1 - k^2 \sin^2 \vartheta)^{\mp 1/2} = \int_0^1 dt \frac{(1 - k^2 t^2)^{\mp 1/2}}{(1 - t^2)^{1/2}} \quad (\text{B.33})$$

for the parameter  $k \in [0, 1]$ . The identity (B.32) is the results of the following calculation:

$$\begin{aligned} K(k), E(k) &= \int_0^{\pi/2} d\vartheta (1 - k^2 \sin^2 \vartheta)^{\mp 1/2} = \int_0^{\pi/2} d\vartheta \sum_{n=0}^{\infty} \binom{\mp 1/2}{n} (-k^2 \sin^2 \vartheta)^n \\ &= \sum_{n=0}^{\infty} \frac{(\mp 1/2)^n}{n!} (-1)^n k^{2n} \int_0^{\pi/2} d\vartheta \sin^{2n} \vartheta = \sum_{n=0}^{\infty} \frac{(-1)^n (\mp 1/2)^n}{n!} k^{2n} \frac{\pi}{2} \frac{(1/2)^{\bar{n}}}{n!} \\ &= \frac{\pi}{2} \sum_{n=0}^{\infty} \frac{(\pm 1/2)^{\bar{n}} (1/2)^{\bar{n}}}{1^{\bar{n}} n!} (k^2)^n = \frac{\pi}{2} \cdot {}_2F_1 \left( \pm \frac{1}{2}, \frac{1}{2}; 1; k^2 \right), \end{aligned} \quad (\text{B.34})$$

using (B.7) and (B.14), as well as  $\Gamma(n+1) = n! = 1^{\bar{n}}$ .

As the last example, the Mellin-transform  $\mathcal{M}\{f(x)\}(s) = \int_0^\infty dx x^{s-1} f(x)$  with  $s \in \mathbb{C}$  for the function  $f(x) = [x^2 + 2zyx + y^2]^{-q}$  with the parameters  $q \in \mathbb{C}$ ,  $y \in \mathbb{R}$  and  $z \in \mathbb{C} \setminus \mathbb{R}_{\leq -1}$  is given by [91]:

$$\int_0^\infty dt \frac{t^{s-1}}{[t^2 + 2zyt + y^2]^q} = y^{s-2q} \text{B}(s, -s+2q) {}_2F_1 \left( s, -s+2q; \frac{1}{2} + q; \frac{1}{2} - \frac{z}{y} \right) \quad (\text{B.35})$$

for  $0 < \text{Re}(s) < 2 \text{Re}(q)$ .

Not only the mathematical elementary functions, but also almost all of the special functions in physics can be represented by the hypergeometric function. Since the special functions in physics arises from the solutions of the differential equations of Gauss type (B.2), they have expressions in terms of the hypergeometric functions: the orthogonal polynomials like Jacobi-, Laguerre- and Hermite polynomials as well as the spherical harmonics (via the Legendre function), and the Bessel functions, to name a few [77, 86].



# References

- [1] A. Altland and B. Simons, *Condensed Matter Field Theory*, 2 ed. (Cambridge University Press, New York, 2010).
- [2] S. Bose, *Plancks Gesetz und Lichtquantenhypothese*, *Zeitschrift für Physik* **26**, 178 (1924).
- [3] A. Einstein, *Quantentheorie des einatomigen idealen Gases*, Sitzungsberichte der preussischen Akademie der Wissenschaften 12 (1924).
- [4] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, *Observation of Bose-Einstein condensation in a dilute atomic vapor*, *Science* **269**, 198 (1995).
- [5] K. B. Davis, M. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, *Bose-Einstein condensation in a gas of sodium atoms*, *Phys. Rev. Lett.* **75**, 3969 (1995).
- [6] E. Cornell, *Very Cold Indeed: The Nanokelvin Physics of Bose-Einstein Condensation*, *J. Res. Natl. Inst. Stand. Technol.* **101**, 419 (1996).
- [7] M. R. Andrews, C. G. Townsend, H. Miesner, D. S. Durfee, D. M. Kurn, and W. Ketterle, *Observation of Interference Between Two Bose Condensates*, *Science* **275**, 637 (1997).
- [8] S. J. Blundell, *Superconductivity: A Very Short Introduction*, (Oxford University Press, Oxford, 2009).
- [9] D. Fraser and A. Koberinski, *The Higgs mechanism and superconductivity: A case study of formal analogies*, *Studies in History and Philosophy of Science Part B: Studies in History and Philosophy of Modern Physics* **55**, 72 (2016).
- [10] SFB/TR 185 “OSCAR”, B5: *The BEC-BCS crossover in a gas with controlled disorder*, WWW document, (<https://www.physik.uni-kl.de/oscar/index.php/projects/project-area-b/b5>) (stand: 2023.01.15.).
- [11] S. Yong, S. Barbosa, J. Koch, F. Lang, A. Pelster, and A. Widera, *Unravelling Interaction and Temperature Contributions in Unpolarized Trapped Fermionic Atoms in the BCS Regime*, *arXiv:2311.08853* (2023).
- [12] H. K. Onnes, *Further experiments with liquid helium. C. The resistance of pure mercury at helium temperatures*, Commun. Phys. Lab., Leiden University (1911).
- [13] H. Fröhlich, *Theory of the Superconducting State. I. The Ground State at the Absolute Zero of Temperature*, *Phys. Rev.* **79**, 845 (1950).
- [14] E. Maxwell, *Isotope Effect in the Superconductivity of Mercury*, *Phys. Rev.* **78**, 477 (1950).
- [15] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, *Theory of Superconductivity*, *Phys. Rev.* **108**, 1175 (1957).

