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Theory of Quantum and Complex systems

Probing itinerant ferromagnetism with ultracold quantum gases

Studie van itinerant ferromagnetisme vanuit het perspectief van ultrakoude kwantumgassen

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Preface

Itinerant ferromagnetism is spontaneous polarization of non-localized (itinerant or "wandering") particles, i.e. ferromagnetism in a gas. Although it has already been predicted in a free electron gas by F. Bloch in 1929, it has proven to be notoriously hard to find experimentally. Due to the recent successes of ultracold atomic gases as a quantum simulator for condensed matter systems and their experimental tunability, this experimental system has been suggested as a model system for the realization of pure itinerant ferromagnetism. In 2009, experimentalists from the Ketterle group at MIT have been able to reach the strongly interacting regime where itinerant ferromagnetism was predicted to occur. However, the experimental instability towards molecular pairing prevented the formation of any equilibrium state (including the itinerant ferromagnetic state).

On the theoretical side, itinerant ferromagnetism is very hard to model due to the strong interactions and correlations involved. In order to understand why it could not yet be observed in ultracold atomic gases, the current theoretical models have to be updated and improved. That is the main goal of this doctoral dissertation: to improve the theoretical description of itinerant ferromagnetism in the context of ultracold atomic gases. In order to meet this goal, I went back to the basic theory of itinerant ferromagnetism in the path-integral formalism. In particular, I studied how the direct and exchange interactions are treated in the Hartree channel of the path-integral formalism and how this treatment can be improved.

First, I identified an important stability issue in the conventional description of the interactions in the saddle-point approximation for contact interactions. In order to understand this stability issue, I extended the current formalism to general interaction potentials and demonstrated that the Pauli exclusion principle is not necessarily observed in the saddle-point approximation. In order to solve this problem, I proposed to enforce the Pauli exclusion principle using a modified interaction potential. Afterwards, I applied this new method to the example of itinerant ferromagnetism in 3D. The results suggest that dynamical stability is an important factor to take into account when studying itinerant ferromagnetism, as it greatly constrains the itinerant ferromagnetic region in the phase diagram. Finally, I demonstrated that the new method is not exact: the Pauli exclusion principle is not the same as an interaction potential and both behave differently under a Fourier transform.

Overview

This dissertation consists of three large parts and a conclusion:

- **Part I Background:** In the first part of this dissertation, the necessary background for the remainder of this dissertation will be given.
 - Chapter 1 History of itinerant ferromagnetism: A brief introduction to itinerant ferromagnetism in the context of condensed matter systems.
 - Chapter 2 Itinerant ferromagnetism in ultracold atomic gases: An introduction to ultracold atomic gases and itinerant ferromagnetism in the context of ultracold atomic gases. A detailed description of recent experiments on itinerant ferromagnetism is given and the research presented in this dissertation is situated in the literature.
 - Chapter 3 Path-integral formalism: The path-integral formalism is introduced, with a focus on path-integral field theory. The concepts introduced in this chapter are important for understanding the theoretical description presented in the subsequent chapters.

- <u>Part II Contact interactions</u>: In the second part, contact interactions are treated in the Hartree channel of the path-integral formalism.
 - Chapter 4 The saddle-point thermodynamic grand potential: In this chapter the basic description for a two-component Fermi gas with contact interactions will be constructed, with a particular focus on the treatment of the interactions. The thermodynamic grand potential will be calculated in the saddle-point approximation, which is equivalent to a mean-field approximation. At temperature zero, the Stoner criterion for itinerant ferromagnetism is rederived in order to demonstrate the equivalency with other theoretical treatments.
 - Chapter 5 Stability analysis of the saddle points: Here I demonstrate that all saddle points of the thermodynamic grand potential are unstable to density (quantum) fluctuations. This implies that the treatment presented in chapter 4 does not provide a valid description of the physics of the system.
- **Part III General interaction potentials:** In the third part, general interaction potentials are treated in the Hartree channel of the path-integral formalism.
 - Chapter 6 The saddle-point thermodynamic grand potential: In this chapter, I extend the description presented in chapter 4 for contact interactions to general interaction potentials. In order to include the Pauli exclusion principle in the saddle-point approximation, I introduced a new modified interaction potential.
 - Chapter 7 Stability analysis of the saddle points: A stability analysis of the saddle points of the thermodynamic potential is performed, resulting in a phase diagram for itinerant ferromagnetism in 3D. The stability requirement greatly constrains the itinerant ferromagnetic region in the phase diagram.
 - Chapter 8 Discussion of implicit assumptions and approximations: The implicit assumptions and approximations made in the previous chapters are discussed. It is shown that the new method is not exact, as the enforcement of the Pauli exclusion principle using a modified interaction potential is not conserved under a Fourier transform. A preliminary analysis in the momentum basis (instead of the position basis) can be found in Appendix A Saddle-point grand potential in momentum space.
- Part IV Conclusion:
 - Chapter 9 Conclusion: A general summary of the conclusions of this dissertation.

Part I Background

Chapter 1

History of itinerant ferromagnetism

In this chapter, I will give a brief overview of the history of itinerant ferromagnetism in the context of condensed matter systems. First, I will explain how ferromagnetism arises from the collective behavior of electrons in condensed matter systems (Sec. 1.1). Next, I will explain the two main theoretical paradigms for ferromagnetism: Heisenberg (or localized) ferromagnetism (Sec. 1.2.1) and itinerant (or non-localized) ferromagnetism (Sec. 1.2.2), with emphasis on the theory of itinerant models. Finally, the occurrence of itinerant ferromagnetism in condensed matter systems will be discussed (Sec. 1.3).

1.1 What is ferromagnetism?

Ferromagnetism is spontaneous magnetization or polarization. Starting with their first use as compass needles in the 12th century in China, ferromagnetic materials have invaded our lives with applications ranging from the magnets on people's refrigerators to the hard disks of our computers. Historically they have been studied even longer than that, but the key ingredients for a macroscopic theory of ferromagnetism have only been discovered in the past two centuries: Maxwell's theory of electromagnetism and quantum mechanics.

Ferromagnetism in condensed matter systems arises from the electrons in the atoms that make up a particular material. In classical electromagnetism, the magnetic moment μ associated with a current *I* along a loop of infinitesimally small area **dS** is given by $d\mu = IdS$ (fig. 1.1 (a)). For a loop of finite size, the contributions from neighboring infinitesimal current loops cancel each other and only the contribution of the current running around the perimeter of the surface remains,

$$\boldsymbol{\mu} = I \int \mathbf{dS} \tag{1.1}$$

(see fig. 1.1 (b)). In a similar way, the angular momentum **L** associated with the motion of an electron around its atomic nucleus gives rise to a magnetic dipole moment $\mu = \gamma \mathbf{L}$ with γ the gyromagnetic ratio. The magnetic dipole moment of an atom is then given by the sum of the contributions of the electrons. If a net magnetic dipole moment remains, the atom behaves as a tiny magnet. Ferromagnetism occurs when the atoms spontaneously align their magnetic dipole moments. However classically, no net magnetization can remain in a solid, as the contributions of the bulk and edge currents cancel each other (Bohr-van Leeuwen theorem, fig. 1.2). Furthermore, the dipole-dipole interactions are much too weak to overcome the thermal fluctuations above $\sim 1 \text{ K}$, while ferromagnetism is known to occur at temperatures up to 1000 K.

These problems are solved when taking into account the *spin* of the electrons. Its classical analog is the angular momentum associated with the rotation of the electrons around their axis. However, as electrons are elementary particles which are considered to be infinitesimally small, there are a multitude of problems with this analogy and it is better to consider the spin as an inherent quantummechanical property. The electron spin is 1/2 and the associated spin states are called spin-up (+1/2or \uparrow) and spin-down $(-1/2 \text{ or }\downarrow)$. In quantum mechanics, there are two important classes of particles, depending on their spin:



Figure 1.1: (a) A current I along an infinitesimally small loop with area dS gives rise to a magnetic moment $d\mu = IdS$. (b) For a loop of finite size, only the contribution of the current running around the perimeter of the surface remains, as the contributions of neighboring infinitesimal current loops cancel each other. Image source: Stephen Blundell, *Magnetism in Condensed Matter* (Oxford University Press, New York, 2012).



Figure 1.2: An illustration of the classical Bohr-van Leeuwen theorem. Electrons in a magnetic field rotate in cyclotron orbits in the bulk of the system. Along the edge, the electrons move in "skipping orbits" due to scattering at the surface. The net current due to the bulk cyclotron orbits is exactly canceled by the edge current due to the skipping orbits, so classically there is no net magnetization of the material. Image source: Stephen Blundell, *Magnetism in Condensed Matter* (Oxford University Press, New York, 2012).

- Bosons: Particles with integer spin (e.g. photons). If you exchange two identical bosons, their quantum-mechanical state remains the same. We can also say that their quantum states are symmetric. Because of this symmetry, bosons are allowed to occupy the same quantum state. As an example, in a perfect laser all photons occupy the same quantum state.
- Fermions: Particles with half-integer spin (e.g. electrons). If you exchange two identical fermions, their quantum-mechanical state does not remain the same: a minus sign appears in front of the two-particle state. We can also say their quantum states are antisymmetric. Because of this antisymmetry, fermions are not allowed to occupy the same quantum state. This property is called the Pauli exclusion principle.

Each spatial quantum state can be occupied by up to two electrons: one for each spin state. The interaction energy of an electron at position \mathbf{r}_1 in the electric field of an electron at position \mathbf{r}_2 is determined by the Coulomb potential

$$V_C\left(\mathbf{r}_1 - \mathbf{r}_2\right) = \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|},\tag{1.2}$$

where ε_0 is the vacuum permittivity and e the electric charge. The Coulomb potential between two electrons is repulsive. The closer the electrons are to each other, the stronger the repulsion. On average, two electrons of opposite spin states are able to come closer to each other than two electrons of the same spin state. This effectively screens a part of the Coulomb interactions and reduces the interaction energy between electrons of the same spin state. The repulsion is strongest between two electrons of opposite spin states with the same spatial quantum state. The difference in interaction energy between particles of opposite and particles of the same spin states is called the exchange energy. The exchange energy can cause spontaneous polarization or alignment of the electron spins in a material. This is a purely quantum-mechanical effect, arising from the fermionic symmetry properties of the electrons.

The energy cost of polarization is mainly caused by the fact that a given number of electrons have to be loaded into higher kinetic energy levels (or spatial quantum states) if they have the same spin state. In order for materials to become ferromagnetic, the exchange interactions have to be sufficiently strong with respect to the kinetic energy difference. Because of this energy cost, only a limited number of the electrons in a material take part in the collective polarization. Furthermore, thermal excitations will cause fluctuations of the electron spin states and destroy the spin alignment, so ferromagnetism can only occur up to a maximum temperature (the Curie temperature). Depending on the material, other forces (e.g. dipole-dipole interactions) may also counteract the polarizing effect of the exchange interactions.

For a more complete overview of magnetism in condensed matter systems, the reader is referred to ref. [1].

1.2 Exchange interactions

There are two main paradigms for describing the exchange interactions in ferromagnets. The first is Heisenberg or localized ferromagnetism [2], where the electrons are assumed to be confined to their respective atoms. The second paradigm for ferromagnetism is itinerant or non-localized ferromagnetism [3]. Itinerant literally means "wandering", so itinerant ferromagnetism means ferromagnetism of particles which are freely moving with respect to each other (i.e. in a gas). Next, I will discuss both types of ferromagnetism.

1.2.1 Heisenberg or localized ferromagnetism

If the electrons are assumed to be confined to their respective atoms, the distribution of the electrons over the energy levels of each atom can be studied. At low temperatures, the electrons will completely fill the lowest energy shells and only the upper occupied shell may remain partially filled. In order to avoid double occupation of the same spatial quantum state (the situation where the Coulomb repulsion is strongest), the electrons in the partially filled shell will aim to align their spin states. This effect is called the Hund-rule coupling and it gives rise to a local dipole moment of each atom.

In the Heisenberg model, a local dipole moment is associated with each atom (localized in a lattice) and these local dipole moments are allowed to interact with each other. In most cases, the nearest-neighbor interactions are dominant and other interactions are neglected. In that case, the Heisenberg model corresponds to the mathematical Ising model with Hamiltonian

$$\hat{H} = -\sum_{\langle i,j \rangle} J_{ij} \hat{\mathbf{S}}_i \hat{\mathbf{S}}_j, \qquad (1.3)$$

where the notation $\langle i, j \rangle$ denotes that the sum is taken over neighboring lattice sites *i* and *j*, with J_{ij} the interaction parameter and $\hat{\mathbf{S}}_i$ the spin operator of lattice site *i*. Many different physical effects can come into play when determining the values of J_{ij} . An overview of the most important effects (e.g. dipole-dipole interactions, exchange, superexchange, double exchange) is given in ref. [1]. The interactions favor spin alignment (or ferromagnetism) if $J_{ij} > 0$. In first order perturbation theory, J_{ij} is given by the exchange integral

$$J_{ij} = \int \psi_i^* \left(\mathbf{r}_1 \right) \psi_j^* \left(\mathbf{r}_2 \right) H_{int} \psi_j \left(\mathbf{r}_1 \right) \psi_i \left(\mathbf{r}_2 \right) d\mathbf{r}_1 d\mathbf{r}_2, \tag{1.4}$$

with H_{int} the Hamiltionian of the interactions between the electrons.

The Heisenberg model works reasonably well for electrically insulating materials, as in that case the electrons can be assumed to be confined to their respective atoms. However, in metals not all of the electrons are confined to their atoms and the use of local moments may not always be valid. Especially in d-band transition metals such as iron, nickel and cobalt, the Heisenberg model fails to predict the non-integer magnetic moment per atom and the large specific heat capacity [4].

1.2.2 Itinerant or non-localized ferromagnetism

Itinerant ferromagnetism was first suggested by F. Bloch in 1929 [3], when he showed that the exchange interactions between conduction electrons could also cause ferromagnetism. To support his statement, he treated the conduction electrons as a free electron gas with single-particle wave functions

$$\psi_{k,l,m}\left(x,y,z\right) = \frac{1}{\sqrt[3]{L}} \exp\left[\frac{2\pi i}{L}\left(kx + ly + mz\right)\right].$$
(1.5)

Here (x, y, z) are the 3D position coordinates, (k, l, m) the three quantum numbers denoting the number of nodes of the wave function in each direction and L the length of the cubic sample. Each (k, l, m)-state can contain up to two electrons: one for each spin state. The kinetic energy of the electron gas is given by

$$E_{free} = \sum_{i=1}^{N} E_{k_i, l_i, m_i}$$
(1.6)

$$E_{k,l,m} = \frac{1}{2m_e} \left(\frac{h}{L}\right)^2 \left(k^2 + l^2 + m^2\right),$$
(1.7)

where N is the number of conduction electrons, (k_i, l_i, m_i) the quantum state of the *i*-th electron, h the Planck constant and m_e the electron mass. The interaction energy is given by

$$E_{int} = E_{Coulomb} - \sum_{\text{spin } r \parallel \text{ spin } s} J_{rs}, \qquad (1.8)$$

where $E_{Coulomb}$ is the electrostatic interaction between the charges of the electrons. The second term in (1.8) represents the exchange energy, so the sum over the electrons r and s is only taken over electrons with parallel spins. The exchange energy J_{rs} between electrons r and s is given by

$$J_{rs} = \frac{e^2}{4\pi\varepsilon_0} \int d\mathbf{r}_1 d\mathbf{r}_2 \left\{ \frac{\psi_r\left(\mathbf{r}_1\right)\psi_s\left(\mathbf{r}_2\right)\left[\psi_r\left(\mathbf{r}_2\right)\psi_s\left(\mathbf{r}_1\right)\right]^*}{|\mathbf{r}_1 - \mathbf{r}_2|} \right\}.$$
(1.9)

F. Bloch explicitly calculated J_{rs} and found

$$J_{k,l,m;k',l',m'} = \frac{e^2}{4\pi^2 \varepsilon_0 \left[(k-k')^2 + (l-l')^2 + (m-m')^2 \right] L}.$$
(1.10)

He also calculated the number of different microconfigurations of identical electrons which corresponds to a given macroconfiguration. Each macroconfiguration is characterized by the total number of electrons 2N, the number $2N_s$ of singly-occupied (k, l, m)-states (so there are $2N - 2N_s$ doublyoccupied sites which contain two electrons of opposite spin states) and the total magnetization M = $\mu_B (N_{\uparrow} - N_{\downarrow}) = \mu_B \Delta N/2$, with N_{σ} the number of electrons in spin state σ and μ_B the Bohr magneton. At zero temperature and under the assumption that all electrons in singly-occupied states have the same spin state $(N_s = \Delta N)$, the total energy of the system up to first order in perturbation theory, with the free electron gas as the unperturbed state, is given by

$$E(\Delta N) = \frac{4\pi}{5} \frac{1}{2m_e} \left(\frac{h}{L}\right)^2 \left(\frac{3}{4\pi}\right)^{5/3} \left[(N + \Delta N)^{5/3} + (N - \Delta N)^{5/3} \right] - \left(\frac{3}{4\pi}\right)^{4/3} \frac{e^2}{2\varepsilon_0 L} \left[(N + \Delta N)^{4/3} + (N - \Delta N)^{4/3} \right].$$
 (1.11)

The first term is the kinetic energy, while the second term is the interaction energy. Only the exchange part of the interaction remains, as the direct Coulomb interaction was exactly canceled by a homogeneous positive background in the limit $N \to +\infty$ (Jellium model). Polarization causes an increase in the kinetic energy, but a decrease in the exchange energy. In this model it is energetically advantageous to polarize if

$$a = \frac{L}{\sqrt[3]{2N}} \ge 0.9 \left(\frac{3}{8\pi}\right)^{1/3} \frac{2\pi\varepsilon_0}{m_e} \left(\frac{h}{e}\right)^2 \approx 0.6 \times 10^{-7} \,\mathrm{cm}\,.$$
(1.12)

For one conduction electron per atom, a is the lattice constant.

Bloch's analysis for free electrons is a proof of principle. It was later expanded to include the effects of a periodic lattice potential and temperature by E. C. Stoner in the 1930's [5,6]. The main effect of a periodic potential is that it modifies the distribution of states into a series of energy bands. That is why itinerant models are also called band models.

1.3 Itinerant ferromagnetism in metals

Itinerant ferromagnetism requires moving electrons, so it can only occur in conductive materials. Furthermore, a very flat conduction band is required in order to reduce the kinetic energy cost of polarization. The main example of such materials are d-band transition metals (e.g. iron, nickel and cobalt) [4]. In those materials, itinerant models have succeeded in explaining the non-integer magnetic moment per atom and the large specific heat capacity. However, the temperature dependence of their magnetization and their magnetic susceptibilities are better described by the Heisenberg model of local moments.

In pure itinerant models, the ferromagnetic-to-paramagnetic phase transition occurs through a uniform shrinking of the magnetic moments in the material. In the Heisenberg model, this phase transition is realized by a directional disorder of the local moment caused by thermal fluctuations (see fig. 1.3). In d-band transition metals, electron correlations and electron spin density fluctuations are responsible for the ferromagnetic-to-paramagnetic phase transition and these effects are better described by the interaction of local moments. Since the acknowledgment of this problem in the 1950's, hybrid models have been developed which capture both localized and non-localized ferromagnetic behaviors. An overview of those models is given in the review paper [4]. Despite the major progress in our understanding of d-band transition metals, the construction of a hybrid model that captures their full ferromagnetic behavior remains an open problem in solid state physics.

In condensed matter systems, itinerant ferromagnetism always occurs together with localized ferromagnetism. So far, pure itinerant ferromagnetism has never been observed. This has impeded



Figure 1.3: In the Heisenberg model (with $J_{ij} > 0$), at temperature zero all local moments are aligned with each other (upper panel). As the temperature increases, thermal fluctuations will cause directional disorder of the local moments and a decrease of the total magnetization (lower panel).

verification of itinerant models. This verification is especially important since the strong interactions and correlations involved are very challenging theoretically. Almost all theoretical models have to rely on approximations and it is still unclear to what extent those approximations are valid. In fact, it is still debated whether a free electron gas (with a uniform positive background) can become itinerant ferromagnetic at all without auxiliary conditions (e.g. coupling to a periodic potential, coupling to lattice vibrations, presence of Heisenberg ferromagnetism, ...). Only for certain lattice models with specific band fillings has itinerant ferromagnetism been rigorously proven to occur [7,8].

In order to solve these theoretical questions, researchers have started looking for itinerant ferromagnetism in other experimental systems. The first was liquid ³He, where some models predicted itinerant ferromagnetism at high pressure (for low temperatures). However, liquid ³He solidifies long before it gets close to the itinerant ferromagnetic phase transition [9]. Ultracold atomic gases are the next promising system for verification of pure itinerant ferromagnetic models [10–15]. The quest for itinerant ferromagnetism in ultracold atomic gases will be discussed in the next chapter.

Chapter 2

Itinerant ferromagnetism in ultracold atomic gases

In this chapter I will give a general introduction to the field of ultracold atomic gases (Sec. 2.1) and its most important experimental tools (Sec. 2.2). Next, the quest for the experimental realization of itinerant ferromagnetism in ultracold atomic gases will be discussed (Sec. 2.3). First the Stoner criterion for the occurrence of itinerant ferromagnetism is derived (Sec. 2.3.1). Then the experimental results will be compared to the expected experimental signatures (Sec. 2.3.2) and their interpretation will be discussed (Sec. 2.3.3). The current consensus is that itinerant ferromagnetism has not yet been realized experimentally in ultracold atomic gases. Finally, the future outlook will be discussed and the research presented in this dissertation will be situated in the recent literature (Sec. 2.3.4).

2.1 What are ultracold atomic gases?

In quantum mechanics, a particle with mass m corresponds to a wave packet, the size of which is given by the *de Broglie wavelength* $\lambda_{dB} = \sqrt{2\pi\hbar^2/mk_BT}$ (fig. 2.1), where k_B is the Boltzmann constant and T the temperature. When cooling down atoms, their λ_{dB} increases. In experiments with ultracold atoms, atoms are cooled down to such low temperatures that λ_{dB} becomes of the order of the interparticle distance, or $n\lambda_{dB}^3 \approx 1$ with n the particle density of the gas. The criterion $n\lambda_{dB}^3 \gtrsim 1$ defines the *ultracold* regime. In this regime, the wave packets of the atoms overlap and quantum effects are enhanced.



Figure 2.1: Classically, a gas is described as a group of freely moving particles. In quantum mechanics, these particles can be represented by wave packets.

Obviously, reaching the ultracold regime is experimentally challenging. In order to prevent solidification, the gases are kept very dilute, lowering the required temperature even further to the order of μ K or 100 nK. Special cooling techniques were developed in order to reach these temperatures, e.g. laser cooling (Nobel prize 1997) and evaporation cooling. Furthermore, no physical container is able to hold the gas, as atoms colliding with the walls of the container would immediately evaporate. Instead, optical and magnetic traps (usually harmonic traps) are used to keep the gas contained during the experiment. However, the rewards are great: quantum effects become macroscopic and can be studied in unprecedented detail. This effect is most obvious for bosonic atoms (e.g. ⁸⁷Rb, ²³Na and ⁷Li).

When $n\lambda_{dB}^3 \approx 1$ for bosons, most bosons will acquire the same phase and occupy the same singleparticle ground state. This macroscopic occupation of the ground state is called a Bose-Einstein condensate or BEC (Nobel prize 2001, fig. 2.2). When two BEC's collide, an interference pattern appears, confirming the quantum-mechanical nature of this special phase of matter (fig. 2.3). A BEC is also superfluid: it flows without friction and is irrotational. It can only rotate if a "hole" or vortex is made in the BEC. This causes quantization of the circulation around a vortex in a BEC (fig. 2.4).



Figure 2.2: When bosons are cooled down, their wave packets will start to overlap and most of the particles will gather in the ground state. Eventually, this ground state occupation will become macroscopic. Image adapted from the MIT Ketterle group website.



Figure 2.3: When two Bose-Einstein condensates are allowed to expand and overlap with each other, interference fringes appear. This is an important confirmation of the quantum-mechanical nature of this state. Image source: MIT Ketterle group website.

Fermionic atoms (e.g. ⁴⁰K and ⁶Li) are not allowed to occupy the same quantum state, so in principle they cannot form a BEC. However, in a two-component Fermi gas, where the components are called (pseudo)spin-up and (pseudo)spin-down, pairs of up and down fermions can be formed. These pairs effectively behave themselves as bosons and are allowed to Bose-condense [16–25].



Figure 2.4: When a BEC is stirred, an increasing number of vortices are created. At large rotation frequencies, the vortices form an Abrikosov lattice.

2.1.1 Interactions

The alkali atoms are easiest to use (and magnetically trapped) experimentally, although more recently isotopes of earth alkali elements and lanthanides have also been used in ultracold gas experiments. For the alkali atoms, the interactions between the atoms are best described by a short-range Van der Waals potential. In dilute gases at low temperatures, spherical s-wave scattering dominates and scattering into higher order partial waves is negligible. Because of the short range of the interactions and the dominance of the s-wave scattering, the interactions between two atoms at positions \mathbf{x}_1 and \mathbf{x}_2 are often approximated by a contact potential:

$$V_{contact}\left(\mathbf{x}_{2}-\mathbf{x}_{1}\right)=g\delta\left(\mathbf{x}_{2}-\mathbf{x}_{1}\right)$$
(2.1)

with $\delta(\Delta \mathbf{x})$ the Dirac delta function. The parameter g is determined by requiring that the contact potential has the same s-wave scattering length a_s as the true interaction potential. In 3D,

$$g = \frac{4\pi\hbar^2 a_s}{m} \tag{2.2}$$

with m the mass of the atoms. Because s-wave scattering between fermions of the same (pseudo)spin state is forbidden by the Pauli principle, only the s-wave scattering length $a_s^{\uparrow\downarrow}$ between up and down atoms is relevant in most ultracold Fermi gas experiments. The effect of the interactions is then fully described by the dimensionless parameter $a_s^{\uparrow\downarrow}k_F$, with $k_F = \sqrt[3]{3\pi^2 n}$ the Fermi wavenumber.