## BIBLIOGRAPHY

- [16] W. Meissner and R. Ochsenfeld, *Ein neuer Effekt bei Eintritt der Supraleitfähigkeit*, *Die Naturwissenschaften* **21**, 787 (1933).
- [17] P. Coleman, *Introduction to Many-Body Physics*. (Cambridge University Press, Cambridge, 2015).
- [18] Britannica, The Editors of Encyclopaedia. *Meissner effect*. Encyclopedia Britannica, 14 Aug. 2023, <https://www.britannica.com/science/Meissner-effect>. Accessed 30 January 2024.
- [19] D. M. Eagles, *Possible Pairing without Superconductivity at Low Carrier Concentrations in Bulk and Thin-Film Superconducting Semiconductors*, *Phys. Rev.* **186**, 456 (1969).
- [20] A. J. Leggett, *Diatomic molecules and cooper pairs*, edited by A. Pekalski and J. A. Przys-tawa (Springer Berlin Heidelberg, 1980), pp. 13-27.
- [21] W. Zwerger (editor), *The BCS-BEC Crossover and the Unitary Fermi Gas*, (Springer, Berlin 2012).
- [22] P. Nozières and S. Schmitt-Rink, *Bose condensation in an attractive fermion gas: From weak to strong coupling superconductivity*, *J. Low Temp. Phys.* **59**, 195 (1985).
- [23] C. A. R. Sá de Melo, *When fermions become bosons: Pairing in ultracold gases*, *Physics Today* **61**, 45 (2008).
- [24] S. Jochim, M. Bartenstein, A. Altmeyer, G. Hendl, S. Riedl, C. Chin, J. Hecker Denschlag, and R. Grimm, *Bose-Einstein condensation of molecules*, *Science* **302**, 2101 (2003).
- [25] M. W. Zwierlein, C. A. Stan, C. H. Schunck, S. M. F. Raupach, A. J. Kerman, and W. Ketterle, *Condensation of Pairs of Fermionic Atoms near a Feshbach Resonance*, *Phys. Rev. Lett.* **92**, 120403 (2004).
- [26] M. Greiner, C. A. Regal, and D. S. Jin, *Emergence of a molecular Bose-Einstein condensate from a Fermi gas*, *Nature* **426**, 537 (2003).
- [27] M. W. Zwierlein, J. R. Abo-Shaeer, A. Schirotzek, C. H. Schunck, and W. Ketterle, *Vortices and superfluidity in a strongly interacting Fermi gas*, *Nature* **435**, 1047 (2005).
- [28] B. Gänger, J. Phieler, B. Nagler and A. Widera, *A versatile apparatus for fermionic lithium quantum gases based on an interference-filter laser system*, *Rev. Sci. Instr.* **89**, 093105 (2018).
- [29] H. T. C. Stoof, *Coherent Versus Incoherent Dynamics During Bose-Einstein Condensation in Atomic Gases* *J. Low Temp. Phys.* **114**, 11 (1999).
- [30] C. A. R. Sá de Melo, M. Randeria, and J. R. Engelbrecht, *Crossover from BCS to Bose superconductivity: Transition temperature and time-dependent Ginzburg-Landau theory*, *Phys. Rev. Lett.* **71**, 3202 (1993).
- [31] J. R. Engelbrecht, M. Randeria, and C. A. R. Sá de Melo, *BCS to Bose crossover: Broken-symmetry state*, *Phys. Rev. B* **55**, 15153 (1997).
- [32] M. Combescot and S.-Y. Shiau, *Excitons and Cooper Pairs: Two Composite Bosons in Many-Body Physics*. (Oxford University Press, Oxford, 2015).
- [33] S. M. Girvin and K. Yang, *Modern Condensed Matter Physics*, (Cambridge University Press, Cambridge, 2019).