The contact potential approximation is valid if the range of the interaction potential is smaller than the relevant length scales of the problem. In dilute ultracold atomic gases, there are several important length scales:

- The size L of the experimental system. In this dissertation, we will assume that the size of the system is much larger than all other relevant length scales.
- The de Broglie wavelength $\lambda_{dB} = \sqrt{2\pi\hbar^2/mk_BT}$, which is a measure of the width of the atomic wave packet.
- The average distance *d* between the atoms.
- The range R of the interaction potential.

Ultracold implies $\lambda_{dB} > d$ and dilute implies $d \gtrsim R$, so generally $L > \lambda_{dB} > d \gtrsim R$ and the contact potential approximation can be used for most dilute ultracold Fermi gases.

2.2 Experimental tunability

Since the achievement of Bose-Einstein condensation, many other physical phenomena have been probed in ultracold atomic gases. This has been enabled by the great experimental tunability of ultracold atoms. Here I will discuss the most important experimental tools which are responsible for this tunability, with a focus on the two-component Fermi gases which are important for itinerant ferromagnetism. A more complete overview of ultracold atomic gases is given in the following recent theoretical [26] and experimental [27] review papers.

2.2.1 Atom number and spin-imbalance

The possible quantum states of an atom are determined by a complex interaction between the orbital angular momentum \mathbf{L} of the electrons, the spin \mathbf{S} of the electrons and the nuclear spin \mathbf{I} . The total angular momentum of the atom is given by $\mathbf{F} = \mathbf{L} + \mathbf{S} + \mathbf{I}$. The different total angular momentum states of an atom are called hyperfine states. They are labeled as $|F, m_F \rangle$, with $F = |\mathbf{F}|$ and $m_F \in \{-F, -F + 1, \dots, F - 1, F\}$ related to the orientation of the total angular momentum vector \mathbf{F} .

In experiments with ultracold atomic gases, it is possible to accurately control the number of atoms in each hyperfine state. In order to study a two-component Fermi gas, atoms are usually prepared in the two lowest energy hyperfine states, often an $|F, m_F = -F >$ and an $|F, m_F = -F + 1 >$ state. In the remainder of this dissertation, where the internal structure of the atoms is not important, those two components will be denoted as (pseudo)spin-up (\uparrow) and (pseudo)spin-down (\downarrow). The number of atoms in each of the hyperfine states determines the spin-imbalance $\Delta N = N_{\uparrow} - N_{\downarrow}$, where N_{σ} is the number of atoms with (pseudo)spin state σ .

Due to angular momentum conservation, the number of atoms in each hyperfine state is conserved in two-body collisions between atoms of the $|F, m_F = -F >$ and $|F, m_F = -F + 1 >$ states. Atoms in higher momentum states can only be created through higher order collisions with three or more particles, but at low temperatures those are unlikely to occur. That is why in ultracold two-component atomic Fermi gases, one can often assume that the number of atoms in each hyperfine state is conserved for the duration of the experiment.

2.2.2 Feshbach resonances

Across a Feshbach resonance, the scattering length can be tuned by changing the magnetic field B applied to the system. A Feshbach resonance occurs when a bound state in a closed scattering channel has an energy close to that in an open scattering channel (fig. 2.5). Near the Feshbach resonance, the normal free particle states and the molecular bound state are mixed, which has a strong influence on the scattering length between the particles. The resulting value of the scattering length depends on the energy difference ΔE between the bound state and the incident energy of the open scattering channel. If the molecular state has a different magnetic moment than the free particles, this energy difference can be tuned by changing the magnetic field B applied to the system, $\Delta E = \delta \mu (B - B_0)$ with $\delta \mu$ the difference in magnetic moments. The resulting scattering length is then given by

$$a \approx a_{bg} \left(1 - \frac{\Delta}{B - B_0} \right), \tag{2.3}$$

where a_{bg} is the background scattering length (or scattering length far from the resonance) and Δ is the width of the resonance (fig. 2.6).

On the repulsive side of the Feshbach resonance (a > 0), the molecular state has a lower energy than the scattering states in the open channel. Near the Feshbach resonance, inelastic collisions producing these molecules are resonantly enhanced. This has multiple implications for experiments with ultracold atoms. First, the molecular binding energy

$$E_b = \frac{\hbar^2}{2\mu a^2},\tag{2.4}$$

where μ is the reduced mass of the atoms, is released in the form of kinetic energy when molecules form. This binding energy is sufficiently large to allow the atoms to escape the trapping potential.



Figure 2.5: The interaction potentials of an open and a closed scattering channel as a function of the distance between the atoms. The closed scattering channel contains many different bound states. When one of those bound states has an energy close to that in an open scattering channel, a Feshbach resonance occurs. Image source: I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008).



Figure 2.6: (a) The scattering length a and (b) the molecular energy E as a function of the magnetic field B near a magnetically tuned Feshbach resonance at $B = B_0$. Δ is the width of the Feshbach resonance and $E_b = -E$ the molecular binding energy. Image source: C. Chin, R. Grimm, P. Julienne, and E. Tiesinga, Rev. Mod. Phys. **82**, 1225 (2010).

This causes an increased atom loss rate near the Feshbach resonance. Depending on the isotopes used in the experiments, the dominant channel for decay to the molecular state is mediated by two-body and/or three-body collisions. The increased two-and three-body loss rate near the Feshbach resonance greatly reduces the lifetime of experiments near a Feshbach resonance, especially on the repulsive side.

The main experimental features of a Feshbach resonance are shown in fig. 2.7 for a BEC of 23 Na: an increased atom loss rate and a divergence of the (s-wave) scattering length [28]. A more detailed theoretical analysis and an overview of the experimentally most relevant Feshbach resonances is given in [29]. Most of them are s-wave resonances, but more recently also p-wave Feshbach resonances (where the *p*-wave scattering length diverges) are being explored in experiments.



Figure 2.7: The most important experimental features of a Feshbach resonance as observed in a Bose-Einstein condensate of 23 Na atoms: (a) the increased atom loss and (b) the divergence of the scattering length. Image source: S. Inouye *et al.*, Nature **392**, 151154 (1998).

The tunability of the scattering length has allowed study of many important physical phenomena, including the BCS-BEC crossover of superfluid pairing in ultracold two-component Fermi gases [18– 25] (fig. 2.8). For weak attractive interactions, the pairs are very tightly bound and form a Bose-Einstein condensate. For weak repulsive interactions, the pairs are very large and their behavior is best described by the BCS (Bardeen-Cooper-Schrieffer) model which was originally developed to describe superconductivity (or superfluid pairing of electrons). By tuning the interactions over a Feshbach resonance in ultracold atomic gases, the crossover between both models could be studied. This clearly demonstrated that the BEC and BCS models for superfluidity in two-component Fermi gases are two sides of the same coin.

The regime in which the scattering length diverges is called the unitarity limit. Note that, as you can clearly see in fig. 2.8, nothing catastrophic happens at unitarity. It is only the divergence of a theoretical parameter which is used to describe the interactions, not of the interaction energy.

2.2.3 Optical lattices

When two laser beams of the same wavelength λ are aimed at each other, a standing wave of wavelength $\lambda/2$ is created in between the two lasers (fig. 2.9). This standing wave induces a small dipole moment



Figure 2.8: Phase diagram of fermionic pairing in a two-component Fermi gas as a function of the inverse s-wave scattering length $1/a_s$ between spin-up and spin-down particles (in units of the Fermi wavenumber k_F) and the temperature T (in units of the Fermi temperature T_F). T_{pair} is the critical temperature below which fermionic pair formation occurs, while T_c is the critical temperature for Bose-Einstein condensation of the fermion pairs. By tuning a_s over a Feshbach resonance, the BCS-BEC crossover can be studied. Image source: C. A. R. Sá de Melo, Phys. Today **61**, 45 (2008).

in the atoms which are trapped between the lasers. The standing wave acts as a periodic potential on the atoms through interaction with the induced dipole moment of the atoms. This periodic potential is called an optical lattice in the context of ultracold atomic gases [30–33].



Ultracold gas

Figure 2.9: When two laser beams with the same wavelength are aimed at each other, a standing wave is created between them. This standing wave acts as a periodic potential on the atoms and is called an optical lattice. Image source: I. Bloch, Nature **453**, 1016 (2008).

If the lattice depth is very large, a series of 2D "pancakes" is created and the dimensionality of the system is effectively reduced. By adding extra pairs of laser beams in perpendicular directions, the dimensionality can be further reduced to 1D tubes or an artificial crystal of 0D lattice sites (fig. 2.10). By combining pairs of laser beams along different angles, different lattice geometries can be created (e.g. triangular lattices).

2.2.4 Quantum simulation

To summarize, in ultracold atomic gases the geometry, dimensionality, particle numbers per spin state and interaction strengths can all be accurately controlled. This tunability has created enormous experimental possibilities. The purity of the system allows us to check the predictions of many-body



Figure 2.10: By adding pairs of laser beams in perpendicular directions, the dimensionality of the system can be reduced. Image source: I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008).

theories with unprecedented accuracy, hence ultracold atomic gases are also known as a quantum simulator [34] for many-body theories. Consequently, it has also been suggested that ultracold atomic gases could be used to "quantum simulate" itinerant ferromagnetism [10–15]. The tunability of the interaction strength and the possibility to exclude the presence of a crystal lattice may give us a chance to observe pure itinerant ferromagnetism in ultracold atomic gases, something which has so far proven impossible in conventional materials. In the next section, a mean-field toy model will be used to explain the main expected experimental features of the normal-to-itinerant-ferromagnetic phase transition.

2.3 The experimental quest for itinerant ferromagetism

In 2009, experimentalists at MIT were able to probe the strongly interacting regime where itinerant ferromagnetism is expected and they reported its observation [35]. Although they observed all expected experimental features of the normal-to-itinerant-ferromagnetic phase transition, with the exception of magnetic domains, it was later proven that they did not observe itinerant ferromagnetism. The instability of the repulsive branch of the Feshbach resonance to molecular pairing prevented the formation of any equilibrium state, including the itinerant ferromagnetic state [36].

In this section I will first derive the Stoner criterion for itinerant ferromagnetism using a mean-field theoretical toy model. Next, I will discuss the expected experimental signatures and the results of recent experiments. Finally, I will give an overview of the most recent proposals for the realization of the itinerant ferromagnetic state in ultracold atomic gases.

2.3.1 Stoner criterion

In order to understand the physics of the normal-to-itinerant-ferromagnetic phase transition, the free energy of a homogeneous spin-1/2 Fermi gas can be studied as a function of the polarization $P = \delta n/n$ (here $n = n_{\uparrow} + n_{\downarrow}$ is the total particle density and $\delta n = n_{\uparrow} - n_{\downarrow}$ the particle density difference). As an approximation to the short-ranged Van der Waals interactions, contact interactions will be used. Within this approximation, no net interactions between particles of equal spin states remain, as their direct and exchange contributions exactly cancel each other. This implies that it is sufficient to only describe the (direct) interactions between particles of different spin states, whereas for electrons the exchange interactions have to be treated explicitly. Despite the fact that only direct interactions have to be treated, also in the Stoner model itinerant ferromagnetism is caused by the exchange interactions. This is illustrated in fig. 2.11.



Figure 2.11: If the (contact) interaction potential of the Stoner model is assumed to be spinindependent, the physics of the Bloch and Stoner model is very similar. In both cases, the total direct interactions are independent of the polarization and the exchange interactions are responsible for the energy gained by polarizing. However, due to different compensation mechanisms (canceling the terms circled in black) the final expressions for the interaction energy are very different in both models. In the Stoner model, only the direct interactions between particles of different spin states have to be studied, while in Bloch's model only the exchange interactions remain.

In units of $\hbar = 1$, the atomic mass m = 1/2, the Boltzmann constant $k_B = 1$ and the Fermi wavevector $k_F = 1$, the mean-field free energy F per unit volume V of this system is given by [35]

$$\frac{F(P)}{V} = \frac{2}{9\pi^3} a_s k_F \left(1 - P^2\right) + \frac{1}{10\pi^2} \left[(1+P)^{5/3} + (1-P)^{5/3} \right], \qquad (2.5)$$

with a_s the s-wave scattering length for collisions between particles of different spin states. The effect of the contact interactions is fully captured by the dimensionless parameter $a_s k_F$, which is the ratio between the two most important length scales in the system. The total particle density n is fixed to $n = 1/3\pi^2$ due to the choice of the length unit $k_F = \sqrt[3]{3\pi^2 n}$, therefore the free energy (2.5) only depends on $a_s k_F$ and P.

The first term in (2.5), the interaction energy, is a parabola with an extremum in P = 0. This extremum is a minimum if $a_s k_F < 0$ and a maximum if $a_s k_F > 0$. The second term in (2.5), the free-particle energy or kinetic energy, has one minimum in P = 0.

If $a_s k_F < 0$, both terms are minimal in P = 0 and the free energy has only one minimum in P = 0. If $a_s k_F > 0$, the two terms will compete: the interaction term favors spin-polarization, while the kinetic energy favors the unpolarized state with P = 0.

The extrema of the free energy can be calculated using its first derivative:

$$0 = \frac{1}{V} \frac{\partial F}{\partial P} = -\frac{4}{9\pi^3} a_s k_F P + \frac{1}{6\pi^2} \left[(1+P)^{2/3} - (1-P)^{2/3} \right], \qquad (2.6)$$

with the exception of the extrema at the borders |P| = 1 of the allowed values of the polarization. Note that P = 0 is always a solution of eq. (2.6). The extremum at P = 0 is a minimum if

$$0 \le \left. \frac{1}{V} \frac{\partial^2 F}{\partial P^2} \right|_{P=0} = -\frac{4}{9\pi^3} a_s k_F + \frac{2}{9\pi^2} \Leftrightarrow a_s k_F \le \frac{\pi}{2}.$$
(2.7)

This means we expect partially and fully polarized minima of the free energy and thus polarization for

$$a_s k_F > \frac{\pi}{2} \approx 1.571. \tag{2.8}$$

This is called the *Stoner criterion* for itinerant ferromagnetism. Improved theoretical models find different critical values of $a_s k_F$, but they are all of the order of one. Second order models in a_s predict $a_s k_F > 1.054$ [14].

A plot of the mean-field free energy (2.5) as a function of the polarization for different values of $a_s k_F$ can be found in fig. 2.12. Full polarization is expected for $a_s k_F \ge 2^{-7/3} 3\pi \approx 1.87$. The continuous behavior of the order parameter P as a function of $a_s k_F$ (fig. 2.13) signifies that the normal-to-itinerant-ferromagnetic phase transition is of second order in the Stoner model.



Figure 2.12: The free energy F(P) as a function of the polarization for several different values of the dimensionless interaction parameter a_sk_F , relative to the free energy F_0 at $a_sk_F = 0$ and P = 0. Depending on the value of a_sk_F , the minima of the free energy will be unpolarized (P = 0), partially polarized (0 < |P| < 1) or fully polarized (|P| = 1). If $a_sk_F \ge \pi/2$, the polarization of the minima will increase as a function of a_sk_F until they become fully polarized at $a_sk_F = 2^{-7/3}3\pi$.



Figure 2.13: The polarization P as a function of the dimensionless interaction parameter $a_s k_F$. If $a_s k_F \ge \pi/2$, the polarization will increase as a function of $a_s k_F$ until full polarization is reached at $a_s k_F = 2^{-7/3} 3\pi$.

2.3.2 Experimental signatures

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In a true spin-1/2 system, the expectation value of the spin can be represented by a "spin vector" of fixed length. The number of atoms per spin state is not fixed and polarization occurs through alignment of the spin vectors of the particles. In contrast, in ultracold atomic gases there is no true spin state and the number of atoms in each pseudospin state is fixed. This has important implications for

itinerant ferromagnetism: polarization in ultracold atomic gases can only occur through the formation of magnetic domains, i.e. spatial separation of the atoms in each pseudospin state. The difference between both cases is illustrated in fig. 2.14.



Figure 2.14: In a true spin-1/2 system, polarization occurs through alignment of the spins of the particles (above). In ultracold atomic gases, the number of particles in each pseudospin state is fixed and polarization necessarily occurs through magnetic domain formation (below).

In the 2009 experiment by the Ketterle group at MIT [35], an equal mixture of approximately 6.5×10^5 ⁶Li atoms in the lowest two hyperfine states was prepared at B = 590G on the weakly interacting repulsive side of the Feshbach resonance. Next, the magnetic field was increased towards the Feshbach resonance at B = 834G, providing an opportunity to study the strongly interacting regime. The temperature during the experiment varied between $T/T_F = 0.12$ and $T/T_F = 0.6$ with the Fermi temperature $T_F \approx 1.4 \,\mu$ K for this specific experimental system.

There are four expected experimental signatures of the normal-to-itinerant-ferromagnetic phase transition:

- 1. The suppression of elastic and inelastic collisions, and thus a decreased three-body loss rate: Due to the Pauli exclusion principle and the short range of the interaction potential, atoms of the same spin state are close to non-interacting. This causes suppression of the elastic and inelastic collisions in the itinerant ferromagnetic state. Near the Feshbach resonance, inelastic three-body collisions are the dominant decay channel from atoms to molecules. Furthermore, they cause production of atoms which can escape the trapping potential. Monitoring the atom loss rate and the molecular fraction of the gas is a way of measuring the rate of the inelastic three-body collisions.
- 2. A minimum in the kinetic energy: As the magnetic field is increased, the interaction strength will increase and cause expansion of the unpolarized gas in the trap. This expansion lowers the particle density n and the Fermi energy $E_F = \hbar^2 k_F^2/2m$, and thus the kinetic energy. When the gas starts to polarize, the kinetic energy will rapidly increase due to the larger local particle density per spin state. This causes a minimum in the kinetic energy near the phase transition.
- 3. A maximum in the cloud size: The pressure of the gas is given by

$$p = \frac{2}{3}\frac{E_{kin}}{V} + \frac{E_{int}}{V}.$$
(2.9)

where E_{kin} is the kinetic energy and E_{int} is the interaction energy. Polarization causes the interaction energy to (almost) disappear, while the kinetic energy is increased by a factor $2^{2/3}$

(for full polarization). At constant volume, polarization would result in a decrease of the pressure of the system. As the experimental system is kept at constant pressure, the volume of the gas has to decrease after the phase transition to the itinerant ferromagnetic state.

4. Magnetic domain formation

In the experiment, the first three experimental signatures were observed. The atom loss rate, the kinetic energy and the chemical potential μ (related to the cloud size σ_z along the z-direction through $\mu = \frac{1}{2}m\omega_z^2\sigma_z^2$ with ω_z the frequency of the harmonic trap along the z-direction) are shown in fig. 2.15, fig. 2.16 and fig. 2.17, respectively. Consequently in [35], the observation of the normal-toitinerant-ferromagnetic phase transition was reported. However, the experimental results suggested the onset of itinerant ferromagnetism at $a_s k_F = 1.9 \pm 0.2$, which is significantly higher than the value $a_s k_F = \pi/2$ predicted by the Stoner criterion and the value $a_s k_F = 1.054$ predicted by secondorder calculations [14]. Furthermore, without the observation of magnetic domains, the nature of the observed phase transition could not be confirmed. A large discussion in the literature ensued, which will be discussed in the next section.



Figure 2.15: The atom loss rate observed during the experiment as a function of the interaction parameter $a_s k_F$ for different temperatures T/T_F : 0.55 (triangles, dashed line), 0.22 (open circles, dotted line) and 0.12 (closed circles, solid line). The curves are guides to the eye. In the gray shaded region, the maximum of the atom loss rate at $T/T_F = 0.12$ suggests the onset of the normal-to-itinerant-ferromagnetic phase transition. Image source: G.-B. Jo *et al.*, Science **325**, 1521 (2009).

2.3.3 Interpretation of the experimental results

From the start, it was clear that the experimental results could not correspond to itinerant ferromagnetism in equilibrium [37]. Some researchers suggested physical effects which could delay the onset of the normal-to-itinerant-ferromagnetic phase transition to higher values of $a_s k_F$ [38,39]. However, it was shown that, without the observation of magnetic domains, the experimental observations could also be explained by the formation of a strongly short-range correlated state (without itinerant ferromagnetism) [40]. The atom loss rate could even be reproduced in a theoretical model without itinerant ferromagnetism [41]. Next, the stability of the itinerant ferromagnetic state was considered: first against a single spin-flip [42] and next against Feshbach molecular pairing [43]. The results suggested that molecular pairing would occur slightly faster than magnetic domain formation.

Clearly, a follow-up experiment was needed to establish whether the itinerant ferromagnetic state was realized in the experiment. First the spin-drag coefficient [44] and next the magnetic susceptibility (determined from spin correlations) [45] were suggested as a way to characterize the observed phase transition.

In 2011, the Ketterle group at MIT repeated their experiment with a significantly higher imaging resolution (both spatial and temporal) [36]. They measured the spin correlations by speckle imaging.



Figure 2.16: The measured kinetic energy for different values of the interaction parameter $a_s k_F$ and the temperature T/T_F . In the gray shaded region, the kinetic energy minimum at $T/T_F = 0.12$ suggests the observation of the normal-to-itinerant-ferromagnetic phase transition. Image source: G.-B. Jo *et al.*, Science **325**, 1521 (2009).

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Figure 2.17: The chemical potential μ for different values of the interaction parameter $a_s k_F$ and the temperature T/T_F . The chemical potential was determined from experimental measurements of the cloud size σ_z along the z-direction using $\mu = \frac{1}{2}m\omega_z^2\sigma_z^2$, with m the atomic mass and ω_z the harmonic trap frequency along the z-direction. In the gray shaded region, the maximum of the chemical potential (and thus the volume) of the gas at $T/T_F = 0.12$ suggests the observation of the normal-to-itinerant-ferromagnetic phase transition. Image source: G.-B. Jo *et al.*, Science **325**, 1521 (2009).

This measurement was based on the fact that for an appropriate choice of the laser frequency, the local refractive index varies as a function of the local polarization of the gas. Spin fluctuations cause spatial fluctuations in the local refractive index, which affect the phase pattern imprinted on the light passing through the gas. After propagation, those phase fluctuations are transformed into amplitude fluctuations. The measured amplitude fluctuations are then used as a measure for the spin fluctuations.

Near the normal-to-itinerant-ferromagnetic phase transition, a large increase in the spin fluctuations is expected. In the experiment, no such increase of the spin fluctuations was observed (fig. 2.18). Furthermore, it was established that the physics of the system is dominated by the formation of Feshbach molecules. The fast molecular pairing prevented the formation of any equilibrium state, including the itinerant ferromagnetic state. Even if tiny magnetic domains should be formed, the faster molecular pairing would take over the magnetic domain formation and prevent their growth. This seriously decreases the prospects for realizing the short-ranged Stoner model in ultracold atomic gases.



Figure 2.18: The spin fluctuations (a) as a function of the magnetic field, and (b) at the Feshbach resonance as a function of the hold time in the trap, relative to the spin fluctuations measured at 527G. The spin fluctuations show only a limited increase, while a much larger increase is expected at the normal-to-itinerant-ferromagnetic phase transition. Image source: C. Sanner *et al.*, Phys. Rev. Lett. **106**, 010402 (2011).

2.3.4 Future outlook

The experiment in 2011 [36] by the Ketterle group closed one discussion, but it also opened up the next one: are there other ways to realize itinerant ferromagnetism in ultracold atomic gases? How do we suppress the molecular pairing? How do we increase our theoretical understanding of itinerant ferromagnetism? Can we lower the critical value of $a_s k_F$ in the Stoner criterion? Here I will give an overview of the most recent research proposals for the realization and study of the itinerant ferromagnetic state in ultracold atomic gases. A more general overview can be found in the review article [46].

The most important proposals aim to reduce the molecular pairing and the atom loss rate near the Feshbach resonance:

- Narrow Feshbach resonances [36]: At a narrow Feshbach resonance, the Feshbach molecules have a dominant closed channel character and less overlap with the atoms from the open channel. This makes decay from the metastable atomic branch to the molecular branch less likely. However, the range of the interactions is longer near a narrow Feshbach resonance, precluding realization of the short-ranged Stoner model.
- Mass imbalance [47]: Mass imbalance can be introduced by using a mixture of two different isotopes or elements instead of two hyperfine states of the same isotope. Mass imbalanced pairs are harder to form, so mass imbalance is expected to reduce the molecular pairing rate. The

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mixture may consist of two fermionic atom species (e.g. ⁴⁰K and ⁶Li [48]), or one fermionic and one bosonic atom species (e.g. ⁴⁰K and ⁸⁷Rb [49]). In the latter case, the particle numbers and interaction strengths have to be tuned in such a way that (almost) all bosons are tightly bound to a fermionic atom. The Bose-Fermi pair acts as a (composite) fermion and can be considered as the second fermionic component. Mass imbalance is currently the most promising proposal for the realization of the itinerant ferromagnetic state, so there have been several theoretical studies of the associated phase diagram [50–53].

- Reduced dimensions (especially 1D): A (quasi-)1D two-component Fermi gas has been experimentally realized recently [54]. Three-body collisions are suppressed in 1D [55], so this is a promising system for the experimental realization of itinerant ferromagnetism. However, fully polarized itinerant ferromagnetism cannot be the ground state in 1D under certain symmetry conditions [56, 57]. A small symmetry breaking field could be used to circumvent this problem and enable realization of the itinerant ferromagnetic state [58].
- Optical lattices: Optical lattices (especially 3D optical lattices) limit the mobility of the atoms and therefore also the collision rate and atom loss rate. There have been several proposals for the realization of itinerant ferromagnetism in lattice models [59–65]. However, ferromagnetism realized in optical lattices may not be purely itinerant.