## BIBLIOGRAPHY

- [34] W. Demtröder, *Experimentalphysik* 4, 5 ed. (Springer, Berlin, 2017).
- [35] C. J. Pethick and H. Smith, *Bose–Einstein Condensation in Dilute Gases*. (Cambridge University Press, New York, 2008).
- [36] F. Werner, L. Tarruell, and Y. Castin, *Number of closed-channel molecules in the BEC-BCS crossover*, *Eur. Phys. J. B* **68**, 401 (2009).
- [37] E. Neri, S. F. Caballero-Benítez, V. Romero-Rochín, and R. Paredes, *Pairing and molecule formation along the BCS-BEC crossover for finite range potentials*, *Phys. Scr.* **95**, 034013 (2020).
- [38] A. Korolyuk, J. J. Kinnunen, and P. Törmä, *Collective excitations of a trapped Fermi gas at finite temperature*, *Phys. Rev. A* **89**, 013602 (2014).
- [39] J. J. Kinnunen, M. Rodriguez, and P. Törmä, *Pairing Gap and In-Gap Excitations in Trapped Fermionic Superfluids*, *Science* **305**, 1131 (2004).
- [40] S. Simonucci and G. C. Strinati, *Equation for the superfluid gap obtained by coarse graining the Bogoliubov–de Gennes equations throughout the BCS-BEC crossover*, *Phys. Rev. B* **89**, 054511 (2014).
- [41] A. Barresi, A. Boulet, P. Magierski, and G. Wlazlowski, *Dissipative Dynamics of Quantum Vortices in Fermionic Superfluid*, *Phys. Rev. Lett.* **130**, 043001 (2023).
- [42] C. Timm, lecture script on *Theory of Superconductivity*, (TU Dresden, Dresden, 2020).
- [43] A. Klein and E. R. Marshalek, *Boson Realizations of Lie-Algebras with Applications to Nuclear-Physics*, *Rev. Mod. Phys.* **63**, 375 (1991).
- [44] N. Hamamoto, M. Oi, and N. Onishi, *Equation for the superfluid gap obtained by coarse graining the Bogoliubov–de Gennes equations throughout the BCS-BEC crossover*, *Phys. Rev. A* **75**, 054511 (2007).
- [45] P. Ring, P. Schuck and M. R. Strayer, *The Nuclear Many-Body Problem*. (Springer, Berlin, 1983).
- [46] G. C. Strinati, P. Pieri, G. Röpke, P. Schuck, and M. Urban, *The BCS–BEC crossover: From ultra-cold Fermi gases to nuclear systems*, *Phys. Rep.* **738**, 1 (2018).
- [47] A. Becker, *BCS Mean-Field Theory for Trapped Fermions*, thesis for M.Sc., RPTU Kaiserslautern-Landau (2021).
- [48] C. Zhao, L. Jiang, X. Liu, W. M. Liu, X. Zou, and H. Pu, *Hartree-Fock-Bogoliubov theory of dipolar Fermi gases*, *Phys. Rev. A* **81**, 063642 (2010).
- [49] L. Pitaevskii and S. Stringari, *Bose–Einstein Condensation and Superfluidity*. (Oxford University Press, Oxford, 2016).
- [50] P. Zhang and Y. Gu, *Periodically and quasi-periodically driven dynamics of Bose-Einstein condensates*, *SciPost Phys.* **9**, 079 (2020).
- [51] S. Giorgini, L. P. Pitaevskii, and S. Stringari, *Theory of ultracold atomic Fermi gases*, *Rev. Mod. Phys.* **80**, 1215 (2008).
- [52] F. J. Sevilla and L. Olivares-Quiroz, *Chemical potential for the interacting classical gas and the ideal quantum gas obeying a generalized exclusion principle*, *Eur. J. Phys.* **33**, 709 (2012).

## BIBLIOGRAPHY

- [53] F. W. J. Olver, D. W. Lozier, R. F. Boisvert, and C. W. Clark (ed.), *NIST Handbook of Mathematical Functions*. (Cambridge University Press, New York, 2010).
- [54] F. Schwabl, *Statistische Mechanik*, 3 ed. (Springer, Berlin, 2006).
- [55] L. P. Kadanoff, *Slippery Wave Functions*, *J. Stat. Phys.* **152**, 805 (2013)
- [56] C. Berthod, M. Köhl, and T. Giamarchi, *Second-order response theory of radio-frequency spectroscopy for cold atoms*, *Phys. Rev. A* **92**, 013626 (2015).
- [57] G. M. Bruun, Y. Castin, R. Dum, and K. Burnett, *BCS theory for trapped ultracold fermions*, *Eur. Phys. J. D* **7**, 433 (1999).
- [58] M. Grasso and M. Urban, *Hartree-Fock-Bogoliubov theory versus local-density approximation for superfluid trapped fermionic atoms*, *Phys. Rev. A* **68**, 033610 (2003).
- [59] R. B. Diener, R. Sensarma, and M. Randeria, *Quantum fluctuations in the superfluid state of the BCS-BEC crossover*, *Phys. Rev. A* **77**, 023626 (2008).
- [60] W. Ketterle and M. W. Zwierlein, *Making, probing and understanding ultracold Fermi gases* *La Rivista del Nuovo Cimento* **5-6**, 247 (2008).
- [61] M. W. Zwierlein, C. H. Schunck, A. Schirotzek, and W. Ketterle, *Direct observation of the superfluid phase transition in ultracold Fermi gases*, *Nature* **442**, 54 (2006).
- [62] C. N. Yang, *Concept of Off-Diagonal Long-Range Order and the Quantum Phases of Liquid He and of Superconductors*, *Rev. Mod. Phys.* **34**, 694 (1962).
- [63] D. C. Wood, *The computation of polylogarithms*, University of Kent (1992).
- [64] N. W. Ashcroft and N. D. Mermin, *Solid State Physics*, International ed. (Saunders College Publishing, New York, 1976).
- [65] R. D. Mattuck, *A Guide to Feynman Diagrams in the Many-body Problem*, 2 ed. (Dover Publications, 1992).
- [66] A. Ghosal, M. Randeria, and N. Trivedi, *Inhomogeneous pairing in highly disordered s-wave superconductors*, *Phys. Rev. B* **65**, 014501 (2001).
- [67] C. Gruber and A. Pelster, *A theory of finite-temperature Bose-Einstein condensates in neutron stars*, *Eur. Phys. J. D* **68**, 1434 (2014).
- [68] A. Perali, P. Pieri, L. Pisani, and G. C. Strinati, *BCS-BEC Crossover at Finite Temperature for Superfluid Trapped Fermi Atoms*, *Phys. Rev. Lett.* **92**, 220404 (2004).
- [69] M. Houbiers, H. T. C. Stoof, W. I. McAlexander, and R. G. Hulet, *Elastic and inelastic collisions of  $6\text{Li}$  atoms in magnetic and optical traps*, *Phys. Rev. A* **57**, R1497, (1998).
- [70] M. Bartenstein, A. Altmeyer, S. Riedl, R. Geursen, S. Jochim, C. Chin, J. H. Denschlag, R. Grimm, A. Simoni, E. Tiesinga, C. J. Williams, and P. S. Julienne, *Precise determination of  $6\text{Li}$  cold collision parameters by radio-frequency spectroscopy on weakly bound molecules*, *Phys. Rev. Lett.* **94**, 103201 (2005).
- [71] R. Grimm, *Ultracold Fermi gases in the BEC-BCS crossover: a review from the Innsbruck perspective*, in *Proceedings of the International School of Physics “Enrico Fermi”*, edited by C. S. M. Inguscio and W. Ketterle (Academic Press, Cambridge, 2007).