Other proposals are aimed at avoiding the Feshbach resonance, e.g. by lowering the value of $a_s k_F$ where the normal-to-itinerant-ferromagnetic phase transition is expected to occur:

- Dipolar interactions: Recently, ultracold dipolar Fermi gases have been experimentally realized. The dipole interaction is achieved by using dipolar molecules (e.g. KRb [66]) or atoms with large magnetic moments (e.g. ¹⁶¹Dy [67] or ¹⁶⁷Er [68]). With dipolar interactions, the Feshbach resonance may be avoided alltogether. It would be interesting to study whether itinerant ferromagnetism can be realized in dipolar atomic gases [69–71].
- Spin-orbit coupling: Spin-orbit coupling couples the spin state and momentum of the atoms, favoring alignment of the momentum and spin states of the atoms. One study suggested that the change in the dispersion relation caused by spin-orbit coupling may lower the critical value of $a_s k_F$ required to find itinerant ferromagnetism [72]. However, other studies suggest that the alignment of the spin state with the momentum would impede the formation of magnetic domains [73,74]. So far in experiments with ultracold atomic gases, only equal Rashba-Dresselhaus spin-orbit coupling has been realized [75–77], where the momentum and spin state are coupled along one direction. At the moment, experiments with other types of spin-orbit coupling still suffer from heating problems.

A third possibility is to avoid the competition between the magnetic domain formation and the molecular pairing, by preparing the gas in the fully polarized state:

• Demagnetization experiment: In this experiment two spin-polarized Fermi gases with opposite spins are prepared and brought into contact with each other. By studying the spin diffusion time as a function of the interaction strength one can probe itinerant ferromagnetism. In the ferromagnetic state, the spins should not diffuse and the domain boundary should be long-lived. Even if this state is metastable, the thermalization time can offer information on the metastability barrier [78].

The final trend is a return to the basic theory of itinerant ferromagnetism. As itinerant ferromagnetism is so notoriously hard to find experimentally, there are doubts about the existence and stability of the itinerant ferromagnetic state. By improving the basics, researchers are hoping to resolve these doubts. The research presented in this dissertation falls into this category:

• Few fermion systems: It is possible to exactly calculate the ground state of systems with a given small number of fermions. Furthermore, few fermion systems have also become accessible experimentally [79]. This can be used to test the validity of the current models for itinerant ferromagnetism [80–82].

• Dynamical stability of itinerant ferromagnetism: Dynamical stability is stability against density and polarization changes. A dynamical instability of itinerant ferromagnetism may explain why it is so notoriously hard to find experimentally. Studies of this topic are limited [42, 46, 57, 83]. In this dissertation, the dynamical stability of the itinerant ferromagnetic state is studied.

The goal of this dissertation is to improve the theoretical description of itinerant ferromagnetism in a homogeneous two-component ultracold atomic Fermi gas using the path-integral formalism. This formalism is introduced in the next chapter.
Chapter 3

Path-integral formalism

In this chapter, the theoretical toolbox that will be used in the remainder of this dissertation will be introduced. The basics of the path-integral formalism will be explained, with a focus on the field theoretical formulation. For more details about the path-integral formalism and its applications, the reader is referred to [84-87].

3.1 Principle of stationary action

The path-integral formalism was originally formulated by Richard P. Feynman as an answer to the question of how to extend the classical principle of stationary action (also called the principle of least action) to quantum mechanics [84]. That is why the principle of stationary action is introduced first.

3.1.1 Systems with N degrees of freedom

The aim of both classical and quantum mechanics is to predict the time evolution of the system, starting from knowledge of the state of the system at a given point in time. In classical mechanics, the state of a system with N degrees of freedom is represented by the 2N generalized coordinates q_i and $\dot{q}_i = dq_i/dt$ (i = 1, 2, ..., N and $N \in \mathbb{N}$). During the time evolution from time t_0 to time t_1 , the system will follow a certain path ($q_i(t)$) in configuration space. The action S of each path in configuration space is given by

$$S = \int_{t_0}^{t_1} L(q_i(t), \dot{q}_i(t)) dt, \qquad (3.1)$$

where the function $L(q_i, \dot{q}_i)$ is called the Lagrangian. The Lagrangian of the system is defined as the difference between the kinetic energy and the potential energy V of the system:

$$L(q_i, \dot{q}_i) = \sum_{i=1}^{N} \frac{m_i}{2} \dot{q}_i^2 - V(q_1, q_2, \dots, q_N), \qquad (3.2)$$

where m_i is the mass associated with the i^{th} generalized coordinate. There are many possible paths in configuration space, but in classical mechanics only one path is actually realized: the classical path. This path is determined from the principle of stationary action: $\delta S = 0$. This variation of the action is taken over all possible paths of the system in configuration space during the time evolution (with appropriate boundary conditions).

The principle of stationary action can be used to derive the Euler-Lagrange equations of motion,

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) = \frac{\partial L}{\partial q_i}.$$
(3.3)

This is a set of N equations, one for each (q_i, \dot{q}_i) -pair. The solution to these equations is the classical path.

3.1.2 Classical field theory

The principle of stationary action can be extended to continuous fields $\phi(x, t)$, which have an infinite number of degrees of freedom. This formulation is especially useful in the context of special relativity and electromagnetism. That is why in the field-theoretical formulation

$$S = \int \mathcal{L}(\phi, \partial_{\mu}\phi) d^{4}x \qquad (3.4)$$

of the action the four-vector notation is used: $\mu = 0, 1, 2, 3$ with $\mu = 0$ indicating the time coordinate and $\mu = 1, 2, 3$ indicating the spatial coordinates. The calligraphic $\mathcal{L}(\phi, \partial_{\mu}\phi)$ represents the Lagrangian density, which is related to the Lagrangian L through integration over the spatial coordinates:

$$L = \int \mathcal{L} d\mathbf{x}.$$
 (3.5)

The principle of stationary action $\delta S = 0$ remains the same, but now the variation of the action is taken over all possible configurations of the field ϕ (with the appropriate boundary conditions). The resulting field equations are given by

$$\frac{\partial \mathcal{L}(\phi, \partial_{\mu}\phi)}{\partial \phi} - \partial_{\mu} \left[\frac{\partial \mathcal{L}(\phi, \partial_{\mu}\phi)}{\partial (\partial_{\mu}\phi)} \right] = 0.$$
(3.6)

3.2 The path-integral formalism

In classical mechanics, only one path in configuration space is realized: the classical path (with $\delta S = 0$). However, in the path-integral formulation of quantum mechanics all paths in configuration space contribute and interfere with each other. This results in a probability distribution to find a particle at a given time and position.

In the path-integral formalism, only two postulates are needed. For a single particle in a onedimensional system (1D), represented by position coordinate x, they were originally formulated by R. P. Feynman as [84]

- 1. If an ideal measurement is performed to determine whether a particle has a path lying in a region of space time, then the probability that the result will be affirmative is the absolute square of a sum of complex contributions, one from each path in the region.
- 2. The paths contribute equally in magnitude, but the phase of their contribution is the classical action S in units of \hbar ; i.e., the time integral of the Lagrangian taken along the path.

The probability amplitude of the particle to propagate from position x_a at time t_a to position x_b at time t_b is given by the *propagator*

$$K(x_b, t_b; x_a, t_a) = \int_{x_a, t_a}^{x_b, t_b} \mathcal{D}[x] \exp\left\{\frac{iS[x(t)]}{\hbar}\right\}.$$
(3.7)

Here, $\int \mathcal{D}[x]$ represents the sum over all possible paths. Using the time-slicing method [85], the path integral can be rewritten as

$$\int_{x_a,t_a}^{x_b,t_b} \mathcal{D}\left[x\right] = \prod_{t\in]t_a,t_b[} \int_{-\infty}^{+\infty} dx_t.$$
(3.8)

This is a sum over all possible values of the coordinates x_t at each time $t \in]t_a, t_b[$. The complex quantum-mechanical wave function $\psi(x, t)$, which is defined in such a way that $|\psi(x, t)|^2$ is the probability to find the particle in position x at time t, must obey the following integral equation:

$$\psi\left(x_{b}, t_{b}\right) = \int K\left(x_{b}, t_{b}; x_{a}, t_{a}\right) \psi\left(x_{a}, t_{a}\right) dx_{a}.$$
(3.9)

If the action in (3.7) is chosen to be equal to the classical action (3.1), (3.9) becomes the integral representation of the Schrödinger equation. The path-integral formulation of quantum mechanics is fully equivalent with the Schrödinger and Heisenberg pictures.

If $|\delta S|$ is large with respect to \hbar , i.e. if small changes in the path induce large changes in the action, the phase factor exp $\{iS[x(t)]/\hbar\}$ changes rapidly and nearby paths will cancel each other's contributions to the path integral due to destructive interference. Paths where the action is stationary $(\delta S = 0)$ will experience the least destructive interference, so the largest contribution to the path integral is given by these classical paths. This links the path-integral formalism with the principle of stationary action in classical mechanics.

Feynman's original postulates for a single particle in 1D can easily be extended to multiple particles and higher-dimensional systems.

3.2.1 Statistical physics

Consider a system that consists of a single particle which is in thermal equilibrium with a bath of temperature T. In the path-integral formalism, it can be shown that the *partition function* of this system is given by

$$\mathcal{Z} = \int dx K \left(x, -i\hbar\beta | x, 0 \right), \tag{3.10}$$

with K the propagator as defined in eq. (3.7) and $\beta = 1/k_B T$ the inverse temperature of the system [85]. The partition function is a very important quantity in statistical physics, as it can be used to derive many other important statistical quantities, e.g. the free energy $F(T, V) = -k_B T \ln(\mathcal{Z})$ (with V the volume) and the internal energy $U(S, V) = k_B T^2 \partial [\ln(\mathcal{Z})] / \partial T$ (with S the entropy).

Note that the time coordinate $-i\hbar\beta$ is imaginary, so eq. (3.10) assumes that the propagator has been analytically extended into the imaginary time plane. In order to avoid working explicitly with imaginary numbers, the imaginary time coordinate $\tau = it$ is used. In this notation, the action

$$S[x] = \int_{0}^{-i\hbar\beta} dt \left\{ \frac{m [\dot{x}(t)]^{2}}{2} - V [x(t)] \right\}$$
(3.11)

is replaced by the Euclidean action

$$S_E[x] = \int_{0}^{h\beta} d\tau \left\{ \frac{m \left[\dot{x}(\tau) \right]^2}{2} + V[x(\tau)] \right\}$$
(3.12)

and the partition sum is given by

$$\mathcal{Z} = \int \mathcal{D}x \exp\left\{-\frac{S_E\left[x\left(\tau\right)\right]}{\hbar}\right\}$$
(3.13)

with

$$\int \mathcal{D}x = \prod_{\tau \in [0,\hbar\beta]} \int_{-\infty}^{+\infty} d\left[x\left(\tau\right)\right].$$
(3.14)

In contrast with eq. (3.8), in statistical physics the path integral (3.14) is also taken over the boundary values. Furthermore, there is an important sign difference between the Euclidean (3.12) and the normal (3.11) action. Note that the conversion between both notations is more complicated if there is also a vector potential involved, as this changes the kinetic energy part.

Just as Feynman's original postulates, these path-integral statistical physics expressions for a single particle in 1D can be extended to multiple particles and higher-dimensional systems.

3.3 Path-integral field theory

For very large particle numbers or if the number of particles in the system is not conserved, it is easier to use fields in order to describe the state of the system. For this purpose, quantum field theory was developed. In this context, the sum over all paths becomes a sum over all possible configurations of the fields. This is also called a functional integral.

3.3.1 Bosonic fields

Bosons are represented by complex scalar fields $\phi_{\mathbf{x},t}$. As an example, we can consider a "simpleverse", where there are only 5 possible values for the time and position coordinates (thus 25 possible (x,t) coordinates). In fig. 3.1, three possible configurations of a real field are shown. A sum over all configurations of the real field ϕ in the simpleverse is given by

$$\int \mathcal{D}\phi = \prod_{i=1}^{5} \prod_{j=1}^{5} \int d\left[\phi\left(x_i, t_j\right)\right]$$
(3.15)

with $\phi(x_i, t_j) \in \mathbb{R}$. For a complex bosonic field, it is necessary to sum over both the real and imaginary parts. This is commonly written as a path integral over the complex field ϕ and its complex conjugate $\overline{\phi}$:

$$\int \mathcal{D}\bar{\phi} \int \mathcal{D}\phi = \prod_{i=1}^{5} \prod_{j=1}^{5} \left\{ \int d\left[\bar{\phi}\left(x_{i}, t_{j}\right)\right] \int d\left[\phi\left(x_{i}, t_{j}\right)\right] \right\}$$
(3.16)

with $\bar{\phi}(x_i, t_j), \phi(x_i, t_j) \in \mathbb{C}$. This expression can be extended to other spaces than the simpleverse:

$$\int \mathcal{D}\bar{\phi} \int \mathcal{D}\phi = \prod_{\mathbf{x},t} \int d\bar{\phi}_{\mathbf{x},t} \int d\phi_{\mathbf{x},t}, \qquad (3.17)$$

where the product is taken over all possible values of \mathbf{x} and t.



Figure 3.1: Three possible configurations of the bosonic field $\phi(x,t)$ with $x, t \in \{1, 2, 3, 4, 5\}$ in the simpleverse.

3.3.2 Fermionic fields and Grassmann algebra

A path integral over all possible configurations of a fermionic field ψ is defined in a similar way as for the bosonic systems,

$$\int \mathcal{D}\bar{\psi} \int \mathcal{D}\psi = \prod_{\mathbf{x},t} \int d\bar{\psi}_{\mathbf{x},t} \int d\psi_{\mathbf{x},t}.$$
(3.18)

However, the values of the fermionic fields at each position \mathbf{x} and time t are no longer given by complex numbers, but by Grassmann numbers.

Grassmann numbers have very special algebraic properties. Especially the antisymmetry of a product of Grassmann numbers η_1 and η_2 is important,

$$\eta_1 \eta_2 = -\eta_2 \eta_1, \tag{3.19}$$

as this enables automatic inclusion of the fermionic antisymmetry property [88, 89]. Due to the antisymmetry, a product of two identical Grassmann variables is zero: $\eta_1^2 = 0$. This in turn implies that any function of N Grassmann variables can be exactly Taylor expanded into a function that is linear in each of the N Grassmann variables.

Grassmann integrals (also called Berezin integrals [90]) have some peculiar properties. They are defined as

$$\int d\eta = 0 \text{ and } \int d\eta \eta = 1.$$
(3.20)

Integrals of other functions can be easily calculated using the exact linear Taylor expansion:

$$\int d\eta f(\eta) = \int d\eta \left\{ f(0) + \left[\partial_{\eta} f(0) \right] \eta \right\} = \partial_{\eta} f(0) \,. \tag{3.21}$$

For the path-integral formalism, the Gaussian Grassmann integral has special importance. It is given by

$$\int d\bar{\eta} \int d\eta \exp\left(-a\eta\bar{\eta}\right) = \int d\bar{\eta} \int d\eta \left(1 - a\bar{\eta}\eta\right)$$
$$= \int d\bar{\eta} \left[a\bar{\eta} \left(\int d\eta\eta\right)\right]$$
$$= \int d\bar{\eta} \left(a\bar{\eta}\right) = a. \tag{3.22}$$

Note that interchanging $d\eta$ and $\bar{\eta}$ causes the corresponding term to change sign.

3.3.3 Partition function

In the context of itinerant ferromagnetism in ultracold atomic gases, it is important to study the statistical properties of a (pseudo)spin-1/2 Fermi gas. These can be derived from the partition function, given by

$$\mathcal{Z} = \left(\prod_{\sigma=\uparrow,\downarrow} \int \mathcal{D}\bar{\psi}_{\sigma} \int \mathcal{D}\psi_{\sigma}\right) \exp\left(-S_E\left[\bar{\psi}_{\sigma},\psi_{\sigma}\right]\right)$$
(3.23)

with $S_E[\bar{\psi}_{\sigma}, \psi_{\sigma}]$ the Euclidean action of the system. The statistical quantity most relevant to the remainder of this dissertation is the *thermodynamic grand potential per unit volume*, defined as

$$\Omega\left(\beta,\mu_{\uparrow},\mu_{\downarrow}\right) = -\frac{1}{\beta V}\ln\mathcal{Z},\tag{3.24}$$

because the ground state of the system that will be considered in the subsequent chapters can be found by minimizing $\Omega(\beta, \mu_{\uparrow}, \mu_{\downarrow})$. In eq. (3.24), μ_{\uparrow} and μ_{\downarrow} are the chemical potentials associated with particles of the respective spin states mentioned in the subscript.

If the Euclidean action is quadratic in the fermionic fields, the fermionic path integral in (3.23) can be performed exactly:

$$\int \mathcal{D}\bar{\psi} \int \mathcal{D}\psi \exp\left(-\sum_{j,j'=1}^{N} \bar{\psi}_j A_{jj'} \psi_{j'}\right) = \det A.$$
(3.25)

A free, non-interacting gas of neutral fermions is one of the few systems whose partition sum can be calculated exactly, as its Euclidean action (in units $\hbar = 1$ and 2m = 1) is given by the quadratic expression

$$S_E\left[\bar{\psi}_{\sigma},\psi_{\sigma}\right] = \sum_{\sigma=\uparrow,\downarrow} \int_0^{\rho} d\tau \int_V d\mathbf{x} \bar{\psi}_{\sigma,\mathbf{x},\tau} \left(\frac{\partial}{\partial \tau} - \boldsymbol{\nabla}_{\mathbf{x}}^2 - \mu_{\sigma}\right) \psi_{\sigma,\mathbf{x},\tau}$$
(3.26)

with $\tau = it$ the imaginary time, $\beta = 1/k_B T$ the inverse temperature, V the volume and μ_{σ} the chemical potential of spin state σ . Despite the limited number of systems where the path integral in (3.23) can be performed analytically, the path-integral formalism has become an important tool in quantum field theory [91].

In the remainder of this dissertation, only the Euclidean action will be used, so this will no longer be explicitly specified.

Part II

Contact interactions

Chapter 4

The saddle-point thermodynamic grand potential

The formalism presented in this chapter was published as:

E. Vermeyen and J. Tempere, Contact Potential Instability in the Path-Integral description of Itinerant Ferromagnetism, Journal of Low Temperature Physics 179, 175-185 (2015).

4.1 Introduction

In this chapter, the thermodynamic grand potential of a free, uniform spin-1/2 Fermi gas with contact potential interactions will be derived in the saddle-point approximation with density fields. The thermodynamic grand potential was introduced in Sec. 3.3.3. It is related to the partition sum as follows: $\Omega(\beta, \mu_{\uparrow}, \mu_{\downarrow}) = -\ln(\mathcal{Z})/\beta V$, with $\beta = 1/k_B T$ the inverse temperature and V the volume. In the path-integral formalism, the partition sum of a spin-1/2 Fermi gas is given by

$$\mathcal{Z} = \left(\prod_{\sigma=\uparrow,\downarrow} \int \mathcal{D}\bar{\psi}_{\sigma} \int \mathcal{D}\psi_{\sigma}\right) \exp\left(-S\left[\bar{\psi}_{\sigma},\psi_{\sigma}\right]\right).$$
(4.1)

The action $S\left[\bar{\psi}_{\sigma}, \psi_{\sigma}\right]$ depends on the system that is studied. In this chapter, the following action for a spin-1/2 Fermi gas with contact interactions and without an external interaction potential will be used (in units $\hbar = 1, 2m = 1, k_B = 1$ and $k_F = 1$):

$$S\left[\bar{\psi}_{\sigma},\psi_{\sigma}\right] = \sum_{\sigma=\uparrow,\downarrow} \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \bar{\psi}_{\sigma,\mathbf{x},\tau} \left(\frac{\partial}{\partial\tau} - \boldsymbol{\nabla}_{\mathbf{x}}^{2} - \mu_{\sigma}\right) \psi_{\sigma,\mathbf{x},\tau} + g \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \bar{\psi}_{\uparrow,\mathbf{x},\tau} \bar{\psi}_{\downarrow,\mathbf{x},\tau} \psi_{\downarrow,\mathbf{x},\tau} \psi_{\uparrow,\mathbf{x},\tau}, \qquad (4.2)$$

with $\tau = it$ the imaginary time and **x** the position vector. The first term in eq. (4.2) is the freeparticle energy, where $\nabla_{\mathbf{x}}^2$ is related to the kinetic energy and the chemical potentials μ_{σ} are used to fix the particle numbers. The second term in eq. (4.2) is the interaction energy, with g the interaction strength. In 3D, g is related to the s-wave scattering length a_s by eq. (2.2), or $g = 8\pi a_s k_F$ in the chosen units.

Because the interaction energy is of fourth order in the fermionic fields, the functional integral (4.1) with the action from eq. (4.2) can not be calculated exactly. The main theoretical challenge is to find the best way to convert the interaction term into terms which are of second order in the fermionic fields. The tool which is used to perform this conversion is called the Hubbard-Stratonovich transformation.

4.2 The Hubbard-Stratonovich transformation

4.2.1 Definition

In the Hubbard-Stratonovich transformation, a bosonic auxiliary field is introduced which acts as a mediator for the interactions. The transformation is based on an algebraic property of a path integral over the bosonic fields, which we choose to call A and B:

$$\mathcal{Z}_{AB} = \int \mathcal{D}A \int \mathcal{D}B \exp\left(c \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} A_{\mathbf{x},\tau} B_{\mathbf{x},\tau}\right), \qquad (4.3)$$

with $c, A_{\mathbf{x},\tau}, B_{\mathbf{x},\tau} \in \mathbb{C}$. As we sum over all possible configurations of the bosonic fields A and B, \mathcal{Z}_{AB} remains unchanged after shifting the fields A and B by the reference fields A^0 and B^0 ,

$$\mathcal{Z}_{AB} = \int \mathcal{D}A \int \mathcal{D}B \exp\left[c \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \left(A_{\mathbf{x},\tau} - A_{\mathbf{x},\tau}^{0}\right) \left(B_{\mathbf{x},\tau} - B_{\mathbf{x},\tau}^{0}\right)\right].$$
(4.4)

The factor that contains the product of the reference fields can then be isolated,

$$\exp\left(-c\int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} A^{0}_{\mathbf{x},\tau} B^{0}_{\mathbf{x},\tau}\right)$$
$$= \frac{1}{\mathcal{Z}_{AB}} \int \mathcal{D}A \int \mathcal{D}B \exp\left[c\int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \left(A_{\mathbf{x},\tau} B_{\mathbf{x},\tau} - A_{\mathbf{x},\tau} B^{0}_{\mathbf{x},\tau} - A^{0}_{\mathbf{x},\tau} B_{\mathbf{x},\tau}\right)\right].$$
(4.5)

If the reference fields are chosen in such a way that the left-hand side of eq. (4.5) becomes equal to the interaction term in the fermionic partition sum from eqs. (4.1) and (4.2),

$$\exp\left(-c\int_{0}^{\beta}d\tau\int_{V}d\mathbf{x}A^{0}_{\mathbf{x},\tau}B^{0}_{\mathbf{x},\tau}\right) = \exp\left(-g\int_{0}^{\beta}d\tau\int_{V}d\mathbf{x}\bar{\psi}_{\uparrow,\mathbf{x},\tau}\bar{\psi}_{\downarrow,\mathbf{x},\tau}\psi_{\downarrow,\mathbf{x},\tau}\psi_{\uparrow,\mathbf{x},\tau}\right),\tag{4.6}$$

eq. (4.5) can be used to convert the interaction term into terms of second order in the fermionic fields.

In this transformation, pairs of fermionic fields are treated as a complex bosonic field, even though in a strict mathematical sense these are products of Grassmann numbers. This issue will be dealt with in more detail in chapter 6. There are three possible ways to pair the four fermionic fields in the interaction term [92]:

- 1. Bogoliubov: $\bar{\psi}_{\uparrow,\mathbf{x},\tau}\bar{\psi}_{\downarrow,\mathbf{x},\tau}$ and $\psi_{\downarrow,\mathbf{x},\tau}\psi_{\uparrow,\mathbf{x},\tau}$,
- 2. Hartree: $\bar{\psi}_{\uparrow,\mathbf{x},\tau}\psi_{\uparrow,\mathbf{x},\tau}$ and $\bar{\psi}_{\downarrow,\mathbf{x},\tau}\psi_{\downarrow,\mathbf{x},\tau}$,
- 3. Fock: $\bar{\psi}_{\uparrow,\mathbf{x},\tau}\psi_{\downarrow,\mathbf{x},\tau}$ and $\bar{\psi}_{\downarrow,\mathbf{x},\tau}\psi_{\uparrow,\mathbf{x},\tau}$.

The Bogoliubov channel corresponds to superfluid pairing and has been used successfully to describe the BCS-BEC crossover [25,93]. The Hartree channel corresponds to density-density interactions and the Fock channel represents spin-flip interactions. In the remainder of this dissertation the Hartree channel will be used, as density-density interactions are most suitable to describe the interactions in the normal, paramagnetic and ferromagnetic phases [89, 94, 95].

4.2.2 Construction of the transformation

After the choice of the channel, it is still necessary to construct the transformation itself using the complex bosonic density fields ρ_{\uparrow} and ρ_{\downarrow} and their conjugate counterparts $\bar{\rho}_{\uparrow}$ and $\bar{\rho}_{\downarrow}$. In eq. (4.5), only two bosonic fields were used. To introduce four bosonic fields, we will need two transformations.

Both transformations are constructed from the definitions

$$\begin{cases} \rho^{0}_{\uparrow,\mathbf{x},\tau} = \bar{\rho}^{0}_{\uparrow,\mathbf{x},\tau} = \bar{\psi}_{\uparrow,\mathbf{x},\tau}\psi_{\uparrow,\mathbf{x},\tau}\\ \rho^{0}_{\downarrow,\mathbf{x},\tau} = \bar{\rho}^{0}_{\downarrow,\mathbf{x},\tau} = \bar{\psi}_{\downarrow,\mathbf{x},\tau}\psi_{\downarrow,\mathbf{x},\tau} \end{cases}$$
(4.7)

of the reference fields.