## BIBLIOGRAPHY

- [72] V. L. Berezinskii, *Destruction of long-range order in one-dimensional and two-dimensional systems possessing a continuous symmetry group. II. Quantum systems*, *Sov. Phys. JETP* **34**, 610 (1971).
- [73] J. M. Kosterlitz and D. J. Thouless, *Ordering, metastability and phase transitions in two-dimensional systems*, *J. Phys. C: Solid State Physics* **6**, 1181 (1973).
- [74] P. Christodoulou, M. Galka, N. Dogra, R. Lopes, J. Schmitt, and Z. Hadzibabic, *Observation of first and second sound in a BKT superfluid*, *Nature* **594**, 191 (2021).
- [75] N. S. Möller, F. E. A. dos Santos, V. S. Bagnato, and A. Pelster, *Bose–Einstein condensation on curved manifolds*, *New J. Phys.* **22**, 063059 (2020).
- [76] Y. He, H. Guo, and C.-C. Chien, *BCS-BEC crossover of atomic Fermi superfluid in a spherical bubble trap*, *Phys. Rev. A* **105**, 033324 (2022).
- [77] A. F. Nikiforov and V. B. Uvarov, *Special Functions of Mathematical Physics*, (Birkhäuser Boston, 1988).
- [78] P. Fulde and R. A. Ferrell, *Superconductivity in a Strong Spin-Exchange Field*, *Phys. Rev.* **135**, A550 (1964).
- [79] A. I. Larkin and Yu. N. Ovchinnikov, *Nonuniform state of superconductors*, *Sov. Phys. JETP* **20**, 762 (1965).
- [80] T. K. Koponen, T. Paananen, J. P. Martikainen, M. R. Bakhtiari, and P. Törmä, *FFLO state in 1-, 2- and 3-dimensional optical lattices combined with a non-uniform background potential*, *New J. Phys.* **10**, 045014 (2008).
- [81] Y. A. Liao, A. S. Rittner, T. Paprotta, W. Li, G. B. Partridge, R. G. Hulet, S. K. Baur, and E. J. Mueller, *Spin-imbalance in a one-dimensional Fermi gas*, *Nature* **467**, 567 (2010).
- [82] N. Kaschewski, A. Pelster, and C. A. R. Sá de Melo, *Self-consistently generalized Hartree–Fock–Bogoliubov approximation* (in preparation)
- [83] H. Kleinert, *Hubbard-Stratonovich Transformation: Successes, Failure, and Cure*, *arXiv:1104.5161* (2011).
- [84] G. B. Arfken, H. J. Weber, and F. E. Harris, *Mathematical methods for physicists*, 7 ed. (Academic Press, London, 2012).
- [85] K. Aomoto and M. Kita, *Theory of Hypergeometric Functions*, (Springer, Berlin, 2011).
- [86] S. Hassani, *Mathematical Physics*, 2 ed. (Springer, Berlin, 2013).
- [87] H. Kleinert, *Multivalued Fields*, (World Scientific, Singapore, 2008).
- [88] J. B. Seaborn, *Hypergeometric Functions and Their Applications*, (Springer, New York, 1991).
- [89] Wolfram Research, Inc. (www.wolfram.com), Wolfram—One, *PolyLog: Representations through more general functions: Through hypergeometric functions*, Champaign, Illinois (2023). (2023.10.20)
- [90] W. Magnus, F. Oberhettinger, and R. P. Soni, *Formulas and Theorems for the Special Functions of Mathematical Physics*, (Springer, New York, 1966).
- [91] F. Oberhettinger, *Tables of Mellin Transforms*, (Springer, New York, 1974).

## BIBLIOGRAPHY

- [92] P. Marian, *Second-order squeezed states*, *Phys. Rev. A* **55**, 3051 (1997).
- [93] L. Salasnich, P. A. Marchetti, and F. Toigo, *Superfluidity, sound velocity, and quasicondensation in the two-dimensional BCS-BEC crossover*, *Phys. Rev. A* **88**, 053612 (2013).
- [94] A. Pelster, lecture script on *Bose-Einstein-Kondensation*, (University of Duisburg-Essen, Essen, 2004).
- [95] N. Andrenacci, A. Perali, P. Pieri, and G. C. Strinati, *Density-induced BCS to Bose-Einstein crossover*, *Phys. Rev. B* **60**, 12410 (1999).
- [96] L. Landau, *Theory of the Superfluidity of Helium II*, *Phys. Rev.* **60**, 356 (1941).
- [97] J. E. Robinson, *Note on the Bose-Einstein Integral Functions*, *Phys. Rev.* **83**, 678 (1951).

## **Declaration of Authorship**

I hereby declare that the presented thesis with the title “Hartree-Fock-Bogoliubov Mean-Field Theory of trapped fermionic atoms” is my original work. All direct or indirect sources used are acknowledged as references. Unless not cited, every contents in this thesis are generated by my own research.

Kaiserslautern, February 5, 2023.

---

Sejung Yong