In the first transformation, $A_{\mathbf{x},\tau} = \bar{\rho}_{\downarrow,\mathbf{x},\tau}$, $B_{\mathbf{x},\tau} = \rho_{\uparrow,\mathbf{x},\tau}$ and c = g/2 are chosen in eq. (4.5). The resulting transformation is given by

$$\exp\left(-\frac{g}{2}\int_{0}^{\beta}d\tau\int_{V}d\mathbf{x}\bar{\psi}_{\downarrow,\mathbf{x},\tau}\psi_{\downarrow,\mathbf{x},\tau}\bar{\psi}_{\uparrow,\mathbf{x},\tau}\psi_{\uparrow,\mathbf{x},\tau}\right)$$
(4.8)

$$=\frac{1}{\mathcal{Z}_{\rho,1}}\int \mathcal{D}\bar{\rho}_{\downarrow}\int \mathcal{D}\rho_{\uparrow} \exp\left[\frac{g}{2}\int\limits_{0}^{\beta}d\tau\int\limits_{V}d\mathbf{x}\left(-\bar{\rho}_{\downarrow,\mathbf{x},\tau}\bar{\psi}_{\uparrow,\mathbf{x},\tau}\psi_{\uparrow,\mathbf{x},\tau}+\bar{\rho}_{\downarrow,\mathbf{x},\tau}\rho_{\uparrow,\mathbf{x},\tau}-\bar{\psi}_{\downarrow,\mathbf{x},\tau}\psi_{\downarrow,\mathbf{x},\tau}\rho_{\uparrow,\mathbf{x},\tau}\right)\right].$$

The second transformation is constructed using the choice $A_{\mathbf{x},\tau} = \bar{\rho}_{\uparrow,\mathbf{x},\tau}$, $B_{\mathbf{x},\tau} = \rho_{\downarrow,\mathbf{x},\tau}$ and c = g/2 in eq. (4.5),

$$\exp\left(-\frac{g}{2}\int_{0}^{\beta}d\tau\int_{V}d\mathbf{x}\bar{\psi}_{\uparrow,\mathbf{x},\tau}\psi_{\downarrow,\mathbf{x},\tau}\bar{\psi}_{\downarrow,\mathbf{x},\tau}\psi_{\downarrow,\mathbf{x},\tau}\right) \tag{4.9}$$

$$=\frac{1}{\mathcal{Z}_{\rho,2}}\int \mathcal{D}\bar{\rho}_{\uparrow}\int \mathcal{D}\rho_{\downarrow} \exp\left[\frac{g}{2}\int\limits_{0}^{\rho}d\tau\int\limits_{V}d\mathbf{x}\left(-\bar{\rho}_{\uparrow,\mathbf{x},\tau}\bar{\psi}_{\downarrow,\mathbf{x},\tau}\psi_{\downarrow,\mathbf{x},\tau}+\bar{\rho}_{\uparrow,\mathbf{x},\tau}\rho_{\downarrow,\mathbf{x},\tau}-\bar{\psi}_{\uparrow,\mathbf{x},\tau}\psi_{\uparrow,\mathbf{x},\tau}\rho_{\downarrow,\mathbf{x},\tau}\right)\right].$$

Using the antisymmetry of a product of Grassmann variables,

$$\bar{\psi}_{\uparrow,\mathbf{x},\tau}\bar{\psi}_{\downarrow,\mathbf{x},\tau}\psi_{\downarrow,\mathbf{x},\tau}\psi_{\uparrow,\mathbf{x},\tau} = \bar{\psi}_{\downarrow,\mathbf{x},\tau}\psi_{\downarrow,\mathbf{x},\tau}\bar{\psi}_{\uparrow,\mathbf{x},\tau}\psi_{\uparrow,\mathbf{x},\tau} = \bar{\psi}_{\uparrow,\mathbf{x},\tau}\psi_{\uparrow,\mathbf{x},\tau}\bar{\psi}_{\downarrow,\mathbf{x},\tau}\psi_{\downarrow,\mathbf{x},\tau}, \qquad (4.10)$$

so (4.8) and (4.9) can be used to construct the Hubbard-Stratonovich transformation that will be used in the remainder of this chapter:

$$\exp\left(-g\int_{0}^{\beta}d\tau\int_{V}d\mathbf{x}\bar{\psi}_{\uparrow,\mathbf{x},\tau}\bar{\psi}_{\downarrow,\mathbf{x},\tau}\psi_{\downarrow,\mathbf{x},\tau}\psi_{\uparrow,\mathbf{x},\tau}\right)$$

$$=\frac{1}{\mathcal{Z}_{\rho,1}\mathcal{Z}_{\rho,2}}\int\mathcal{D}\bar{\rho}_{\uparrow}\int\mathcal{D}\rho_{\uparrow}\int\mathcal{D}\bar{\rho}_{\downarrow}\int\mathcal{D}\rho_{\downarrow}\exp\left[g\int_{0}^{\beta}d\tau\int_{V}d\mathbf{x}\left(\frac{\bar{\rho}_{\uparrow,\mathbf{x},\tau}\rho_{\downarrow,\mathbf{x},\tau}+\bar{\rho}_{\downarrow,\mathbf{x},\tau}\rho_{\uparrow,\mathbf{x},\tau}}{2}\right)\right]$$

$$-\frac{\bar{\rho}_{\uparrow,\mathbf{x},\tau}+\rho_{\uparrow,\mathbf{x},\tau}}{2}\bar{\psi}_{\downarrow,\mathbf{x},\tau}\psi_{\downarrow,\mathbf{x},\tau}-\frac{\bar{\rho}_{\downarrow,\mathbf{x},\tau}+\rho_{\downarrow,\mathbf{x},\tau}}{2}\bar{\psi}_{\uparrow,\mathbf{x},\tau}\psi_{\uparrow,\mathbf{x},\tau}}\right)\right].$$
(4.11)

For symmetry reasons, the transformations in eqs. (4.8) and (4.9) contribute equally to eq. (4.11). Both transformations are each other's complex conjugate and they can be viewed as two directions of the same interaction process (fig. 4.1).

Because the reference fields of the bosonic fields are equal to the reference fields of their conjugated counterparts, it is also possible to construct a transformation with real density fields ρ_{\uparrow} and ρ_{\downarrow} :

$$\exp\left(-g\int_{0}^{\beta}d\tau\int_{V}d\mathbf{x}\bar{\psi}_{\uparrow,\mathbf{x},\tau}\bar{\psi}_{\downarrow,\mathbf{x},\tau}\psi_{\downarrow,\mathbf{x},\tau}\psi_{\uparrow,\mathbf{x},\tau}\right)$$
(4.12)

$$= \frac{1}{\mathcal{Z}_{\rho}} \int \mathcal{D}\rho_{\uparrow} \int \mathcal{D}\rho_{\downarrow} \exp\left[g \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \left(\rho_{\uparrow,\mathbf{x},\tau}\rho_{\downarrow,\mathbf{x},\tau} - \rho_{\uparrow,\mathbf{x},\tau}\bar{\psi}_{\downarrow,\mathbf{x},\tau}\psi_{\downarrow,\mathbf{x},\tau} - \rho_{\downarrow,\mathbf{x},\tau}\bar{\psi}_{\uparrow,\mathbf{x},\tau}\psi_{\uparrow,\mathbf{x},\tau}\right)\right].$$



Figure 4.1: A diagrammatic representation of the two Hubbard-Stratonovich transformations in eqs. (4.8) and (4.9). Both transformations are complementary, as they can be viewed as opposite directions of the same interaction process.

In the saddle-point approximation, this transformation is equivalent to the transformation in eq. (4.11). In this chapter, the full transformation with complex fields will be used in order to demonstrate this equivalency. In part II, we will immediately use real density fields in the Hubbard-Stratonovich transformation.

As a side note, it is also possible to rewrite eq. (4.11) using the notation $\rho = (\rho_{\uparrow} + \rho_{\downarrow})/2$ and $\phi = (\rho_{\uparrow} - \rho_{\downarrow})/2$ for the average and half density difference fields. This notation is often used in the literature [96].

4.2.3 Result

After the Hubbard-Stratonovich transformation in eq. (4.11), the partition sum is given by

$$\mathcal{Z} = \left(\prod_{\sigma=\uparrow,\downarrow} \int \mathcal{D}\bar{\psi}_{\sigma} \int \mathcal{D}\psi_{\sigma} \int \mathcal{D}\bar{\rho}_{\sigma} \int \mathcal{D}\rho_{\sigma}\right) \exp\left(-S_{eff}\left[\bar{\psi}_{\sigma},\psi_{\sigma},\bar{\rho}_{\sigma},\rho_{\sigma}\right]\right),\tag{4.13}$$

where we defined a new effective action $S_{eff} \left[\bar{\psi}_{\sigma}, \psi_{\sigma}, \bar{\rho}_{\sigma}, \rho_{\sigma} \right]$ given by

$$S_{eff}\left[\bar{\psi}_{\sigma},\psi_{\sigma},\bar{\rho}_{\sigma},\rho_{\sigma}\right] = \sum_{\sigma=\uparrow,\downarrow} \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \left[\bar{\psi}_{\sigma,\mathbf{x},\tau} \left(\frac{\partial}{\partial\tau} - \boldsymbol{\nabla}_{\mathbf{x}}^{2} - \mu_{\sigma}\right)\psi_{\sigma,\mathbf{x},\tau} + g \frac{\bar{\rho}_{-\sigma,\mathbf{x},\tau} + \rho_{-\sigma,\mathbf{x},\tau}}{2} \bar{\psi}_{\sigma,\mathbf{x},\tau} \psi_{\sigma,\mathbf{x},\tau} - \frac{g}{2}\bar{\rho}_{\sigma,\mathbf{x},\tau}\rho_{-\sigma,\mathbf{x},\tau}\right].$$
(4.14)

The proportionality factors $\mathcal{Z}_{\rho,1}$ and $\mathcal{Z}_{\rho,2}$ from the Hubbard-Stratonovich transformation (4.11) will only show up as a shift in the zero point of the thermodynamic grand potential. They were left out in eqs. (4.13) and (4.14), as they were used to define a new energy reference.

4.3 Fourier transformation

The fermionic path integral in eq. (4.13) can not yet be performed due to the remaining derivatives in the effective action (4.14). In order to remove these derivatives, eq. (4.14) is Fourier transformed. The Fourier transformation of the fermionic and bosonic fields is defined as

$$\psi_{\sigma,\mathbf{x},\tau} = \frac{1}{\sqrt{\beta V}} \sum_{\mathbf{k},n} \exp\left(i\mathbf{k}\cdot\mathbf{x} - i\omega_n\tau\right)\psi_{\sigma,\mathbf{k},n}$$

$$\bar{\psi}_{\sigma,\mathbf{x},\tau} = \frac{1}{\sqrt{\beta V}} \sum_{\mathbf{k},n} \exp\left(-i\mathbf{k}\cdot\mathbf{x} + i\omega_n\tau\right)\bar{\psi}_{\sigma,\mathbf{k},n}$$
(4.15)

$$\begin{cases} \bar{\psi}_{\sigma,\mathbf{x},\tau} = \frac{1}{\sqrt{\beta V}} \sum_{\mathbf{k},n}^{\mathbf{k},n} \exp\left(-i\mathbf{k}\cdot\mathbf{x} + i\omega_{n}\tau\right) \bar{\psi}_{\sigma,\mathbf{k},n} \\ \\ \rho_{\sigma,\mathbf{x},\tau} = \frac{1}{\sqrt{\beta V}} \sum_{\mathbf{q},m} \exp\left(i\mathbf{q}\cdot\mathbf{x} - i\Omega_{m}\tau\right) \rho_{\sigma,\mathbf{q},m} \\ \bar{\rho}_{\sigma,\mathbf{x},\tau} = \frac{1}{\sqrt{\beta V}} \sum_{\mathbf{q},m} \exp\left(-i\mathbf{q}\cdot\mathbf{x} + i\Omega_{m}\tau\right) \bar{\rho}_{\sigma,\mathbf{q},m} \end{cases}$$
(4.15)

with $\omega_n = (2n+1)\pi/\beta$ $(n \in \mathbb{Z})$ the fermionic and $\Omega_m = 2\pi m/\beta$ $(m \in \mathbb{Z})$ the bosonic Matsubara frequencies. Furthermore, the following representations of the Dirac delta function will be used:

$$\delta\left(\mathbf{k}\right) = \frac{1}{V} \int_{V} d\mathbf{x} \exp\left(\pm i\mathbf{k} \cdot \mathbf{x}\right),\tag{4.17}$$

$$\delta_m = \frac{1}{\beta} \int_0^\beta d\tau \exp\left(\pm i\Omega_m \tau\right). \tag{4.18}$$

The first term of the effective action (4.14), the free-particle part, Fourier transforms as

$$\sum_{\sigma=\uparrow,\downarrow} \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \bar{\psi}_{\sigma,\mathbf{x},\tau} \left(\frac{\partial}{\partial \tau} - \boldsymbol{\nabla}_{\mathbf{x}}^{2} - \mu_{\sigma} \right) \psi_{\sigma,\mathbf{x},\tau}$$

$$= \sum_{\sigma=\uparrow,\downarrow} \sum_{\mathbf{k},n} \sum_{\mathbf{k}',n'} \frac{1}{\beta V} \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \left[\exp\left(-i\mathbf{k} \cdot \mathbf{x} + i\omega_{n}\tau\right) \bar{\psi}_{\sigma,\mathbf{k},n} \left(\frac{\partial}{\partial \tau} - \boldsymbol{\nabla}_{\mathbf{x}}^{2} - \mu_{\sigma} \right) \right]$$

$$\times \exp\left(i\mathbf{k}' \cdot \mathbf{x} - i\omega_{n'}\tau\right) \psi_{\sigma,\mathbf{k}',n'}$$

$$= \sum_{\sigma=\uparrow,\downarrow} \sum_{\mathbf{k},n} \sum_{\mathbf{k}',n'} \left\{ \frac{1}{\beta} \int_{0}^{\beta} d\tau \exp\left[i\left(\omega_{n} - \omega_{n'}\right)\tau\right] \right\} \left\{ \frac{1}{V} \int_{V} d\mathbf{x} \exp\left[-i\left(\mathbf{k} - \mathbf{k}'\right) \cdot \mathbf{x}\right] \right\}$$

$$\times \bar{\psi}_{\sigma,\mathbf{k},n} \left[-i\omega_{n'} + (\mathbf{k}')^{2} - \mu_{\sigma} \right] \psi_{\sigma,\mathbf{k}',n'}$$

$$= \sum_{\sigma=\uparrow,\downarrow} \sum_{\mathbf{k},n} \sum_{\mathbf{k}',n'} \bar{\psi}_{\sigma,\mathbf{k},n} \left(-i\omega_{n} + \mathbf{k}^{2} - \mu_{\sigma} \right) \delta_{\Delta n} \delta\left(\Delta\mathbf{k}\right) \psi_{\sigma,\mathbf{k}',n'}.$$

$$(4.19)$$

with $\Delta \mathbf{k} = \mathbf{k} - \mathbf{k}'$ and $\Delta n = n - n'$. Fourier transforming the interaction terms in (4.14) is similar. In the four-vector notation $k = (\mathbf{k}, \omega_n)$ and $q = (\mathbf{q}, \Omega_m)$, the resulting Fourier transformed effective action is given by

$$S_{eff}\left[\bar{\psi}_{\sigma},\psi_{\sigma},\bar{\rho}_{\sigma},\rho_{\sigma}\right] = \sum_{\sigma=\uparrow,\downarrow} \left\{ \sum_{k,k'} \bar{\psi}_{\sigma,\mathbf{k},n} \left[-G_{\sigma}^{-1}\left(k,k'\right) \right] \psi_{\sigma,\mathbf{k}',n'} - \frac{g}{2} \sum_{q} \bar{\rho}_{\sigma,q} \rho_{-\sigma,q} \right\}.$$
(4.20)

with the inverse Green's function defined as

$$-G_{\sigma}^{-1}(k,k') = \left(-i\omega_n + \mathbf{k}^2 - \mu_{\sigma}\right)\delta\left(\Delta k\right) + g\frac{\bar{\rho}_{-\sigma,-\Delta k} + \rho_{-\sigma,\Delta k}}{2\sqrt{\beta V}}.$$
(4.21)

After the Fourier transformation of the effective action, the standard formula (3.25) for a Gaussian fermionic path integral can be used to carry out the fermionic path integral. The resulting expression for the partition sum is given by

$$\mathcal{Z} = \left(\prod_{\sigma=\uparrow,\downarrow} \int \mathcal{D}\bar{\rho}_{\sigma} \int \mathcal{D}\rho_{\sigma}\right) \exp\left[\sum_{\sigma=\uparrow,\downarrow} \left(\frac{g}{2} \sum_{q} \bar{\rho}_{\sigma,q} \rho_{-\sigma,q} + \operatorname{Tr}\left\{\ln\left[-G_{\sigma}^{-1}\left(k,k'\right)\right]\right\}\right)\right].$$
(4.22)

The term Tr $\{\ln \left[-G_{\sigma}^{-1}(k,k')\right]\}$ is problematic. Due to the contributions of the bosonic density fields in eq. (4.21), $-G_{\sigma}^{-1}$ is a highly non-diagonal infinitely large matrix in k-space. Diagonalizing that matrix in order to take the logarithm is not feasible, so the remaining bosonic path integral cannot be performed exactly. In order to overcome this problem, the saddle-point approximation will be used next.

4.4 Saddle-point approximation

In the saddle-point approximation, the main contribution to the path integral over bosonic fields is assumed to come from a configuration where the field is constant:

$$\begin{cases} \rho_{\sigma,q} = \sqrt{\beta V} \delta(q) \rho_{\sigma} \\ \bar{\rho}_{\sigma,q} = \sqrt{\beta V} \delta(q) \rho_{\sigma}^{*} \end{cases}$$

$$(4.23)$$

and only the combination of values $(\rho_{\uparrow}, \rho_{\downarrow})$ that extremizes (preferably minimizes) the thermodynamic grand potential will be counted in the path integral. In this approximation, the inverse Green's function matrix becomes diagonal in k-space,

$$-G_{\sigma}^{-1}(k,k') = \left(-i\omega_n + \mathbf{k}^2 - \mu_{\sigma} + g\operatorname{Re}\left[\rho_{-\sigma}\right]\right)\delta\left(\Delta k\right)$$
(4.24)

and the resulting partition sum is given by

$$\mathcal{Z} = \exp\left\{\sum_{\sigma=\uparrow,\downarrow} \left[\frac{g}{2}\beta V \rho_{\sigma}^* \rho_{-\sigma} + \sum_k \ln\left(-i\omega_n + \mathbf{k}^2 - \mu_{\sigma} + g\operatorname{Re}\left[\rho_{-\sigma}\right]\right)\right]\right\}$$
(4.25)

Using the definition in eq. (3.24) of the thermodynamic grand potential per unit volume, we find

$$\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow},\rho_{\downarrow}\right) = -g\rho_{\uparrow}^{R}\rho_{\downarrow}^{R} - g\rho_{\uparrow}^{I}\rho_{\downarrow}^{I} - \sum_{\sigma=\uparrow,\downarrow}\frac{1}{\beta V}\sum_{k}\ln\left(-i\omega_{n} + \mathbf{k}^{2} - \mu_{\sigma} + g\rho_{-\sigma}^{R}\right),\qquad(4.26)$$

with $\rho_{\sigma}^{R} = \operatorname{Re} [\rho_{\sigma}]$ and $\rho_{\sigma}^{I} = \operatorname{Im} [\rho_{\sigma}]$. The imaginary parts of ρ_{\uparrow} and ρ_{\downarrow} only occur in the second term of (4.26) as a shift in Ω_{sp} , so we can choose $\rho_{\uparrow}^{I} = \rho_{\downarrow}^{I} = 0$. This shows that it would have been possible to use the Hubbard-Stratonovich transformation with real bosonic density fields from Sec. 4.2.2. The real parts of ρ_{\uparrow} and ρ_{\downarrow} still have to be determined using the saddle-point equations

$$\frac{\partial\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}^{R},\rho_{\downarrow}^{R}\right)}{\partial\rho_{\sigma}^{R}}\bigg|_{\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{-\sigma}^{R}} = 0.$$
(4.27)

The remaining Matsubara sum in (4.26) was performed using contour integration and the residue theorem. The result was also checked numerically. After taking the continuum limit of the remaining sum over **k** in (4.26), we find

$$\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}^{R},\rho_{\downarrow}^{R}\right) = -g\rho_{\uparrow}^{R}\rho_{\downarrow}^{R} + \Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)$$
(4.28)

$$\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right) = -\sum_{\sigma=\uparrow,\downarrow} \int \frac{d^D k}{(2\pi)^D} \left(\frac{1}{\beta} \ln\left\{1 + \exp\left[\beta\left(\mathbf{k}^2 - \mu_{\sigma}'\right)\right]\right\} - \mathbf{k}^2 + \mu_{\sigma}'\right)$$
(4.29)

in D dimensions. $\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)$ has the same form as the non-interacting free-particle energy, but with a shift in the chemical potentials due to the interactions. The new effective chemical potentials are defined as

$$\mu'_{\sigma} = \mu_{\sigma} - g\rho^R_{-\sigma}.\tag{4.30}$$

To summarize, we find in the saddle-point approximation that the contact interactions cause

- 1. an extra term in $\Omega_{sp}\left(\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho^R_{\uparrow}, \rho^R_{\downarrow}\right)$, the interaction energy $-g\rho^R_{\uparrow}\rho^R_{\downarrow}$, and
- 2. a shift $-g\rho_{-\sigma}^R$ of the effective chemical potential.

The saddle-point equations have to be solved for each value of the thermodynamic variables β , μ_{\uparrow} and μ_{\downarrow} . The resulting thermodynamic grand potential after determining the values of ρ_{\uparrow}^R and ρ_{\downarrow}^R will from now on be called Ω_{sp} (β , μ_{\uparrow} , μ_{\downarrow}).

4.4.1 The number equations

The particle number densities are determined by the number equations

$$n_{\sigma} = -\left. \frac{\partial \Omega_{sp} \left(\beta, \mu_{\uparrow}, \mu_{\downarrow}\right)}{\partial \mu_{\sigma}} \right|_{\beta, \mu_{-\sigma}}.$$
(4.31)

The saddle-point equations need to be solved together with the number equations, as the choice of k_F as a unit implies that the total particle density $n = n_{\uparrow} + n_{\downarrow}$ is given by $n = k_F^3/3\pi^2 = 1/3\pi^2$.

The number equations (4.31) can be rewritten as a function of $\Omega_{sp}\left(\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\uparrow}^{R}, \rho_{\downarrow}^{R}\right)$,

$$n_{\sigma} = -\frac{\partial\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}^{R},\rho_{\downarrow}^{R}\right)}{\partial\mu_{\sigma}}\bigg|_{\beta,\mu_{-\sigma};\rho_{\uparrow}^{R},\rho_{\downarrow}^{R}} - \frac{\partial\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}^{R},\rho_{\downarrow}^{R}\right)}{\partial\rho_{\uparrow}^{R}}\bigg|_{\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\downarrow}^{R}}\frac{\partial\rho_{\uparrow}^{R}}{\partial\mu_{\sigma}}\bigg|_{\beta,\mu_{-\sigma}} - \frac{\partial\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\downarrow}^{R},\rho_{\downarrow}^{R}\right)}{\partial\rho_{\downarrow}^{R}}\bigg|_{\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}^{R}}\frac{\partial\rho_{\downarrow}^{R}}{\partial\mu_{\sigma}}\bigg|_{\beta,\mu_{-\sigma}}.$$

$$(4.32)$$

For solutions to the saddle-point equations (4.27), this simplifies to

$$n_{\sigma} = -\left. \frac{\partial \Omega_{sp} \left(\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\uparrow}^{R}, \rho_{\downarrow}^{R} \right)}{\partial \mu_{\sigma}} \right|_{\beta, \mu_{-\sigma}; \rho_{\uparrow}^{R}, \rho_{\downarrow}^{R}} = -\left. \frac{\partial \Omega_{sp,0} \left(\beta, \mu_{\uparrow}', \mu_{\downarrow}' \right)}{\partial \mu_{\sigma}'} \right|_{\beta, \mu_{-\sigma}'}.$$
(4.33)

This expression can in turn be used to rewrite the saddle-point equations (4.27) after taking the first derivatives of $\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}^{R},\rho_{\downarrow}^{R}\right)$ (given by eqs. (4.28), (4.29) and (4.30)) to ρ_{\uparrow}^{R} and ρ_{\downarrow}^{R} ,

$$0 = \frac{\partial\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}^{R},\rho_{\downarrow}^{R}\right)}{\partial\rho_{\uparrow}^{R}}\bigg|_{\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\downarrow}^{R}} = -g\rho_{\downarrow}^{R} + \frac{\partial\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)}{\partial\mu_{\downarrow}'}\bigg|_{\beta,\mu_{\uparrow}'}\frac{\partial\mu_{\downarrow}'}{\partial\rho_{\uparrow}}\bigg|_{\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\downarrow}^{R}}$$
$$= -g\rho_{\downarrow}^{R} + gn_{\downarrow} \tag{4.34}$$

$$\Leftrightarrow \rho_{\downarrow}^R = n_{\downarrow}. \tag{4.35}$$

In a similar way, the other saddle-point equation becomes $\rho^R_{\uparrow} = n_{\uparrow}$. This validates the interpretation of ρ^R_{\uparrow} and ρ^R_{\downarrow} as density fields.

4.5 Stoner criterion

It is still necessary to check whether the saddle-point thermodynamic grand potential (4.28) can be used to study itinerant ferromagnetism. As the saddle-point approximation is equivalent to a meanfield approximation, at temperature zero in 3D we should be able to recover the Stoner criterion and the mean-field Stoner model from Sec. 2.3.1. As itinerant ferromagnetism is spontaneous polarization, the assumption $\mu_{\uparrow} = \mu_{\downarrow} = \mu$ is necessary to exclude polarization induced by chemical potential differences.

In the remainder of this section, the saddle-point thermodynamic grand potential will be calculated and studied for the case T = 0 ($\beta \to +\infty$) and $\mu_{\uparrow} = \mu_{\downarrow} = \mu$ in 3D.

4.5.1 Temperature zero limit

In the temperature zero limit $(\beta \to +\infty)$, expression (4.29) for the free-particle energy is greatly simplified,

$$\lim_{\beta \to +\infty} \Omega_{sp,0} \left(\beta, \mu_{\uparrow}', \mu_{\downarrow}' \right) = -\sum_{\sigma=\uparrow,\downarrow} \int \frac{d^3k}{(2\pi)^3} \left[\lim_{\beta \to +\infty} \left(\frac{1}{\beta} \ln \left\{ 1 + \exp \left[\beta \left(\mathbf{k}^2 - \mu_{\sigma}' \right) \right] \right\} \right) - \mathbf{k}^2 + \mu_{\sigma}' \right] \right]$$
$$= -\sum_{\sigma=\uparrow,\downarrow} \int_{0}^{+\infty} \frac{dk}{2\pi^2} k^2 \left(k^2 - \mu_{\sigma}' \right) \left[\Theta \left(k^2 - \mu_{\sigma}' \right) - 1 \right]$$
$$= -\sum_{\sigma=\uparrow,\downarrow} \Theta \left(\mu_{\sigma}' \right) \int_{0}^{\sqrt{[\mu_{\sigma}]_+}} \frac{dk}{2\pi^2} \left(-k^2 + \mu_{\sigma}' \right) = -\sum_{\sigma=\uparrow,\downarrow} \frac{[\mu_{\sigma}']_+^{5/2}}{15\pi^2}, \qquad (4.36)$$

where the new notation $[x]_{+} = \max[x, 0]$ was introduced. The saddle-point thermodynamic grand potential is then given by

$$\Omega_{sp}^{T=0}\left(\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}^{R},\rho_{\downarrow}^{R}\right) = \lim_{\beta \to +\infty} \Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}^{R},\rho_{\downarrow}^{R}\right)$$
$$= -g\rho_{\uparrow}^{R}\rho_{\downarrow}^{R} - \frac{\left[\mu_{\uparrow}'\right]_{+}^{5/2} + \left[\mu_{\downarrow}'\right]_{+}^{5/2}}{15\pi^{2}}.$$
(4.37)

4.5.2 Solving the saddle-point equations

Instead of solving the saddle-point equations for each value of the chemical potentials, it is easier to start from given particle number densities n_{\uparrow} and n_{\downarrow} . In that case we know the solutions to the saddle-point equations, as they are given by $\rho_{\sigma} = n_{\sigma}$. What remains is to calculate the values of the chemical potentials which correspond to this particular solution to the saddle-point equations.

First, the effective chemical potentials are calculated from the number equations (4.33),

$$n_{\sigma} = \frac{[\mu_{\sigma}']_{+}^{3/2}}{6\pi^{2}} \Leftrightarrow [\mu_{\sigma}']_{+} = (6\pi^{2}n_{\sigma})^{2/3}.$$
(4.38)

If $n_{\uparrow} \neq 0$ and $n_{\downarrow} \neq 0$, i.e. for unpolarized and partially polarized saddle points, $\mu'_{\sigma} = (6\pi^2 n_{\sigma})^{2/3}$. For a given polarization $P = (n_{\uparrow} - n_{\downarrow}) / (n_{\uparrow} + n_{\downarrow})$ with $n = 1/3\pi^2$ by the choice of $k_F = 1$ as a unit, this implies

$$\begin{cases} n_{\uparrow} = \frac{(1+P)}{6\pi^2} \\ n_{\downarrow} = \frac{(1-P)}{6\pi^2} \end{cases} \Rightarrow \begin{cases} \mu_{\uparrow}' = (1+P)^{2/3} \\ \mu_{\downarrow}' = (1-P)^{2/3} \end{cases} .$$
(4.39)

 $\Omega_{sp}^{T=0}$ is then given by

$$\Omega_{sp}^{T=0}\left(P\right) = -\frac{2}{9\pi^3} a_s k_F \left(1 - P^2\right) - \frac{\left(1 + P\right)^{5/3} + \left(1 - P\right)^{5/3}}{15\pi^2},\tag{4.40}$$

where $g = 8\pi a_s k_F$ was used. Note that in order to recover the free energy per unit volume (2.5) from the Stoner model (Sec. 2.3.1), eq. (4.40) still needs to be converted from the grand-canonical to the canonical ensemble.

Finally, the chemical potentials can be derived from the definition (4.30) of the effective chemical potentials,

$$\mu_{\uparrow} = (1+P)^{2/3} + \frac{4}{3\pi} a_s k_F (1-P)$$
(4.41)

$$\mu_{\downarrow} = (1-P)^{2/3} + \frac{4}{3\pi} a_s k_F (1+P)$$
(4.42)

The requirement $\mu_{\uparrow} = \mu_{\downarrow}$ results in an equation for the value of the interaction parameter $a_s k_F$ where solutions with polarization P to the saddle-point equations occur:

$$\frac{8P}{3\pi}a_sk_F = (1+P)^{2/3} - (1-P)^{2/3}.$$
(4.43)

The unpolarized solution (P = 0) to this equation always exists. For the partially polarized solutions,

$$a_s k_F = \frac{3\pi}{8} \frac{(1+P)^{2/3} - (1-P)^{2/3}}{P}.$$
(4.44)

The onset of the polarization can be found using a Taylor expansion of the numerator,

$$a_s k_F \approx \frac{3\pi}{8} \frac{1 + \frac{2}{3}P - 1 + \frac{2}{3}P}{P} = \frac{\pi}{2}.$$
 (4.45)

This is equal to the Stoner criterion (2.8) for the onset of itinerant ferromagnetism.

In the fully polarized case, $n_{\uparrow} = 0$ or $n_{\downarrow} = 0$ and there is an indeterminacy in eq. (4.38): if $n_{\uparrow} = 0$ (or $n_{\downarrow} = 0$), any negative value of μ'_{\uparrow} (or μ'_{\downarrow} respectively) is a valid solution of eq. (4.38). For positive full polarization (P = 1 and $n_{\downarrow} = 0$), this modifies eq. (4.42) to

$$\mu_{\downarrow} < \frac{8}{3\pi} a_s k_F \tag{4.46}$$

and the condition (4.44) to $a_s k_F > 2^{-7/3} 3\pi$. For negative full polarization (P = -1 and $n_{\uparrow} = 0$), a similar modification of eq. (4.41) results in the same condition $a_s k_F > 2^{-7/3} 3\pi$. The onset of full polarization occurs at $a_s k_F = 2^{-7/3} 3\pi$.

4.5.3 Grand-canonical vs. canonical ensemble

The saddle-point thermodynamic grand potential per unit volume $\Omega_{sp}^{T=0}(P)$ is shown in fig. 4.2 as a function of $1/a_sk_F$. It is hard to compare results with different polarization at the same value of a_sk_F as they correspond to different chemical potentials, but the general conclusion is clear: polarization (and thus also itinerant ferromagnetism) is not favored in the grand canonical ensemble. This conclusion remains when comparing partially and fully polarized solutions to the saddle-point equations with the unpolarized solution at the same values of the chemical potentials.

In the canonical ensemble, where we keep both the number of spin-up and spin-down particles fixed, the saddle-point free energy per unit volume $F_{sp}^{T=0}(n_{\uparrow}, n_{\downarrow}) = \Omega_{sp}^{T=0}(\mu_{\uparrow}, \mu_{\downarrow}) + \mu_{\uparrow}n_{\uparrow} + \mu_{\downarrow}n_{\downarrow}$ has to be minimized instead of the thermodynamic grand potential $\Omega_{sp}^{T=0}(\mu_{\uparrow}, \mu_{\downarrow})$. $F_{sp}^{T=0}(n_{\uparrow}, n_{\downarrow})$ is given by

$$F_{sp}^{T=0}(P) = \frac{2}{9\pi^3} a_s k_F \left(1 - P^2\right) + \frac{\left(1 + P\right)^{5/3} + \left(1 - P\right)^{5/3}}{10\pi^2}$$
(4.47)

if $n = 1/3\pi^2$. Note that only values of P for which an extremum of $\Omega_{sp}^{T=0}$ exists are allowed. These can be determined through eq. (4.43) for partial and full polarization, and through the condition $a_s k_F > 2^{-7/3} 3\pi$ for full polarization. $F_{sp}^{T=0}(P)$ is shown in fig. 4.3 as a function of $1/a_s k_F$. Eq. (4.47) is equal to the mean-field free energy in eq. (2.5). Furthermore, the solutions to the saddle-point equations correspond to the extrema (or saddle-points) of $F_{sp}^{T=0}(P)$.

We find a strange paradox. Spontaneous polarization and thus itinerant ferromagnetism is energetically favorable for strong repulsive interactions in the canonical ensemble, but in that ensemble the particle number densities are not allowed to change. In the grand-canonical ensemble the particle number densities are allowed to change, but in that ensemble itinerant ferromagnetism is never energetically favorable.

A possible solution to this paradox is the use of a hybrid ensemble, in which the total number of particles is kept fixed, but not the number of particles in individual spin components. In this ensemble, the free energy depends on the total density $n = n_{\uparrow} - n_{\downarrow} = 1/3\pi^2$ and $\zeta = (\mu_{\uparrow} - \mu_{\downarrow})/2 = 0$. The free energy associated with this ensemble can be defined as $\mathcal{F}_{sp}^{T=0}(n,\zeta) = \Omega_{sp}^{T=0}(\mu_{\uparrow},\mu_{\downarrow}) + \mu n =$



Figure 4.2: The saddle-point thermodynamic grand potential $\Omega_{sp}^{T=0}$ in the temperature zero limit as a function of $1/a_sk_F$. The blue dashed line corresponds to unpolarized saddle points, the green line to partially polarized saddle points and the red line to fully polarized saddle points. Polarization is not energetically favored in the grand canonical ensemble.

 $F_{sp}^{T=0}(n_{\uparrow},n_{\downarrow}) - \zeta \delta n$ with $\mu = (\mu_{\uparrow} + \mu_{\downarrow})/2$ the average chemical potential and $\delta n = n_{\uparrow} + n_{\downarrow} = P/3\pi^2$ the density difference. By rewriting $\mathcal{F}_{sp}^{T=0}(n = 1/3\pi^2, \zeta = 0)$ as a function of the polarization, we find

$$\mathcal{F}_{sp}^{T=0}\left(P\right) = \frac{2}{9\pi^3} a_s k_F \left(1 - P^2\right) + \frac{\left(1 + P\right)^{2/3} \left(2 - P\right) + \left(1 - P\right)^{2/3} \left(2 + P\right)}{15\pi^2},\tag{4.48}$$

where again only values of P for which a corresponding extremum of $\Omega_{sp}^{T=0}$ exists are allowed. In the hybrid ensemble with $n = 1/3\pi^2$ and $\zeta = 0$, polarization is only energetically favorable if $\pi/2 < a_s k_F < 3\pi (2 - 2^{-1/3}) / 5$ (see fig. 4.4). If the interaction strength $a_s k_F$ is increased, polarization will become energetically favorable once the Stoner criterion $a_s k_F > \pi/2$ is met, but the unpolarized state becomes energetically favorable again if the interactions become too strong $(a_s k_F > 3\pi (2 - 2^{-1/3}) / 5)$.

In conclusion, the region where itinerant ferromagnetism may occur strongly depends on the ensemble which is used to describe the system. The polarization of the saddle points as a function of a_sk_F remains the same for each ensemble. Unpolarized saddle points exist for all values of a_sk_F . Partially polarized saddle points exist for $\pi/2 < a_sk_F < 2^{-7/3}3\pi$, with the relation between a_sk_F and P given by eq. (4.44), and fully polarized saddle points exist for $a_sk_F \geq 2^{-7/3}3\pi$. However, the energy associated with each saddle point and the energy difference between the polarized and unpolarized saddle points strongly depends on the ensemble used. In the next chapter, it will be verified whether the extrema of the thermodynamic grand potential correspond to a physical (or metastable) state of the system.



Figure 4.3: The saddle-point free energy $F_{sp}^{T=0}$ in the temperature zero limit as a function of $1/a_s k_F$. The blue dashed line corresponds to unpolarized saddle points, the green line to partially polarized saddle points and the red line to fully polarized saddle points. Polarization is energetically favored in the canonical ensemble provided the Stoner criterion $a_s k_F > \pi/2$ is met.



Figure 4.4: The (hybrid) saddle-point free energy $\mathcal{F}_{sp}^{T=0}$ in the temperature zero limit as a function of $1/a_s k_F$. The blue dashed line corresponds to unpolarized saddle points, the green line to partially polarized saddle points and the red line to fully polarized saddle points. In the hybrid ensemble with constant total density $n = 1/3\pi^2$ and constant half chemical potential difference $\zeta = 0$, polarization is energetically favorable provided $\pi/2 < a_s k_F < 3\pi (2 - 2^{-1/3})/5$. This condition is stricter than the Stoner criterion $a_s k_F > \pi/2$.

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Chapter 5

Stability analysis of the saddle points

The results obtained in this chapter were published as:

E. Vermeyen and J. Tempere, Contact Potential Instability in the Path-Integral description of Itinerant Ferromagnetism, Journal of Low Temperature Physics 179, 175-185 (2015).

5.1 Hessian matrix

The solutions to the saddle-point equations (4.27) (hereafter often called saddle points) can be minima, maxima or saddle points of the thermodynamic grand potential $\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}^{R},\rho_{\downarrow}^{R}\right)$ as a function of the density fields ρ_{\uparrow}^{R} and ρ_{\downarrow}^{R} . However, only the minima can correspond to a physical (metastable) state of the system, as only the minima are stable against density (quantum) fluctuations.

The nature of a saddle point can be determined by studying the Hessian matrix H of the second derivatives of $\Omega_{sp}\left(\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\uparrow}^{R}, \rho_{\downarrow}^{R}\right)$,

$$H = \begin{pmatrix} \frac{\partial^2 \Omega_{sp} \left(\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\uparrow}^R, \rho_{\downarrow}^R\right)}{\left(\partial \rho_{\uparrow}^R\right)^2} \bigg|_{\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\downarrow}^R} & \frac{\partial^2 \Omega_{sp} \left(\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\uparrow}^R, \rho_{\downarrow}^R\right)}{\partial \rho_{\uparrow}^R \partial \rho_{\downarrow}^R} \bigg|_{\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\downarrow}^R} \\ \frac{\partial^2 \Omega_{sp} \left(\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\uparrow}^R, \rho_{\downarrow}^R\right)}{\partial \rho_{\downarrow}^R \partial \rho_{\uparrow}^R} \bigg|_{\beta, \mu_{\uparrow}, \mu_{\downarrow}} & \frac{\partial^2 \Omega_{sp} \left(\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\uparrow}^R, \rho_{\downarrow}^R\right)}{\left(\partial \rho_{\downarrow}^R\right)^2} \bigg|_{\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\uparrow}^R} \end{pmatrix}.$$
(5.1)

If both eigenvalues of the Hessian are positive for a given solution to the saddle-point equations, this solution is a minimum and stable against density fluctuations. Both eigenvalues are positive if the trace and determinant of the Hessian are both positive.

In order to calculate the Hessian matrix, the first and second derivatives of the saddle-point freeparticle energy $\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)$ with respect to the effective chemical potentials μ_{\uparrow}' and μ_{\downarrow}' will be calculated. The Hessian will then be expressed as a function of these derivatives, which greatly simplifies the subsequent stability analysis.

The first derivatives of eq. (4.29) with respect to μ_{\uparrow}' and μ_{\downarrow}' are given by

$$\frac{\partial\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)}{\partial\mu_{\sigma}'}\bigg|_{\beta,\mu_{-\sigma}'} = \int \frac{d^{D}k}{(2\pi)^{D}} \left\{ \frac{\exp\left[\beta\left(\mathbf{k}^{2}-\mu_{\sigma}'\right)\right]}{1+\exp\left[\beta\left(\mathbf{k}^{2}-\mu_{\sigma}'\right)\right]}+1 \right\}.$$
(5.2)

Next, the second derivatives of eq. (4.29) with respect to μ_{\uparrow}' and μ_{\downarrow}' are given by

$$\frac{\partial^2 \Omega_{sp,0} \left(\beta, \mu_{\uparrow}', \mu_{\downarrow}'\right)}{\left(\partial \mu_{\sigma}'\right)^2} \bigg|_{\beta, \mu_{-\sigma}'} = -I_{\sigma} \left(\beta, \mu_{\sigma}'\right) \text{ and } \frac{\partial^2 \Omega_{sp,0} \left(\beta, \mu_{\uparrow}', \mu_{\downarrow}'\right)}{\partial \mu_{\uparrow}' \partial \mu_{\downarrow}'} \bigg|_{\beta} = 0,$$
(5.3)

where the function $I_{\sigma}(\beta, \mu'_{\sigma})$ is defined as

$$I_{\sigma}\left(\beta,\mu_{\sigma}'\right) = \frac{\beta}{2} \int \frac{d^{D}k}{(2\pi)^{D}} \left\{ \frac{1}{1 + \cosh\left[\beta\left(\mathbf{k}^{2} - \mu_{\sigma}'\right)\right]} \right\}.$$
(5.4)

As the hyperbolic cosine is a positive function, $I_{\sigma}(\beta, \mu'_{\sigma})$ is a positive function, regardless of the values of β , μ'_{\uparrow} and μ'_{\downarrow} .

Using eq. (4.28) and the definition of the effective chemical potential (4.30), the first and second derivatives of $\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}^{R},\rho_{\downarrow}^{R}\right)$ to ρ_{\uparrow}^{R} and ρ_{\downarrow}^{R} can be rewritten as a function of first and second derivatives of $\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)$ to μ_{\uparrow}' and μ_{\downarrow}' . Starting with the first derivatives,

$$\frac{\partial\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}^{R},\rho_{\downarrow}^{R}\right)}{\partial\rho_{\uparrow}^{R}}\bigg|_{\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\downarrow}^{R}} = -g\rho_{\downarrow}^{R} + \frac{\partial\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)}{\partial\mu_{\downarrow}'}\bigg|_{\beta,\mu_{\uparrow}'}\frac{\partial\mu_{\downarrow}'}{\partial\rho_{\uparrow}^{R}} = -g\rho_{\downarrow}^{R} - g\left.\frac{\partial\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)}{\partial\mu_{\downarrow}'}\right|_{\beta,\mu_{\uparrow}'}, \qquad (5.5)$$

$$\frac{\partial\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}^{R},\rho_{\downarrow}^{R}\right)}{\partial\rho_{\downarrow}^{R}}\bigg|_{\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}^{R}} = -g\rho_{\uparrow}^{R} - g\left.\frac{\partial\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)}{\partial\mu_{\uparrow}'}\right|_{\beta,\mu_{\downarrow}'},\tag{5.6}$$

the Hessian matrix of the second derivatives then becomes

$$H = \begin{pmatrix} -g^2 I_{\downarrow} \left(\beta, \mu_{\downarrow}'\right) & -g \\ -g & -g^2 I_{\uparrow} \left(\beta, \mu_{\uparrow}'\right) \end{pmatrix}.$$
(5.7)

Since $I_{\downarrow}\left(\beta,\mu_{\downarrow}'\right)$ and $I_{\uparrow}\left(\beta,\mu_{\uparrow}'\right)$ are positive, the trace of the Hessian

$$\operatorname{Tr} H = -g^2 \left[I_{\downarrow} \left(\beta, \mu_{\downarrow}' \right) + I_{\uparrow} \left(\beta, \mu_{\uparrow}' \right) \right]$$
(5.8)

is always negative and the Hessian always has at least one negative eigenvalue.

This result implies that none of the solutions to the saddle-point equations are stable against density fluctuations. However, the meaning of this instability is still unclear at this point, especially since it was derived for contact interactions. Is this instability caused by the use of the contact pseudopotential, which is not the real interaction potential? Or does it have other implications, e.g. an instability of the itinerant ferromagnetic state for contact interactions? What is the cause of this instability?

In order to solve these questions, in the next part the saddle-point thermodynamic grand potential for a general interaction potential will be calculated and studied.

Part III

General interaction potentials

Chapter 6

The saddle-point thermodynamic grand potential

The formalism presented in this chapter has been submitted for publication as:

E. Vermeyen, C. A. R. Sá de Melo and J. Tempere, Exchange interactions in the Hubbard-Stratonovich transformation for the stability analysis of itinerant ferromagnetism, ArXiv:1511.05402 [cond-mat.quant-gas] (2015).

6.1 Defining a new action

The thermodynamic grand potential can again be calculated from the partition sum, given in the path-integral formalism by eq. (4.1). The action S plays a central role in the calculation of the partition sum. In the previous part, a free spin-1/2 Fermi gas with contact interactions was studied. The action of this system, given by eq. (4.2), consisted of a free-particle part and an interaction part. When defining a new action for a free spin-1/2 Fermi gas with a general interaction potential, only the interaction part has to be changed: the free-particle part remains the same.

In the previous part about contact interactions, we had the luxury that only the interactions between particles of different spin states remained. This is a good approximation for most experiments with dilute ultracold atomic gases, as the range of the potential is usually smaller than the other relevant length scales in the experiment (as discussed in Sec. 2.1.1). There are two reasons to deviate from the contact potential approximation. First, the Pauli exclusion principle forbids two particles of the same spin state to be in the same quantum state. This effectively prevents two particles to come too close to each other. The exchange interactions introduce another length scale (an exclusion length) which may be smaller than the range of the potential. Consequently, it is not certain whether the contact potential approximation remains valid when the exchange interactions become important.

Second, in recent years other interaction potentials have become available in ultracold atomic gases. The most notable examples are dipolar interactions [66–71] and p-wave Feshbach resonances [29]. Dipolar interactions have a longer range than the typical Van der Waals interactions and furthermore they affect particles of both spin states. P-wave Feshbach resonances enhance scattering into the lowest partial wave for interactions between two particles of the same spin state. Scattering between particles of the same spin state cannot be described by a contact pseudopotential, as this potential is completely screened by the Pauli exclusion principle.

In order to cover these different examples, we will consider three interaction potentials $g_{\sigma_1\sigma_2}(\mathbf{x} - \mathbf{x}')$ with $\sigma_1, \sigma_2 = \uparrow, \downarrow$ for interactions between a particle of spin state σ_1 at position \mathbf{x} and a particle of spin state σ_2 at position \mathbf{x}' , under the assumption $g_{\uparrow\downarrow}(\mathbf{\Delta x}) = g_{\downarrow\uparrow}(\mathbf{\Delta x})$. For symmetry reasons, we will also assume $g_{\sigma_1\sigma_2}(\Delta \mathbf{x}) = g_{\sigma_1\sigma_2}(-\Delta \mathbf{x})$. The resulting action is then given by

$$S\left[\bar{\psi}_{\sigma},\psi_{\sigma}\right] = \sum_{\sigma=\uparrow,\downarrow} \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \bar{\psi}_{\sigma,\mathbf{x},\tau} \left(\frac{\partial}{\partial\tau} - \nabla_{\mathbf{x}}^{2} - \mu_{\sigma}\right) \psi_{\sigma,\mathbf{x},\tau} + \sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow} \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \int_{V} d\mathbf{x}' \frac{g_{\sigma_{1}\sigma_{2}}\left(\mathbf{x}-\mathbf{x}'\right)}{2} \bar{\psi}_{\sigma_{1},\mathbf{x},\tau} \bar{\psi}_{\sigma_{2},\mathbf{x}',\tau} \psi_{\sigma_{1},\mathbf{x},\tau}.$$
(6.1)

The factor 1/2 in the interaction term avoids double-counting.

In order to calculate the thermodynamic grand potential, we will essentially have to go through the same steps as in chapter 4: first the Hubbard-Stratonovich transformation, then a Fourier transformation of the action in order to perform the fermionic path integral, and finally the saddle-point approximation of the bosonic path integral. However, the change of the interaction term will complicate most expressions. Furthermore, after the derivation it will be illustrated that a correction has to be applied in order to recover the exchange interactions.

6.2 The Hubbard-Stratonovich transformation

Analogous to the derivation of the Hubbard-Stratonovich transformation in Sec. 4.2, the transformation is constructed by shifting the real bosonic auxiliary fields ρ_{\uparrow} and ρ_{\downarrow} by the reference fields $\rho_{\uparrow,\mathbf{x},\tau}^0 = \bar{\psi}_{\uparrow,\mathbf{x},\tau} \psi_{\uparrow,\mathbf{x},\tau}$ and $\rho_{\downarrow,\mathbf{x},\tau}^0 = \bar{\psi}_{\downarrow,\mathbf{x},\tau} \psi_{\downarrow,\mathbf{x},\tau}$ in the path integral

$$\begin{aligned} \mathcal{Z}_{\rho} &= \int \mathcal{D}\rho_{\uparrow} \int \mathcal{D}\rho_{\downarrow} \exp\left[\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow} \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \int_{V} d\mathbf{x}' \frac{g_{\sigma_{1}\sigma_{2}} \left(\mathbf{x}-\mathbf{x}'\right)}{2} \rho_{\sigma_{1},\mathbf{x},\tau} \rho_{\sigma_{2},\mathbf{x}',\tau}\right] \\ &= \int \mathcal{D}\rho_{\uparrow} \int \mathcal{D}\rho_{\downarrow} \exp\left[\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow} \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \int_{V} d\mathbf{x}' \frac{g_{\sigma_{1}\sigma_{2}} \left(\mathbf{x}-\mathbf{x}'\right)}{2} \right. \\ & \left. \times \left(\rho_{\sigma_{1},\mathbf{x},\tau} - \rho_{\sigma_{1},\mathbf{x},\tau}^{0}\right) \left(\rho_{\sigma_{2},\mathbf{x}',\tau} - \rho_{\sigma_{2},\mathbf{x}',\tau}^{0}\right) \right]. \end{aligned}$$

$$(6.2)$$

The resulting transformation is given by

$$\exp\left[-\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow}\int_{0}^{\beta}d\tau\int_{V}d\mathbf{x}\int_{V}d\mathbf{x}'\frac{g_{\sigma_{1}\sigma_{2}}\left(\mathbf{x}-\mathbf{x}'\right)}{2}\bar{\psi}_{\sigma_{1},\mathbf{x},\tau}\bar{\psi}_{\sigma_{2},\mathbf{x}',\tau}\psi_{\sigma_{2},\mathbf{x}',\tau}\psi_{\sigma_{1},\mathbf{x},\tau}\right] \\
=\exp\left[-\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow}\int_{0}^{\beta}d\tau\int_{V}d\mathbf{x}\int_{V}d\mathbf{x}'\frac{g_{\sigma_{1}\sigma_{2}}\left(\mathbf{x}-\mathbf{x}'\right)}{2}\bar{\psi}_{\sigma_{1},\mathbf{x},\tau}\psi_{\sigma_{1},\mathbf{x},\tau}\bar{\psi}_{\sigma_{2},\mathbf{x}',\tau}\psi_{\sigma_{2},\mathbf{x}',\tau}\right] \\
=\frac{1}{\mathcal{Z}_{\rho}}\int\mathcal{D}\rho\uparrow\int\mathcal{D}\rho\downarrow\exp\left[\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow}\int_{0}^{\beta}d\tau\int_{V}d\mathbf{x}\int_{V}d\mathbf{x}'\frac{g_{\sigma_{1}\sigma_{2}}\left(\mathbf{x}-\mathbf{x}'\right)}{2} \\
\times\left(\rho_{\sigma_{1},\mathbf{x},\tau}\rho_{\sigma_{2},\mathbf{x}',\tau}-\rho_{\sigma_{1},\mathbf{x},\tau}\bar{\psi}_{\sigma_{2},\mathbf{x}',\tau}\psi_{\sigma_{2},\mathbf{x}',\tau}-\bar{\psi}_{\sigma_{1},\mathbf{x},\tau}\psi_{\sigma_{1},\mathbf{x},\tau}\rho_{\sigma_{2},\mathbf{x}',\tau}\right].$$
(6.3)

After the Hubbard-Stratonovich transformation, the partition sum is given by eq. (4.13), with a

new effective action given by

$$S_{eff} \left[\bar{\psi}_{\sigma}, \psi_{\sigma}, \bar{\rho}_{\sigma}, \rho_{\sigma} \right] = \sum_{\sigma=\uparrow,\downarrow} \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \left[\bar{\psi}_{\sigma,\mathbf{x},\tau} \left(\frac{\partial}{\partial \tau} - \nabla_{\mathbf{x}}^{2} - \mu_{\sigma} \right) \psi_{\sigma,\mathbf{x},\tau} \right.$$
(6.4)
$$- \sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow} \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \int_{V} d\mathbf{x}' g_{\sigma_{1}\sigma_{2}} \left(\mathbf{x} - \mathbf{x}' \right) \left(\frac{\rho_{\sigma_{1},\mathbf{x},\tau}\rho_{\sigma_{2},\mathbf{x}',\tau}}{2} - \bar{\psi}_{\sigma_{1},\mathbf{x},\tau}\psi_{\sigma_{1},\mathbf{x},\tau}\rho_{\sigma_{2},\mathbf{x}',\tau} \right) \right].$$

The proportionality factor \mathcal{Z}_{ρ} can be set to one by an appropriate choice of the new zero point of the thermodynamic grand potential, so it no longer has to be written explicitly.

6.3 Fourier transformation

Next, the effective action (6.4) is Fourier transformed. The Fourier transformed fermionic and bosonic fields were defined in eqs. (4.15) and (4.16) of Sec. 4.3. However, as the bosonic fields are now real, $\rho_{\sigma,\mathbf{q},m}^* = \rho_{\sigma,-\mathbf{q},-m}$. Furthermore, the interaction potential has to be Fourier transformed explicitly,

$$g_{\sigma_1 \sigma_2} \left(\mathbf{\Delta} \mathbf{x} \right) = \frac{1}{\sqrt{V}} \sum_{\mathbf{Q}} \exp\left(i \mathbf{Q} \cdot \mathbf{\Delta} \mathbf{x} \right) g_{\sigma_1 \sigma_2} \left(\mathbf{Q} \right).$$
(6.5)

The Fourier transformed free-particle part of the action has already been calculated in eq. (4.19), so only the interaction part needs to be Fourier transformed. The resulting effective action is given in the four-vector notation by

$$S_{eff} \left[\bar{\psi}_{\sigma}, \psi_{\sigma}, \bar{\rho}_{\sigma}, \rho_{\sigma} \right] = \sum_{\sigma_{1}=\uparrow,\downarrow} \left\{ \sum_{k,k'} \bar{\psi}_{\sigma_{1},k} \left[-G_{\sigma_{1}}^{-1} \left(k, k' \right) \right] \psi_{\sigma_{1},k'} - \frac{\sqrt{V}}{2} \sum_{\sigma_{2}=\uparrow,\downarrow} \sum_{q} g_{\sigma_{1}\sigma_{2}} \left(\mathbf{q} \right) \rho_{\sigma_{1},-q} \rho_{\sigma_{2},q} \right\},$$
(6.6)

with the inverse Green's function defined as

$$-G_{\sigma_1}^{-1}(k,k') = \left(-i\omega_n + \mathbf{k}^2 - \mu_{\sigma_1}\right)\delta\left(\Delta k\right) + \frac{1}{\sqrt{\beta}}\sum_{\sigma_2=\uparrow,\downarrow} g_{\sigma_1\sigma_2}\left(\mathbf{\Delta k}\right)\rho_{\sigma_2,\Delta k}.$$
(6.7)

After performing the fermionic path integral, the partition sum becomes

$$\mathcal{Z} = \left(\prod_{\sigma=\uparrow,\downarrow} \int \mathcal{D}\bar{\rho}_{\sigma} \int \mathcal{D}\rho_{\sigma}\right) \exp\left[\sum_{\sigma_{1}=\uparrow,\downarrow} \left(\frac{\sqrt{V}}{2} \sum_{\sigma_{2}=\uparrow,\downarrow} \sum_{q} g_{\sigma_{1}\sigma_{2}}\left(\mathbf{q}\right) \rho_{\sigma_{1},-q}\rho_{\sigma_{2},q} + \operatorname{Tr}\left\{\ln\left[-G_{\sigma_{1}}^{-1}\left(k,k'\right)\right]\right\}\right)\right].$$
(6.8)

The remaining bosonic path integral cannot be performed exactly and has to be approximated.

6.4 Saddle-point approximation

In the saddle-point approximation, the main contribution to the path integral over bosonic fields is assumed to come from a configuration where the field is constant: $\rho_{\sigma,q} = \sqrt{\beta V} \delta(q) \rho_{\sigma}$ with ρ_{σ} a real number. Due to homogeneity it is justified to assume that the saddle-point field is constant. Using the definition from eq. (3.24), the saddle-point thermodynamic grand potential is then given by

$$\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow},\rho_{\downarrow}\right) = -\frac{1}{2}\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow}g_{\sigma_{1}\sigma_{2}}\rho_{\sigma_{1}}\rho_{\sigma_{2}} + \Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right).$$
(6.9)

with $\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)$ the free-particle energy as defined in eq. (4.29), the new interaction parameters

$$g_{\sigma_1 \sigma_2} = \sqrt{V} g_{\sigma_1 \sigma_2} \left(\mathbf{q} = \mathbf{0} \right) = \int_V d\left(\mathbf{\Delta} \mathbf{x} \right) g_{\sigma_1 \sigma_2} \left(\mathbf{\Delta} \mathbf{x} \right)$$
(6.10)

equal to the interaction potential integrated over the whole volume and

$$\mu'_{\sigma_1} = \mu_{\sigma_1} - \sum_{\sigma_2 = \uparrow, \downarrow} g_{\sigma_1 \sigma_2} \rho_{\sigma_2} \tag{6.11}$$

the effective chemical potential of spin state σ_1 .

We find similar results as for the contact potential (Sec. 4.4):

- 1. an extra term in $\Omega_{sp}(\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\uparrow}, \rho_{\downarrow})$, namely the interaction energy $-\frac{1}{2}\sum_{\sigma_1, \sigma_2} g_{\sigma_1\sigma_2}\rho_{\sigma_1}\rho_{\sigma_2}$, and
- 2. a shift $-\sum_{\sigma_2} g_{\sigma_1 \sigma_2} \rho_{\sigma_2}$ of the effective chemical potential μ'_{σ_1} .

Remarkably, in the saddle-point approximation only three parameters are necessary to describe the effect of a general interaction potential: $g_{\uparrow\uparrow}$, $g_{\downarrow\downarrow}$ and $g_{\uparrow\downarrow} = g_{\downarrow\uparrow}$. In the first Born approximation in 3D, $g_{\uparrow\downarrow} = 8\pi a_s k_F$.

The values of ρ_{\uparrow} and ρ_{\downarrow} still need to be determined by solving the saddle-point equations

$$\frac{\partial\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow},\rho_{\downarrow}\right)}{\partial\rho_{\sigma}}\Big|_{\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{-\sigma}} = 0.$$
(6.12)

Because of the choice of $k_F = 1$ as a unit, they need to be solved together with the number equation for $n = n_{\uparrow} + n_{\downarrow}$, with

$$n_{\sigma} = -\left. \frac{\partial \Omega_{sp} \left(\beta, \mu_{\uparrow}, \mu_{\downarrow}\right)}{\partial \mu_{\sigma}} \right|_{\beta, \mu_{-\sigma}}.$$
(6.13)

Through a similar derivation as in Sec. 4.4.1 for contact interactions, it can be shown that the saddlepoint equations are equivalent to $\rho_{\sigma} = n_{\sigma}$.

6.5 Exchange interactions

As a verification of the results, it is important to check whether we can recover the results for contact interactions from Sec. 4.4. In order to do so, the interaction potential is chosen as

$$g_{\sigma_1 \sigma_2} \left(\mathbf{\Delta} \mathbf{x} \right) = g \delta \left(\mathbf{\Delta} \mathbf{x} \right) \tag{6.14}$$

with $g \in \mathbb{R}$ and $\Delta \mathbf{x}$ the Dirac delta function. In this particular case, the interaction parameters $g_{\sigma_1 \sigma_2}$ are given by

$$g_{\sigma_1 \sigma_2} = \int_V d\left(\mathbf{\Delta x}\right) g_{\sigma_1 \sigma_2}\left(\mathbf{\Delta x}\right) = g \int_V d\left(\mathbf{\Delta x}\right) \delta\left(\mathbf{\Delta x}\right) = g$$
(6.15)

and eq. (6.9) becomes

$$\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow},\rho_{\downarrow}\right) = -\frac{1}{2}\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow}g\rho_{\sigma_{1}}\rho_{\sigma_{2}} + \Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)$$
(6.16)

with the effective chemical potential given by

$$\mu'_{\sigma_1} = \mu_{\sigma_1} - \sum_{\sigma_2 = \uparrow, \downarrow} g \rho_{\sigma_2}.$$
(6.17)

There is a problem with this result. Due to the Pauli exclusion principle, which forbids two particles to occupy the same quantum state, contact interactions between two particles of the same spin state are forbidden. However in eqs. (6.16) and (6.17), the contact interactions between particles of the same spin state do contribute to the thermodynamic grand potential. In many theoretical derivations, the

interactions between particles of the same spin state are split into two contributions: the direct and the exchange part. The direct interactions are the interactions that the particles would experience without taking into account the Pauli exclusion principle. The exchange part is defined as the correction that is needed in order to obtain the true interaction energy after taking into account the Pauli exclusion principle. For contact interactions, the direct and exchange contributions are equal and cancel each other completely. In the saddle-point thermodynamic grand potential that was derived in this chapter, only the direct interactions are taken into account and the exchange part has disappeared. Next, it is interesting to investigate where and why the exchange interactions disappeared.

6.5.1 Analysis of the Hubbard-Stratonovich transformation

The key to understanding how the exchange interactions disappeared lies in the Hubbard-Stratonovich transformation, given by eq. (6.3) and repeated here:

$$\exp\left[-\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow}\int_{0}^{\beta}d\tau\int_{V}d\mathbf{x}\int_{V}d\mathbf{x}'\frac{g_{\sigma_{1}\sigma_{2}}\left(\mathbf{x}-\mathbf{x}'\right)}{2}\bar{\psi}_{\sigma_{1},\mathbf{x},\tau}\bar{\psi}_{\sigma_{2},\mathbf{x}',\tau}\psi_{\sigma_{2},\mathbf{x}',\tau}\psi_{\sigma_{1},\mathbf{x},\tau}\right] \\
=\frac{1}{\mathcal{Z}_{\rho}}\int\mathcal{D}\rho_{\uparrow}\int\mathcal{D}\rho_{\downarrow}\exp\left[\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow}\int_{0}^{\beta}d\tau\int_{V}d\mathbf{x}\int_{V}d\mathbf{x}'\frac{g_{\sigma_{1}\sigma_{2}}\left(\mathbf{x}-\mathbf{x}'\right)}{2} \\
\times\left(\rho_{\sigma_{1},\mathbf{x},\tau}\rho_{\sigma_{2},\mathbf{x}',\tau}-\rho_{\sigma_{1},\mathbf{x},\tau}\bar{\psi}_{\sigma_{2},\mathbf{x}',\tau}\psi_{\sigma_{2},\mathbf{x}',\tau}-\bar{\psi}_{\sigma_{1},\mathbf{x},\tau}\psi_{\sigma_{1},\mathbf{x},\tau}\rho_{\sigma_{2},\mathbf{x}',\tau}\right)\right].$$
(6.18)

In the first line of eq. (6.18), the Pauli exclusion principle is automatically included due to the antisymmetry of the Grassmann fields and as a result interactions with $\sigma_1 = \sigma_2$ and $\mathbf{x} = \mathbf{x}'$ do not contribute to the path integral over the fermionic fields. However, in the last two lines of eq. (6.18) there is no similar mechanism to ensure the Pauli principle is observed, therefore interactions with $\sigma_1 = \sigma_2$ and $\mathbf{x} = \mathbf{x}'$ do contribute to the path integral over the fermionic fields. Is this Hubbard-Stratnovich transformation still exact? The answer is yes: the "forbidden terms" with $\sigma_1 = \sigma_2$ and $\mathbf{x} = \mathbf{x}'$ cancel each other when the full path integral over the bosonic field is performed.

The recovery of the exchange interactions in the bosonic path integral can be understood as a transfer of symmetry properties. The antisymmetry properties of a pair of fermionic particles disappear when this pair is treated as a true boson. However, the information contained in those symmetry properties cannot simply disappear: it is transformed into symmetry properties of the integrand of the bosonic path integral. These symmetry properties will ensure observance of the Pauli exclusion principle, as will be demonstrated using two simplified examples.

First simplified example

Here, a proof of principle will be provided using complex (or real) numbers and Grassmann numbers instead of bosonic and fermionic fields. The symmetry properties which lead to observance of the Pauli exclusion principle in the right hand side of eq. (6.18) are best demonstrated using the integral

$$C_{1} = \int_{\mathbb{C}} dz \exp\left(-z\bar{z} + \psi_{1}\psi_{2}z + \bar{z}\psi_{3}\psi_{4}\right), \qquad (6.19)$$

with z a complex number and ψ_1 , ψ_2 , ψ_3 and ψ_4 Grassmann numbers. As each function of Grassmann numbers can be Taylor expanded into a linear function,

$$C_{1} = \int_{\mathbb{C}} dz \exp\left(-z\bar{z}\right) \left(1 + \psi_{1}\psi_{2}z + \bar{z}\psi_{3}\psi_{4} + z\bar{z}\psi_{1}\psi_{2}\psi_{3}\psi_{4}\right).$$
(6.20)

Next, the complex integral can be transformed into two real integrals using z = x + iy and $\overline{z} = x - iy$ with $x, y \in \mathbb{R}$,

$$C_{1} = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \exp\left(-x^{2} - y^{2}\right) \left[1 + \psi_{1}\psi_{2}\left(x + iy\right) + \left(x - iy\right)\psi_{3}\psi_{4} + \left(x^{2} + y^{2}\right)\psi_{1}\psi_{2}\psi_{3}\psi_{4}\right]$$

$$= \left[\int_{-\infty}^{+\infty} \exp\left(-x^{2}\right) dx\right] \left[\int_{-\infty}^{+\infty} \exp\left(-y^{2}\right) dy\right]$$

$$+ \left(\psi_{1}\psi_{2} + \psi_{3}\psi_{4}\right) \left[\int_{-\infty}^{+\infty} \exp\left(-x^{2}\right) dx\right] \left[\int_{-\infty}^{+\infty} \exp\left(-y^{2}\right) dy\right]$$

$$+ i\left(\psi_{1}\psi_{2} - \psi_{3}\psi_{4}\right) \left[\int_{-\infty}^{+\infty} \exp\left(-x^{2}\right) dx\right] \left[\int_{-\infty}^{+\infty} \exp\left(-y^{2}\right) dy\right]$$

$$+ \psi_{1}\psi_{2}\psi_{3}\psi_{4}\left\{\left[\int_{-\infty}^{+\infty} x^{2} \exp\left(-x^{2}\right) dx\right] \left[\int_{-\infty}^{+\infty} \exp\left(-y^{2}\right) dy\right]$$

$$+ \left[\int_{-\infty}^{+\infty} \exp\left(-x^{2}\right) dx\right] \left[\int_{-\infty}^{+\infty} y^{2} \exp\left(-y^{2}\right) dy\right]\right\}.$$
(6.21)

Using

$$\int_{-\infty}^{+\infty} \exp\left(-x^2\right) dx = \sqrt{\pi},\tag{6.22}$$

$$\int_{-\infty}^{+\infty} x \exp\left(-x^2\right) dx = 0, \text{ and}$$
(6.23)

$$\int_{-\infty}^{+\infty} x^2 \exp\left(-x^2\right) dx = \frac{\sqrt{\pi}}{2},$$
(6.24)

the following result is obtained:

$$C_1 = \pi \left(1 + \psi_1 \psi_2 \psi_3 \psi_4 \right) = \pi \exp \left(\psi_1 \psi_2 \psi_3 \psi_4 \right).$$
(6.25)

The terms where the Pauli exclusion principle could have been violated if two of the Grassmann numbers ψ_1 , ψ_2 , ψ_3 and ψ_4 are equal vanished due to the antisymmetry of the integrands $x \exp(-x^2)$ and $y \exp(-y^2)$ in eq. (6.21). This implies that the standard Hubbard-Stratonovich transformation is exact,

$$\exp\left(\psi_1\psi_2\psi_3\psi_4\right) = \frac{1}{\pi} \int_{\mathbb{C}} dz \exp\left(-z\bar{z} + \psi_1\psi_2z + \bar{z}\psi_3\psi_4\right).$$
(6.26)

Second simplified example

A simplified example which is closer to the Hubbard-Stratonovich transformation (6.18) with the real fields ρ_{\uparrow} and ρ_{\downarrow} is given by

$$C_{2} = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \exp\left(-xy + \psi_{1}\psi_{2}x + y\psi_{3}\psi_{4}\right)$$

$$= \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \exp\left(-xy\right) \left(1 + \psi_{1}\psi_{2}x + y\psi_{3}\psi_{4} + xy\psi_{1}\psi_{2}\psi_{3}\psi_{4}\right).$$
(6.27)

Similar symmetry arguments will cause the terms with integrand $x \exp(-xy)$ and $y \exp(-xy)$ to vanish, but it is harder to see as it is impossible to decouple the integrals in this notation. They can be decoupled by transforming the coordinates to $\rho = (x + y)/2$ and $\phi = (x - y)/2$,

$$C_{2} = -2 \int_{-\infty}^{+\infty} d\rho \int_{-\infty}^{+\infty} d\phi \exp(-\rho^{2} + \phi^{2}) \left[1 + \psi_{1}\psi_{2}(\rho + \phi) + (\rho - \phi)\psi_{3}\psi_{4} + (\rho^{2} - \phi^{2})\psi_{1}\psi_{2}\psi_{3}\psi_{4}\right]$$

$$= -2 \left[\int_{-\infty}^{+\infty} \exp(-\rho^{2}) d\rho\right] \left[\int_{-\infty}^{+\infty} \exp(\phi^{2}) d\phi\right]$$

$$-2 (\psi_{1}\psi_{2} + \psi_{3}\psi_{4}) \left[\int_{-\infty}^{+\infty} \rho \exp(-\rho^{2}) d\rho\right] \left[\int_{-\infty}^{+\infty} \exp(\phi^{2}) d\phi\right]$$

$$-2 (\psi_{1}\psi_{2} - \psi_{3}\psi_{4}) \left[\int_{-\infty}^{+\infty} \exp(-\rho^{2}) d\rho\right] \left[\int_{-\infty}^{+\infty} \phi \exp(\phi^{2}) d\phi\right]$$

$$-2 \psi_{1}\psi_{2}\psi_{3}\psi_{4} \left\{\left[\int_{-\infty}^{+\infty} \rho^{2} \exp(-\rho^{2}) d\rho\right] \left[\int_{-\infty}^{+\infty} \exp(\phi^{2}) d\phi\right]$$

$$-\left[\int_{-\infty}^{+\infty} \exp(-\rho^{2}) d\rho\right] \left[\int_{-\infty}^{+\infty} \phi^{2} \exp(\phi^{2}) d\phi\right]\right\}.$$
(6.28)

Note that

$$\int_{-\infty}^{+\infty} \exp\left(\phi^2\right) d\phi = +\infty.$$
(6.29)

Because of the antisymmetry of the integrand

$$\int_{-\infty}^{+\infty} \phi \exp\left(\phi^2\right) d\phi = 0, \tag{6.30}$$

and with partial integration it can be shown that

$$\int_{-\infty}^{+\infty} \phi^2 \exp\left(\phi^2\right) d\phi = -\frac{1}{2} \int_{-\infty}^{+\infty} \exp\left(\phi^2\right) d\phi.$$
(6.31)

Finally, it is found that

$$C_{2} = -2\sqrt{\pi} \left[\int_{-\infty}^{+\infty} \exp\left(\phi^{2}\right) d\phi \right] \left(1 + \psi_{1}\psi_{2}\psi_{3}\psi_{4}\right)$$
$$= -2\sqrt{\pi} \left[\int_{-\infty}^{+\infty} \exp\left(\phi^{2}\right) d\phi \right] \exp\left(\psi_{1}\psi_{2}\psi_{3}\psi_{4}\right).$$
(6.32)

This confirms that

$$\exp(\psi_{1}\psi_{2}\psi_{3}\psi_{4}) = \frac{\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \exp(-xy + \psi_{1}\psi_{2}x + y\psi_{3}\psi_{4})}{\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \exp(-xy)}.$$
(6.33)

In conclusion, the Hubbard-Stratonovich transformation (6.18) is exact.

6.5.2 Modified interaction potential

The Pauli exclusion principle is taken into account exactly if the full path integral over the bosonic field is taken, but this is no longer the case when the bosonic path integral is approximated. In many approximations, only a select number of terms in the bosonic path integral are taken into account. This may inadvertently lead to a violation of the Pauli exclusion principle, especially in the saddle-point approximation.

This violation can easily be demonstrated in the simplified examples from Sec. 6.5.1. If a nonzero value is obtained for the integral (6.23) due to approximations, the interaction terms that are forbidden by the Pauli exclusion principle no longer disappear in eqs. (6.21) and (6.28).

As the exchange interactions are crucial to a correct description of itinerant ferromagnetism, it is important to ensure that the Pauli exclusion principle is observed regardless of the approximation to the bosonic path integral. In order to do this, I propose a new method, where the Pauli exclusion principle is explicitly enforced through a modification of the interaction potential:

$$\tilde{g}_{\sigma_1 \sigma_2} \left(\mathbf{\Delta} \mathbf{x} \right) = g_{\sigma_1 \sigma_2} \left(\mathbf{\Delta} \mathbf{x} \right) \left[1 - \delta_{\sigma_1, \sigma_2} \delta_1 \left(\mathbf{\Delta} \mathbf{x} \right) \right], \tag{6.34}$$

with $\tilde{g}_{\sigma_1\sigma_2}(\Delta \mathbf{x})$ the new modified interaction potential, $g_{\sigma_1\sigma_2}(\Delta \mathbf{x})$ the true interaction potential, $\delta_{\sigma_1,\sigma_2}$ the Kronecker delta and

$$\delta_1 \left(\mathbf{\Delta x} \right) = \begin{cases} 1 & \mathbf{\Delta x} = \mathbf{0} \\ 0 & \mathbf{\Delta x} \neq \mathbf{0} \end{cases}$$
(6.35)

This form ensures that terms with $\sigma_1 = \sigma_2$ and $\mathbf{x} = \mathbf{x}'$ do not contribute to the bosonic path integral in eq. (6.3).

An important side note is the fact that the delta function that excludes terms with $\mathbf{x} = \mathbf{x}'$ only has height one. It is not a Dirac delta function with infinite height. This choice only makes sense in a countable basis of the Hilbert space, whereas the position basis is an uncountable set. However, physical bases are always countable and the position basis is an unphysical limit which is often used to ease calculations. In order to compensate for the fact that the position basis is an unphysical limit, it is also possible to define the modified interaction potential as

$$\tilde{g}_{\sigma_1 \sigma_2} \left(\mathbf{\Delta} \mathbf{x} \right) = g_{\sigma_1 \sigma_2} \left(\mathbf{\Delta} \mathbf{x} \right) \left[1 - \delta_{\sigma_1, \sigma_2} f_{\sigma_1} \left(\mathbf{\Delta} \mathbf{x} \right) \right], \tag{6.36}$$

where the screening function $f_{\sigma_1}(\Delta \mathbf{x})$ is the fraction of the interaction potential that is screened by the Pauli exclusion principle at a distance $\Delta \mathbf{x}$ between two particles of spin state σ_1 . This definition of the modified interaction potential will be used in the remainder of this dissertation, as it is a more general form of eq. (6.34).

The modified interaction potential can be introduced in the Hubbard-Stratonovich transformation by replacing $g_{\sigma_1\sigma_2}(\Delta \mathbf{x})$ with $\tilde{g}_{\sigma_1\sigma_2}(\Delta \mathbf{x})$ in the right-hand side of eq. (6.18),

$$\exp\left[-\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow}\int_{0}^{\beta}d\tau\int_{V}d\mathbf{x}\int_{V}d\mathbf{x}'\frac{g_{\sigma_{1}\sigma_{2}}\left(\mathbf{x}-\mathbf{x}'\right)}{2}\bar{\psi}_{\sigma_{1},\mathbf{x},\tau}\bar{\psi}_{\sigma_{2},\mathbf{x}',\tau}\psi_{\sigma_{2},\mathbf{x}',\tau}\psi_{\sigma_{1},\mathbf{x},\tau}\right] \\
=\frac{1}{Z_{\rho}}\mathcal{D}\rho_{\uparrow}\int\mathcal{D}\rho_{\downarrow}\exp\left[\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow}\int_{0}^{\beta}d\tau\int_{V}d\mathbf{x}\int_{V}d\mathbf{x}'\frac{\tilde{g}_{\sigma_{1}\sigma_{2}}\left(\mathbf{x}-\mathbf{x}'\right)}{2}\left(\rho_{\sigma_{1},\mathbf{x},\tau}\rho_{\sigma_{2},\mathbf{x}',\tau}\right)\right] \\
-\rho_{\sigma_{1},\mathbf{x},\tau}\bar{\psi}_{\sigma_{2},\mathbf{x}',\tau}\psi_{\sigma_{2},\mathbf{x}',\tau}-\bar{\psi}_{\sigma_{1},\mathbf{x},\tau}\psi_{\sigma_{1},\mathbf{x},\tau}\rho_{\sigma_{2},\mathbf{x}',\tau}\right)\right].$$
(6.37)

Even though $\tilde{g}_{\uparrow\downarrow}(\Delta \mathbf{x}) = \tilde{g}_{\downarrow\uparrow}(\Delta \mathbf{x}) = g_{\uparrow\downarrow}(\Delta \mathbf{x}) = g_{\downarrow\uparrow}(\Delta \mathbf{x})$, the notation $\tilde{g}_{\sigma_1\sigma_2}$ is used for notational ease.

6.5.3 Result

After the modified Hubbard-Stratonovich transformation, the saddle-point thermodynamic grand potential can then be derived by replacing $g_{\sigma_1\sigma_2}(\Delta \mathbf{x})$ with $\tilde{g}_{\sigma_1\sigma_2}(\Delta \mathbf{x})$ in the remainder of the calculation (Sec. 6.2, 6.3 and 6.4). The result is given by

$$\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow},\rho_{\downarrow}\right) = -\frac{1}{2}\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow}\tilde{g}_{\sigma_{1}\sigma_{2}}\rho_{\sigma_{1}}\rho_{\sigma_{2}} + \Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right),\tag{6.38}$$

$$\mu'_{\sigma_1} = \mu_{\sigma_1} - \sum_{\sigma_2 = \uparrow, \downarrow} \tilde{g}_{\sigma_1 \sigma_2} \rho_{\sigma_2}, \qquad (6.39)$$

where the new modified interaction parameters are given by

$$\tilde{g}_{\sigma_1 \sigma_2} = \sqrt{V} \tilde{g}_{\sigma_1 \sigma_2} \left(\mathbf{q} = \mathbf{0} \right) = \int_V d\left(\mathbf{\Delta} \mathbf{x} \right) \tilde{g}_{\sigma_1 \sigma_2} \left(\mathbf{\Delta} \mathbf{x} \right).$$
(6.40)

Using the exact definition (6.34) for the modified interaction potential, the modified interaction parameters for the contact interaction potential (6.14) are given by

$$\tilde{g}_{\sigma_1 \sigma_2} = g \int_V d\left(\mathbf{\Delta x}\right) \delta\left(\mathbf{\Delta x}\right) \left[1 - \delta_{\sigma_1, \sigma_2} \delta_1\left(\mathbf{\Delta x}\right)\right] = g \left[1 - \delta_{\sigma_1, \sigma_2}\right].$$
(6.41)

This implies that $\tilde{g}_{\uparrow\uparrow} = \tilde{g}_{\downarrow\downarrow} = 0$, so contact interactions between particles of equal spin states no longer contribute to the saddle-point thermodynamic grand potential. In the saddle-point approximation, the correction term introduced in the modified interaction potential corresponds to the exchange interactions. Using the modified interaction potential, the results from chapter 4 for contact interactions are fully recovered.

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Chapter 7

Stability analysis of the saddle points

The results obtained in this chapter have been submitted for publication as:

E. Vermeyen, C. A. R. Sá de Melo and J. Tempere, Exchange interactions in the Hubbard-Stratonovich transformation for the stability analysis of itinerant ferromagnetism, ArXiv:1511.05402 [cond-mat.quant-gas] (2015).

7.1 Hessian matrix

In chapter 5, it was shown for contact interactions that all saddle points of the saddle-point thermodynamic grand potential are unstable to density fluctuations. In order to understand the contactpotential instability, in this chapter a similar stability analysis of the saddle points will be performed for a general interaction potential.

The stability is studied by studying the Hessian matrix of the second derivatives of the saddle-point thermodynamic grand potential in the saddle points,

$$H = \begin{pmatrix} \frac{\partial^2 \Omega_{sp} \left(\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\uparrow}, \rho_{\downarrow}\right)}{\left(\partial \rho_{\uparrow}\right)^2} \bigg|_{\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\downarrow}} & \frac{\partial^2 \Omega_{sp} \left(\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\uparrow}, \rho_{\downarrow}\right)}{\partial \rho_{\uparrow} \partial \rho_{\downarrow}} \bigg|_{\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\downarrow}} \\ \frac{\partial^2 \Omega_{sp} \left(\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\uparrow}, \rho_{\downarrow}\right)}{\partial \rho_{\downarrow} \partial \rho_{\uparrow}} \bigg|_{\beta, \mu_{\uparrow}, \mu_{\downarrow}} & \frac{\partial^2 \Omega_{sp} \left(\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\uparrow}, \rho_{\downarrow}\right)}{\left(\partial \rho_{\downarrow}\right)^2} \bigg|_{\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\uparrow}} \end{pmatrix}.$$
(7.1)

The first derivatives of eq. (6.38) to ρ_{\uparrow} and ρ_{\downarrow} are given by

$$\frac{\partial\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow},\rho_{\downarrow}\right)}{\partial\rho_{\uparrow}}\Big|_{\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\downarrow}} = -\tilde{g}_{\uparrow\downarrow}\rho_{\downarrow} - \tilde{g}_{\uparrow\uparrow}\rho_{\uparrow} + \frac{\partial\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)}{\partial\mu_{\uparrow}'}\Big|_{\beta,\mu_{\downarrow}'}\frac{\partial\mu_{\uparrow}'}{\partial\rho_{\uparrow}} + \frac{\partial\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)}{\partial\mu_{\downarrow}'}\Big|_{\beta,\mu_{\downarrow}'}\frac{\partial\mu_{\downarrow}'}{\partial\rho_{\uparrow}} = -\tilde{g}_{\uparrow\downarrow}\rho_{\downarrow} - \tilde{g}_{\uparrow\uparrow}\rho_{\uparrow} - \tilde{g}_{\uparrow\uparrow}\frac{\partial\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)}{\partial\mu_{\uparrow}'}\Big|_{\beta,\mu_{\downarrow}'} - \tilde{g}_{\uparrow\downarrow}\frac{\partial\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)}{\partial\mu_{\downarrow}'}\Big|_{\beta,\mu_{\downarrow}'}, \quad (7.2)$$

$$\frac{\partial\Omega_{sp}\left(\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow},\rho_{\downarrow}\right)}{\partial\rho_{\downarrow}}\Big|_{\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}} = -\tilde{g}_{\uparrow\downarrow}\rho_{\uparrow} - \tilde{g}_{\downarrow\downarrow}\rho_{\downarrow} - \tilde{g}_{\uparrow\downarrow} \left.\frac{\partial\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)}{\partial\mu_{\uparrow}'}\right|_{\beta,\mu_{\downarrow}'} - \tilde{g}_{\downarrow\downarrow} \left.\frac{\partial\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)}{\partial\mu_{\downarrow}'}\right|_{\beta,\mu_{\downarrow}'}.$$
(7.3)

Using eq. (5.3) for the second derivatives of $\Omega_{sp,0}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)$ to μ_{\uparrow}' and μ_{\downarrow}' , it can be shown that the Hessian matrix is equal to

$$H = \begin{pmatrix} -\tilde{g}_{\uparrow\uparrow} - \tilde{g}_{\uparrow\uparrow}^2 I_{\uparrow} \left(\beta, \mu_{\uparrow}'\right) - \tilde{g}_{\uparrow\downarrow}^2 I_{\downarrow} \left(\beta, \mu_{\downarrow}'\right) & -\tilde{g}_{\uparrow\downarrow} - \tilde{g}_{\uparrow\downarrow} \left[\tilde{g}_{\uparrow\uparrow} I_{\uparrow} \left(\beta, \mu_{\uparrow}'\right) + \tilde{g}_{\downarrow\downarrow} I_{\downarrow} \left(\beta, \mu_{\downarrow}'\right) \right] \\ -\tilde{g}_{\uparrow\downarrow} - \tilde{g}_{\uparrow\downarrow} \left[\tilde{g}_{\uparrow\uparrow} I_{\uparrow} \left(\beta, \mu_{\uparrow}'\right) + \tilde{g}_{\downarrow\downarrow} I_{\downarrow} \left(\beta, \mu_{\downarrow}'\right) \right] & -\tilde{g}_{\downarrow\downarrow} - \tilde{g}_{\uparrow\downarrow}^2 I_{\uparrow} \left(\beta, \mu_{\uparrow}'\right) - \tilde{g}_{\downarrow\downarrow}^2 I_{\downarrow} \left(\beta, \mu_{\downarrow}'\right) \end{pmatrix} \\ = - \begin{pmatrix} \tilde{g}_{\uparrow\uparrow} & \tilde{g}_{\uparrow\downarrow} \\ \tilde{g}_{\uparrow\downarrow} & \tilde{g}_{\downarrow\downarrow} \end{pmatrix} - \begin{pmatrix} \tilde{g}_{\uparrow\uparrow}^2 & \tilde{g}_{\uparrow\downarrow} \tilde{g}_{\uparrow\uparrow} \\ \tilde{g}_{\uparrow\downarrow} & \tilde{g}_{\uparrow\downarrow} \end{pmatrix} I_{\uparrow} \left(\beta, \mu_{\uparrow}'\right) - \begin{pmatrix} \tilde{g}_{\uparrow\downarrow}^2 & \tilde{g}_{\uparrow\downarrow} \tilde{g}_{\downarrow\downarrow} \\ \tilde{g}_{\uparrow\downarrow} & \tilde{g}_{\downarrow\downarrow} \end{pmatrix} I_{\downarrow} \left(\beta, \mu_{\downarrow}'\right)$$
(7.4)

with $I_{\uparrow}\left(\beta,\mu_{\uparrow}'\right)$ and $I_{\downarrow}\left(\beta,\mu_{\downarrow}'\right)$ given by eq. (5.4).

A solution to the saddle-point equations is stable if its Hessian matrix has two positive eigenvalues, which is equivalent to requiring that the trace and determinant of its Hessian are both positive.

From the structure of eq. (7.4) and the fact that $I_{\uparrow}\left(\beta,\mu_{\uparrow}'\right)$ and $I_{\downarrow}\left(\beta,\mu_{\downarrow}'\right)$ are positive functions, it is immediately clear that the Hessian can never have two positive eigenvalues if all interaction constants are positive. In contrast to the contact-potential instability, for a general interaction potential it cannot be proven that all saddle points are unstable to density fluctuations. Next, it is interesting to investigate under which conditions stable saddle points may occur.

7.2 Stability analysis for itinerant ferromagnetism in 3D

In this section the stability analysis will be performed in the context of itinerant ferromagnetism in 3D. To study whether the gas can spontaneously polarize through exchange interactions, it is important to exclude other sources of polarization: chemical potential differences and interaction parameter differences. For that reason, only the case $\mu_{\uparrow} = \mu_{\downarrow}$ and $\tilde{g}_{\uparrow\uparrow} = \tilde{g}_{\downarrow\downarrow} = \tilde{g}_{eq}$ (the index eq signifies interactions between particles of equal spin states) will be studied. In that case, the trace and determinant of the Hessian (7.4) are given by

$$\operatorname{Tr} H = -2\tilde{g}_{eq} - \left(\tilde{g}_{eq}^2 + \tilde{g}_{\uparrow\downarrow}^2\right) I_{tot}\left(\beta, \mu_{\uparrow}', \mu_{\downarrow}'\right) \text{ and }$$
(7.5)

$$\det H = \left(\tilde{g}_{eq}^2 - \tilde{g}_{\uparrow\downarrow}^2\right) \left[1 + \tilde{g}_{eq} I_{tot} \left(\beta, \mu_{\uparrow}', \mu_{\downarrow}'\right) + \left(\tilde{g}_{eq}^2 - \tilde{g}_{\uparrow\downarrow}^2\right) \frac{z \left(\beta, \mu_{\uparrow}', \mu_{\downarrow}'\right) I_{tot}^2 \left(\beta, \mu_{\uparrow}', \mu_{\downarrow}'\right)}{4} \right], \quad (7.6)$$

where we introduced the new parameters

$$I_{tot}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right) = I_{\uparrow}\left(\beta,\mu_{\uparrow}'\right) + I_{\downarrow}\left(\beta,\mu_{\downarrow}'\right)$$
(7.7)

and

$$z\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right) = \frac{4I_{\uparrow}\left(\beta,\mu_{\uparrow}'\right)I_{\downarrow}\left(\beta,\mu_{\downarrow}'\right)}{I_{tot}^{2}\left(\beta,\mu_{\uparrow}',\mu_{\downarrow}'\right)} \in [0,1].$$

$$(7.8)$$

First, stability conditions as a function of \tilde{g}_{eq} and $\tilde{g}_{\uparrow\downarrow}$ will be derived for given values of I_{tot} and z. Next, $I_{tot}\left(\beta, \mu'_{\uparrow}, \mu'_{\downarrow}\right)$ and $z\left(\beta, \mu'_{\uparrow}, \mu'_{\downarrow}\right)$ will be calculated as a function of the inverse temperature β and the polarization P. Afterwards, the existence conditions of the saddle points will be derived from the definition of the effective chemical potential. Finally, these results will be combined into a stability phase diagram as a function of \tilde{g}_{eq} and $\tilde{g}_{\uparrow\downarrow}$.

7.2.1 Stability conditions

Here the stability conditions Tr H > 0 and $\det H > 0$ will be studied for given values of I_{tot} and z. I_{tot} can be removed from the expressions for the trace (7.5) and determinant (7.6) of the Hessian by rescaling the interaction parameters to $G_{eq} = I_{tot}\tilde{g}_{eq}$ and $G_{\uparrow\downarrow} = I_{tot}\tilde{g}_{\uparrow\downarrow}$,

$$\operatorname{Tr} H = -\frac{1}{I_{tot}} \left(2G_{eq} + G_{eq}^2 + G_{\uparrow\downarrow}^2 \right), \text{ and}$$
(7.9)
$$\det H = \frac{1}{I_{tot}^2} \left(G_{eq}^2 - G_{\uparrow\downarrow}^2 \right) \left[1 + G_{eq} + \frac{z}{4} \left(G_{eq}^2 - G_{\uparrow\downarrow}^2 \right) \right].$$
(7.10)

The stability condition $\operatorname{Tr} H > 0$ now no longer depends explicitly on I_{tot} and z. It can be rewritten as $(G_{eq} + 1)^2 + G_{\uparrow\downarrow}^2 < 1$. $(G_{eq} + 1)^2 + G_{\uparrow\downarrow}^2 = 1$ is the equation of a circle with radius 1 and centre $(G_{\uparrow\downarrow}, G_{eq}) = (0, -1)$. Tr H is positive within that circle. Note that this implies that we can only find stable saddle points for $G_{eq} < 0$.

The stability condition det H > 0 still depends on the parameter $z \in [0, 1]$. If z = 0, it simplifies to $\left(G_{eq}^2 - G_{\uparrow\downarrow}^2\right)\left(1 + G_{eq}\right) > 0$. This inequality holds true if both factors are either positive or negative at the same time, so if $|G_{eq}| > |G_{\uparrow\downarrow}|$ and $G_{eq} > -1$, or if $|G_{eq}| < |G_{\uparrow\downarrow}|$ and $G_{eq} < -1$. The stability conditions for z = 0 were drawn in fig. 7.1. The regions where det H > 0 and Tr H > 0 only overlap each other for $-1 < G_{eq} < -|G_{\uparrow\downarrow}|$. This is the stability condition at z = 0.



Figure 7.1: The stability conditions for z = 0 as a function of the rescaled interaction parameters $G_{\uparrow\downarrow} = I_{tot}\tilde{g}_{\uparrow\downarrow}$ and $G_{eq} = I_{tot}\tilde{g}_{eq}$. Within the black circle, Tr H > 0. At the blue lines, the first factor $\left(G_{eq}^2 - G_{\uparrow\downarrow}^2\right)$ of the determinant is zero. At the red line, the second factor $(1 + G_{eq})$ of the determinant is zero. In the left picture, the regions where $\left(G_{eq}^2 - G_{\uparrow\downarrow}^2\right) > 0$ and $(1 + G_{eq}) > 0$ are shaded (in blue and red respectively). In the right picture, the regions where $\left(G_{eq}^2 - G_{\uparrow\downarrow}^2\right) > 0$ and $(1 + G_{eq}) < 0$ are shaded (in blue and red respectively). Where both shaded regions overlap within the black circle, saddle points with z = 0 are stable. In the left picture, this occurs for $-1 < G_{eq} < -|G_{\uparrow\downarrow}|$. There is no stability region remaining in the right picture.

If $z \neq 0$, the determinant can be rewritten as

$$\det H = \frac{2}{zI_{tot}^2} \left(G_{eq}^2 - G_{\uparrow\downarrow}^2 \right) \left[G_{eq} + \frac{2}{z} - \sqrt{\frac{4(1-z)}{z^2} + G_{\uparrow\downarrow}^2} \right] \\ \times \left[G_{eq} + \frac{2}{z} + \sqrt{\frac{4(1-z)}{z^2} + G_{\uparrow\downarrow}^2} \right].$$
(7.11)

The last two factors are two branches of a hyperbola with centre $(G_{\uparrow\downarrow}, G_{eq}) = (0, -2/z)$. They intersect the G_{eq} -axis at

$$G_{eq} = \frac{2}{z} \left(-1 \pm \sqrt{1-z} \right)$$
(7.12)

As $z \in [0, 1]$, -2/z < -2 and the lower branch of the hyperbola always intersects the G_{eq} -axis below the region where Tr H > 0. Consequently, stable saddle points cannot occur in the region where the third factor of eq. (7.11) is negative. The upper branch intersects the G_{eq} -axis between -1 and -2, so it always passes through the circular region where Tr H > 0. There are again two cases, depending on the sign of the factor $\left(G_{eq}^2 - G_{\uparrow\downarrow}^2\right)$ in the determinant. If $\left(G_{eq}^2 - G_{\uparrow\downarrow}^2\right) > 0 \Leftrightarrow |G_{eq}| > |G_{\uparrow\downarrow}|$, det H > 0 also implies

$$G_{eq} > -\frac{2}{z} + \sqrt{\frac{4(1-z)}{z^2} + G_{\uparrow\downarrow}^2} \text{ or } G_{eq} < -\frac{2}{z} - \sqrt{\frac{4(1-z)}{z^2} + G_{\uparrow\downarrow}^2}.$$
(7.13)

As we already excluded the occurrence of stable saddle points below the lower branch of the hyperbola, stable saddle points can only occur above the upper branch of the hyperbola.

If $\left(G_{eq}^2 - G_{\uparrow\downarrow}^2\right) < 0 \Leftrightarrow |G_{eq}| < |G_{\uparrow\downarrow}|, \det H > 0$ also implies

$$-\frac{2}{z} - \sqrt{\frac{4(1-z)}{z^2} + G_{\uparrow\downarrow}^2} < G_{eq} < -\frac{2}{z} + \sqrt{\frac{4(1-z)}{z^2} + G_{\uparrow\downarrow}^2}$$
(7.14)

and stable saddle points can only occur between the two branches of the hyperbola.



Figure 7.2: The stability conditions for z = 0.9 as a function of the rescaled interaction parameters $G_{\uparrow\downarrow} = I_{tot}\tilde{g}_{\uparrow\downarrow}$ and $G_{eq} = I_{tot}\tilde{g}_{eq}$. Within the black circle, $\operatorname{Tr} H > 0$. At the blue lines, the first factor $\left(G_{eq}^2 - G_{\uparrow\downarrow}^2\right)$ of the determinant is zero. At the red lines, the second factor $\left[1 + G_{eq} + \frac{z}{4}\left(G_{eq}^2 - G_{\uparrow\downarrow}^2\right)\right]$ of the determinant is zero. In the left picture, the regions where $\left(G_{eq}^2 - G_{\uparrow\downarrow}^2\right) > 0$ and $\left[1 + G_{eq} + \frac{z}{4}\left(G_{eq}^2 - G_{\uparrow\downarrow}^2\right)\right] > 0$ are shaded (in blue and red, respectively). In the right picture, the regions where $\left(G_{eq}^2 - G_{\uparrow\downarrow}^2\right) < 0$ and $\left[1 + G_{eq} - G_{\uparrow\downarrow}^2\right] < 0$ are shaded regions overlap within the black circle, saddle points with z = 0.9 are stable. In the left picture, this occurs for $-\frac{2}{z} + \sqrt{\frac{4(1-z)}{z^2} + G_{\uparrow\downarrow}^2} < G_{eq} < -|G_{\uparrow\downarrow}|$. There is no stability region remaining in the right picture.

As an example, the stability conditions were drawn for z = 0.9 in fig. 7.2. By combining the stability conditions derived from det H > 0 and Tr H > 0, finally the stability condition

$$-\frac{2}{z} + \sqrt{\frac{4(1-z)}{z^2} + G_{\uparrow\downarrow}^2} < G_{eq} < -|G_{\uparrow\downarrow}|$$
(7.15)

is obtained. In the limit $z \to 0$ of this expression, the stability condition $-1 < G_{eq} < -|G_{\uparrow\downarrow}|$ is recovered. In the limit $z \to 1$, the two branches of the hyperbolas become two straight lines which intersect each other at $(G_{\uparrow\downarrow}, G_{eq}) = (0, -2/z)$, resulting in the stability conditions $-2 + |G_{\uparrow\downarrow}| < G_{eq} < -|G_{\uparrow\downarrow}|$ (fig. 7.3). The stability regions were drawn for different values of z in fig. 7.4. As z goes from 0 to 1, the relative stability region grows from a triangle to a square.



Figure 7.3: The stability conditions for z = 1 as a function of the rescaled interaction parameters $G_{\uparrow\downarrow} = I_{tot}\tilde{g}_{\uparrow\downarrow}$ and $G_{eq} = I_{tot}\tilde{g}_{eq}$. Within the black circle, $\operatorname{Tr} H > 0$. At the blue lines, the first factor $\left(G_{eq}^2 - G_{\uparrow\downarrow}^2\right)$ of the determinant is zero. At the red lines, the second factor $\left[1 + G_{eq} + \frac{1}{4}\left(G_{eq}^2 - G_{\uparrow\downarrow}^2\right)\right]$ of the determinant is zero. In the left picture, the regions where $\left(G_{eq}^2 - G_{\uparrow\downarrow}^2\right) > 0$ and $\left(G_{eq} + 2 - |G_{\uparrow\downarrow}|\right) > 0$ are shaded (in blue and red, respectively). In the right picture, the regions where $\left(G_{eq}^2 - G_{\uparrow\downarrow}^2\right) < 0$ and $\left(G_{eq} - G_{\uparrow\downarrow}^2\right) < 0$ and $\left(G_{eq} + 2 - |G_{\uparrow\downarrow}|\right) > 0$ are shaded (in blue and red, respectively). In the right picture, the regions overlap within the black circle, saddle points with z = 1 are stable. In the left picture, this occurs for $-2 + |G_{\uparrow\downarrow}| < G_{eq} < -|G_{\uparrow\downarrow}|$. There is no stability region remaining in the right picture.



Figure 7.4: The upper (black dashed line) and lower (colored full lines) boundaries of the stability regions as a function of the rescaled interaction parameters $G_{\uparrow\downarrow} = I_{tot}\tilde{g}_{\uparrow\downarrow}$ and $G_{eq} = I_{tot}\tilde{g}_{eq}$ for different values of z. As z goes from 0 to 1, the relative stability region grows from a triangle to a square.

7.2.2 I_{tot} and z as a function of β and P

The stability condition (7.15) still depends on the functions $I_{tot}\left(\beta, \mu_{\uparrow}', \mu_{\downarrow}'\right)$ and $z\left(\beta, \mu_{\uparrow}', \mu_{\downarrow}'\right)$. Similarly to the derivation in Sec. 4.5, it is convenient to start from a given solution of the saddle-point equations and work backwards to the conditions for which this solution exists. As $k_F = 1$ already fixes the total density $n = n_{\uparrow} + n_{\downarrow}$ to $n = 1/3\pi^2$, we start from a given polarization P at a given temperature β . For symmetry reasons, it is sufficient to consider only P > 0. From eqs. (4.33) and (5.2), n_{\uparrow} and n_{\downarrow} can be expressed in terms of the effective chemical potentials,

$$n_{\sigma} = -\left. \frac{\partial \Omega_{sp,0} \left(\beta, \mu_{\uparrow}', \mu_{\downarrow}' \right)}{\partial \mu_{\sigma}'} \right|_{\beta, \mu_{-\sigma}'} = \int \frac{d^3k}{(2\pi)^3} \left\{ \frac{1}{1 + \exp\left[\beta \left(\mathbf{k}^2 - \mu_{\sigma}'\right)\right]} \right\}.$$
 (7.16)

Using

$$n_{\uparrow} = \frac{(1+P)}{6\pi^2} \text{ and } n_{\downarrow} = \frac{(1-P)}{6\pi^2},$$
(7.17)

eq. (7.16) can be solved numerically to find μ'_{\uparrow} and μ'_{\downarrow} for given values of β and P. Next, $I_{tot}\left(\beta, \mu'_{\uparrow}, \mu'_{\downarrow}\right)$ and $z\left(\beta, \mu'_{\uparrow}, \mu'_{\downarrow}\right)$ can be calculated. Both I_{tot} and z are monotonously decreasing functions of the polarization |P| and the temperature $T = 1/\beta$ (fig. 7.5 and 7.6).



Figure 7.5: I_{tot} as a function of the polarization P for T = 0 ($\beta \to +\infty$ limit, black solid line), $\beta = 10$ (blue dashed line), $\beta = 3.5$ (purple dot-dashed line) and $\beta = 1$ (red dotted line). I_{tot} is a monotonously decreasing function of the polarization |P| and the temperature $T = 1/\beta$.

7.2.3 Existence conditions

By determining I_{tot} and z, the stability conditions (7.15) can be calculated as a function of the interaction parameters $\tilde{g}_{\uparrow\downarrow}$ and \tilde{g}_{eq} for any given value of β and P. However, it is still unclear whether saddle points with that polarization P actually exist in the corresponding stability region. A saddle point with a given polarization can exist at given values of the interaction parameters $(\tilde{g}_{\uparrow\downarrow}, \tilde{g}_{eq})$ if a value $\mu = \mu_{\uparrow} = \mu_{\downarrow}$ of the chemical potential exists which satisfies the equations that define the effective chemical potentials (6.39).

There are three separate cases which need to be considered: unpolarized saddle points (UP, P = 0), partially polarized saddle points (PP, 0 < |P| < 1) and fully polarized saddle points (FP, |P| = 1).



Figure 7.6: z as a function of the polarization P for T = 0 ($\beta \rightarrow +\infty$ limit, black solid line), $\beta = 10$ (blue dashed line), $\beta = 3.5$ (purple dot-dashed line) and $\beta = 1$ (red dotted line). z is a monotonously decreasing function of the polarization |P| and the temperature $T = 1/\beta$. z = 1 at P = 0 and z = 0 at |P| = 1.

Unpolarized saddle points

For the unpolarized saddle points, $\rho_{\uparrow} = \rho_{\downarrow} = n/2 = 1/6\pi^2$ and $\mu'_{\uparrow} = \mu'_{\downarrow} = \mu'$, so eq. (6.39) becomes

$$\mu' = \mu - \frac{(\tilde{g}_{\uparrow\downarrow} + \tilde{g}_{eq})}{6\pi^2}.$$
(7.18)

It is always possible to find a value of μ which satisfies this equation, therefore unpolarized saddle points exist for all values of β and $(\tilde{g}_{\uparrow\downarrow}, \tilde{g}_{eq})$.

As z = 1 for P = 0, the unpolarized stability condition is given by

$$-\frac{2}{I_{tot}} + \tilde{g}_{\uparrow\downarrow} < \tilde{g}_{eq} < -|\tilde{g}_{\uparrow\downarrow}|.$$
(7.19)

This is a square in the $(\tilde{g}_{\uparrow\downarrow}, \tilde{g}_{eq})$ -plane (fig. 7.4) with diagonals of length $2/I_{tot}$.

If I_{tot}^0 is defined as the value of I_{tot} for P = 0, it is given by

$$I_{tot}^{0} = \beta \int \frac{d^{3}k}{(2\pi)^{3}} \left\{ \frac{1}{1 + \cosh\left[\beta \left(\mathbf{k}^{2} - \mu'\right)\right]} \right\}$$
(7.20)

with μ' determined by

$$\frac{1}{3\pi^2} = \int \frac{d^3k}{(2\pi)^3} \left\{ \frac{1}{1 + \exp\left[\beta \left(\mathbf{k}^2 - \mu'\right)\right]} \right\}.$$
 (7.21)

In the high-temperature limit $(\beta \to 0 \text{ and } T \to +\infty)$, $I_{tot}^0 = 0$. In the zero-temperature limit $(\beta \to +\infty)$, $\mu' = 1$ and $I_{tot}^0 = 1/2\pi^2$. I_{tot}^0 is a monotonously increasing function of β (fig. 7.7). As the area of the unpolarized stability region is directly proportional to $1/(I_{tot}^0)^2$, this implies that the unpolarized stability region increases as a function of temperature. In the high-temperature limit, it becomes infinitely large.



Figure 7.7: The value I_{tot}^0 of I_{tot} for the unpolarized saddle points as a function of the inverse temperature β . The gray dashed line is the zero-temperature limit $I_{tot}^0 = 1/2\pi^2$.

Partially polarized saddle points

For the partially polarized saddle points, eq. (6.39) becomes

$$\begin{cases} \mu_{\uparrow}' = \mu - \tilde{g}_{eq} \frac{(1+P)}{6\pi^2} - \tilde{g}_{\uparrow\downarrow} \frac{(1-P)}{6\pi^2} \\ \mu_{\downarrow}' = \mu - \tilde{g}_{\uparrow\downarrow} \frac{(1+P)}{6\pi^2} - \tilde{g}_{eq} \frac{(1-P)}{6\pi^2} \end{cases}$$
(7.22)

$$\Leftrightarrow \zeta' = \frac{\mu_{\uparrow}' - \mu_{\downarrow}'}{2} = \left(-\tilde{g}_{eq} + \tilde{g}_{\uparrow\downarrow}\right) \frac{P}{6\pi^2},\tag{7.23}$$

where we defined ζ' as half the effective chemical potential difference. This existence condition can be rewritten as $\tilde{g}_{eq} = \tilde{g}_{\uparrow\downarrow} - 6\pi^2 \zeta'/P$, or

$$G_{eq} = G_{\uparrow\downarrow} - \frac{6\pi^2 \zeta' I_{tot}}{P}.$$
(7.24)

The second term can be rewritten as twice the ratio χ_{diff}/χ_{tot} between the differential susceptibility

$$\chi_{diff} = \left. \frac{\partial \left(\delta n \right)}{\partial \zeta'} \right|_{\beta,\mu'} = I_{tot} \tag{7.25}$$

and the total susceptibility

$$\chi_{tot} = \frac{\delta n}{\zeta'} = \frac{P}{3\pi^2 \zeta'},\tag{7.26}$$

defined in analogy to the magnetic susceptibilities (with δn instead of the magnetization M and ζ' instead of the magnetic field B).

Eq. (7.24) represents a straight line in the $(G_{\uparrow\downarrow}, G_{eq})$ -plane, which intersects the stability region given by eq. (7.15) (fig. 7.4) if $0 < \chi_{diff}/\chi_{tot} < 1$. In fig. 7.8, the ratio χ_{diff}/χ_{tot} is studied as a function of the polarization for different values of β . At T = 0 ($\beta \rightarrow +\infty$), χ_{diff}/χ_{tot} is a monotonously decreasing function of the polarization. However, for finite values of the inverse temperature β , χ_{diff}/χ_{tot} becomes infinitely large in the fully polarized limit. This is an important qualitative difference between the zero and non-zero temperatures: fully polarized saddle points can only be stable in the zero-temperature limit.



Figure 7.8: The ratio χ_{diff}/χ_{tot} between the differential and the total susceptibility as a function of the polarization P for T = 0 ($\beta \to +\infty$ limit, black solid line), $\beta = 10$ (blue dashed line), $\beta = 3.5$ (purple dot-dashed line) and $\beta = 1$ (red dotted line). The straight line $G_{eq} = G_{\uparrow\downarrow} - \chi_{diff}/\chi_{tot}$ where the partially polarized saddle points exist only intersects the stability region if $0 < \chi_{diff}/\chi_{tot} < 1$.



Figure 7.9: The maximum value P_{max} of the polarization P for which (fully or partially) polarized saddle points can be stable as a function of temperature T (in units of the Fermi temperature T_F). For $P \leq P_{\text{max}}$, $\chi_{diff}/\chi_{tot} \leq 1$ and for $P > P_{\text{max}}$, $\chi_{diff}/\chi_{tot} > 1$. Polarized saddle points can only be stable for $T \leq 0.583$.

At P = 0, χ_{diff}/χ_{tot} equals 1 and for low temperatures (high but finite β) it reaches a minimum as a function of P before increasing towards the fully polarized limit. At those temperatures, partially polarized solutions can exist and be stable up to a certain maximum polarization P_{max} , where χ_{diff}/χ_{tot} reaches 1. If the temperature becomes too high (β too low), χ_{diff}/χ_{tot} is a monotonously increasing function of the polarization and none of the partially polarized saddle points are stable. P_{max} is shown as a function of the temperature T in fig. 7.9. The minimum value of β where partially polarized saddle points can be stable may be estimated by studying χ_{diff}/χ_{tot} for a very low value of the polarization. Using $P = 10^{-4}$, $\beta_{\min} \lesssim 1.715$ (or equivalently $T_{\max} = 1/\beta_{\min} \gtrsim 0.583$) is found.

For 0 < P < 1, $z \in [0, 1[$ and the stability condition is given by eq. (7.15).

Fully polarized saddle points

Full polarization is a special case. Fully polarized saddle points only exist at temperature zero, as $n_{\sigma} = 0$ in (7.16) can only be realized in the limit $\mu'_{\sigma} \to +\infty$ at finite values of the inverse temperature β . The fact that fully polarized saddle points only exist at temperature zero is a second very important qualitative difference between zero and non-zero temperatures.

At zero temperature, the number equations are given by eq. (4.38). If P = 1, $n_{\uparrow} = \rho_{\uparrow} = 1/3\pi^2$ and $n_{\downarrow} = \rho_{\downarrow} = 0$, so $\mu'_{\uparrow} = 2^{2/3}$ and $\mu'_{\downarrow} \leq 0$. These values can be used in eq. (6.39) to find

$$\begin{cases} 2^{2/3} = \mu_{\uparrow}' = \mu - \frac{\tilde{g}_{eq}}{3\pi^2} \\ 0 \ge \mu_{\downarrow}' = \mu - \frac{\tilde{g}_{\uparrow\downarrow}}{3\pi^2} \end{cases}$$
(7.27)

$$\Rightarrow \tilde{g}_{eq} \le \tilde{g}_{\uparrow\downarrow} - 3\pi^2 2^{2/3} \tag{7.28}$$

$$\Leftrightarrow G_{eq} \le G_{\uparrow\downarrow} - 3\pi^2 2^{2/3} I_{tot}. \tag{7.29}$$

This is the existence condition for the fully polarized saddle points at T = 0. The same existence condition is found when starting from P = -1.

At |P| = 1, z = 0 and the fully polarized stability condition is given by

$$-\frac{1}{I_{tot}} < \tilde{g}_{eq} < -\left|\tilde{g}_{\uparrow\downarrow}\right|. \tag{7.30}$$

This is a triangle in the $(\tilde{g}_{\uparrow\downarrow}, \tilde{g}_{eq})$ -plane (fig. 7.4).

In the zero-temperature limit at full polarization, $\mu' = 2/3$ and $I_{tot} = 1/(2^{5/3}\pi^2)$, so at T = 0 the fully polarized saddle points exist and are stable in the triangular region where

$$-2^{5/3}\pi^2 < \tilde{g}_{eq} < \min\left[-\left|\tilde{g}_{\uparrow\downarrow}\right|, -3\pi^2 2^{2/3}\right].$$
(7.31)

7.2.4 Stability-existence phase diagram

By combining the stability and existence conditions from Sec. 7.2.1 and 7.2.3 with the calculated values of I_{tot} and z as a function of β and P from Sec. 7.2.2, phase diagrams can be constructed (fig. 7.10).

There are several conclusions that can be drawn from the phase diagrams in fig. 7.10.

- 1. As was already mentioned in Sec. 7.2.3, the area of the unpolarized stability region increases as a function of temperature. In the high-temperature limit, it becomes infinitely large.
- 2. Fully polarized saddle points only exist at temperature zero (as discussed in Sec. 7.2.3). However, at low temperatures there is still a sizable region with almost full polarization.
- 3. The partially and fully polarized existence-stability regions shrink and become less polarized as the temperature increases, until they are absorbed by the growing unpolarized stability region at $\beta_{\min} \leq 1.715$ (see Sec. 7.2.3). The maximum polarization that can be stable decreases with temperature (see fig. 7.9).



Figure 7.10: The stability-existence phase diagrams as a function of the interaction parameters $\tilde{g}_{\uparrow\downarrow}$ and \tilde{g}_{eq} for T = 0 ($\beta \to +\infty$), $\beta = 10$, $\beta = 3.5$ and $\beta = 1$. The blue diagonally shaded region corresponds to the unpolarized stability-existence region, the colored region to the partially polarized stability-existence region (where the hue depends on the polarization P) and the green horizontally and vertically shaded region to the fully polarized stability-existence region. Stable fully polarized saddle points only occur at T = 0. As the temperature increases (or β decreases), the polarized saddle points get less polarized and are absorbed by the growing unpolarized stability region. The current formalism does not allow to investigate what happens outside of the dashed and colored regions.

4. If the interactions become too strong, all saddle points become unstable to density fluctuations. This significantly reduces the area where the itinerant ferromagnetic partially and fully polarized phases are expected.

As the interaction parameter $g_{\uparrow\downarrow}$ is related to the experimentally relevant interaction parameter $a_s^{\uparrow\downarrow}k_F$ by $g_{\uparrow\downarrow} = 8\pi a_s^{\uparrow\downarrow}k_F$ in the first Born approximation (with $8\pi \approx 25$), $a_s^{\uparrow\downarrow}k_F$ is of order one in the itinerant ferromagnetic regions of the phase diagrams in fig. 7.10. This is in agreement with the zero-temperature mean-field Stoner criterion $a_s^{\uparrow\downarrow}k_F = \pi/2$ and the second-order prediction $a_s^{\uparrow\downarrow}k_F = 1.054$ [14] at the normal-to-itinerant-ferromagnetic phase transition, which are based on a simple energy argument (Sec. 2.3.1).

The extra requirement of stability against density fluctuations adds an upper limit to the range of values of $a_s^{\uparrow\downarrow}k_F$ where itinerant ferromagnetism may occur. Furthermore, the remaining interactions \tilde{g}_{eq} between particles of the same spin states after the screening by the exchange interactions play an important role in the stability of the gas. As the interactions at short distances are screened, an interaction potential which is sufficiently, but not too strongly attractive at mid-to-long ranges between particles of equal spin states is required. For itinerant ferromagnetism to occur, a precarious equilibrium has to be observed: strong density fluctuations and thus strong interactions are necessary in order to create magnetic domains, but the magnetic domains are also destroyed if the density fluctuations become too strong.

In most experiments with ultracold atomic gases, almost no interactions remain between particles of equal spin states, so \tilde{g}_{eq} can be assumed to be very small ($|\tilde{g}_{eq}| << 1$). In that case, the phase diagrams in fig. 7.10 predict that the itinerant ferromagnetic state cannot be stable. This may help explain why the Stoner instability (of the normal state to magnetic domain formation) is dominated by the instability of the Feshbach resonance (to molecule formation) in the experiments [35,36]. An important caveat to this conclusion is that it is as yet unclear to what extent the instabilities found in the grand-canonical ensemble may be extended to the experimental system, where the particle numbers are fixed. This issue will be discussed in Sec. 8.3.

The model constructed and discussed in chapter 6 and 7 is not valid outside of the stability regions, so it cannot predict what occurs there. Possible phases include superfluid pairing, phase separation, non-uniform phases (e.g. density waves in dipolar gases [97]) and crystallization. The itinerant ferromagnetic region in the phase diagram may be extended by phase separation and non-uniform itinerant ferromagnetic phases. However, other physical effects that have not been included in the description may also reduce the normal and itinerant ferromagnetic regions in the phase diagram. This is what occurs in liquid ³He, where the itinerant ferromagnetic region in the phase diagram disappears when including crystallization [9]. For itinerant ferromagnetism, it appears there is a large risk of modeling bias: a model created to describe itinerant ferromagnetism will predict itinerant ferromagnetism to occur in a certain part of the phase diagram, but a more general model may not find itinerant ferromagnetism at all. However, it is very challenging to include more than one physical effect in a physically correct way.

As a final remark, for stable saddle points the results can be improved by including the effects of small fluctuations around the saddle point. This is not possible for unstable saddle points, so fig. 7.10 also serves as a diagnostic tool for the feasibility of corrections beyond the saddle-point approximation. Due to time constraints, these calculations were not attempted in this dissertation.

Chapter 8

Discussion of implicit assumptions and approximations

When creating a theoretical model of a physical system, an equilibrium between two conflicting interests has to be sought. On one hand, one wants to include as many physical effects as possible in order to better describe the system. On the other hand, one wants to include the least amount of extraneous physical effects possible in order to ease the calculations.

During the course of my doctoral research, in each conceptual step in the calculations I learned more about the assumptions and approximations that are included in the model I was using and whether those assumptions and approximations are valid. Many assumptions are made implicitly, so it is not always clear at first sight that there is an assumption. In this chapter, I will discuss the most important of these implicit assumptions and approximations.

8.1 The choice of the action

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When the action used in the model has been chosen, many implicit assumptions have already been made. As the action for contact interactions is only a particular form of the action for general interaction potentials, only the action for general interaction potentials will be discussed. It is given by eq. (6.1),

$$S\left[\bar{\psi}_{\sigma},\psi_{\sigma}\right] = \sum_{\sigma=\uparrow,\downarrow} \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \bar{\psi}_{\sigma,\mathbf{x},\tau} \left(\frac{\partial}{\partial\tau} - \nabla_{\mathbf{x}}^{2} - \mu_{\sigma}\right) \psi_{\sigma,\mathbf{x},\tau} + \sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow} \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \int_{V} d\mathbf{x}' \frac{g_{\sigma_{1}\sigma_{2}}\left(\mathbf{x}-\mathbf{x}'\right)}{2} \bar{\psi}_{\sigma_{1},\mathbf{x},\tau} \bar{\psi}_{\sigma_{2},\mathbf{x}',\tau} \psi_{\sigma_{1},\mathbf{x},\tau}.$$
(8.1)

The main assumptions made in the choice of the action are related to the choice of the interaction term:

- The interaction potentials are time-independent. Furthermore, they only depend on the distance between the particles.
- The interactions are instantaneous: all fermionic fields in eq. (8.1) have the same imaginary time index τ .
- The two interacting particles remain in the same positions \mathbf{x} and \mathbf{x}' during the (instantaneous) interaction. In Fourier space, this corresponds to total momentum conservation during the interaction.
- Only elastic interactions between two particles are taken into account. Collisions of more than two particles and inelastic collisions have been neglected. This is not a good approximation

to the situation in the most recent experiments, as inelastic two-and three-body collisions have been shown to become important [36]. However, as discussed in Sec. 2.3.4, researchers are still looking for a way to reduce the three-body collision rate in order to recreate the theoretical Stoner model (which only takes into account elastic two-body collisions).

• Even for interactions between two particles, four particular interaction processes have been selected. For instantaneous interactions, the full interaction term would be given by

$$\sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4=\uparrow,\downarrow} \int_0^\rho d\tau \int_V d\mathbf{x} \int_V d\mathbf{x}' \frac{g_{\sigma_1\sigma_2\sigma_3\sigma_4} \left(\mathbf{x} - \mathbf{x}'\right)}{2} \bar{\psi}_{\sigma_1,\mathbf{x},\tau} \bar{\psi}_{\sigma_2,\mathbf{x}',\tau} \psi_{\sigma_3,\mathbf{x}',\tau} \psi_{\sigma_4,\mathbf{x},\tau}.$$
 (8.2)

In order to select the four interaction processes in eq. (8.1), conservation of total angular momentum (or total spin) during the interaction was used. This is a reasonable approximation for elastic collisions between two particles.

Furthermore, by calculating the partition sum and minimizing the thermodynamic grand potential the ground state of the system is sought. With this approach only equilibrium states of the system can be studied. Experimentalists are trying to extend the lifetimes of the experiments on the repulsive branch of the Feshbach resonance in order to study equilibrium states of the system, but so far the experimental system could not be considered to be in equilibrium [36]. If itinerant ferromagnetism is created with dipolar interactions [69–71], the match between theory and experiments may be closer as dipolar interactions do not suffer from the instability to molecular pairing near a Feshbach resonance.

The final assumption is that all particles have equal mass. As recent proposals for the reduction of the three-body loss rate in experiments include the use of mass imbalance [47–53], it would be interesting to extend the results of chapter 6 and 7 to mass-imbalanced systems.

8.2 The choice of the density fluctuations

Q

As explained in chapters 5 and 7, the Hessian matrix of the saddle-point thermodynamic grand potential was used in order to study the stability of the saddle points against density fluctuations. This way, only uniform perturbations of the density were considered. However, there are many other possible density fluctuations, as the value of the bosonic field can be perturbed in each value of the position coordinate separately (see fig. 8.1).



Figure 8.1: Two possible density fluctuations in a hypothetical system with only 5 different values of the position coordinate. In a general density fluctuation, the density is perturbed in each value of the position coordinate separately (left). In this dissertation, only uniform perturbations of the density were considered (right).

A saddle point is stable against density fluctuations if it is stable against all possible density fluctuations. Conversely, it only takes an instability against one possible fluctuation to drive the state out of equilibrium. The inclusion of other types of density fluctuations can only reduce the stability regions in the phase diagrams (fig. 7.10). The limitation to uniform density fluctuation thus implies the assumption that this is the dominant mode of instability. This seems to be a reasonable approximation, as large parts of the phase diagram turned out to be unstable to uniform density fluctuations.

Within the saddle-point approximation, only uniform density fluctuations can be considered. In order to study other types of density fluctuations, the contribution of these density fluctuations to the thermodynamic grand potential needs to be calculated. This is a tedious and challenging task. That is the reason why these types of fluctuations have not been considered here. In order to improve our results it would be interesting to calculate these fluctuation contributions in the areas of the phase diagram that are stable to uniform density fluctuations.

8.3 The choice of the ensemble

There are several very important differences between the theoretical calculations in part II and III on one hand, and the experiments on the other hand. These are shown in table 8.1.

Experiments	Theory
Fixed particle numbers n_{σ}	Fixed chemical potentials μ_{σ}
Canonical ensemble	Grand canonical ensemble
Trapping potential (usually harmonic)	No external (trapping) potential
Non-uniform gas	Uniform gas

Table 8.1: The main differences between the experiments in ultracold atomic gases and the theoretical calculations presented in this dissertation.

This essentially comes down to the difference between the two important ensembles which have been used in this thesis: the grand-canonical ensemble (energy and particle numbers fluctuate) and the canonical ensemble (particle numbers are conserved, but the energy of the system fluctuates). How do we match the results of the simplified grand-canonical theoretical calculations to the more complicated canonical experimental conditions? There are two possible solutions to this conundrum.

The first solution is to adapt the theory to the experiment. In the saddle-point approximation, transition from the grand-canonical ensemble to the canonical ensemble occurs by transitioning to the free energy $F(\beta, n_{\uparrow}, n_{\downarrow}) = \Omega(\beta, \mu_{\uparrow}, \mu_{\downarrow}) + \mu_{\uparrow}n_{\uparrow} + \mu_{\downarrow}n_{\downarrow}$. The trapping potential could be included by adapting the action. However, path-integral calculations tend to become cumbersome very quickly when adding extra complications to the action. Furthermore, there is a loss of generality when adapting to a particular experimental system.

The second solution is the use of the Local Density Approximation (LDA). If the density is sufficiently slowly varying in space with respect to the other relevant length scales in the experiment, the gas can be considered as locally uniform. The gas is then assumed to consist of a series of small uniform compartments, characterized by local thermodynamic variables. Furthermore, each compartment is allowed to exchange energy and particles with a "bath" that consists of the other compartments. In this situation, the gas is locally described by the grand-canonical ensemble. If LDA is valid, the results obtained in the path-integral formalism for a uniform gas without an external potential in the grand canonical ensemble can be used to predict the local phase of the gas in the experiments.

LDA provides a powerful argument for extending the instability of itinerant ferromagnetism in large parts of the grand-canonical phase diagram to the experimental system. However, it is not clear whether the same instability mechanisms apply in the canonical ensemble. In the grand-canonical ensemble, density fluctuations can also be realized through the creation and annihilation of particles, while the density fluctuations in the canonical ensemble are limited to density shifts. Further research is needed in order to clarify the link between the phase diagram in fig. 7.10 and the experiments. Given the fact that itinerant ferromagnetism has proven to be notoriously elusive in experiments despite the great number of solid theoretical predictions, it is likely that at least some of the instability mechanisms of itinerant ferromagnetism will persist in the experimental system. This would provide a natural explanation for the discrepancy between theory and experiments.

For a general interaction potential, great care has to be taken when applying LDA, as the range of the interactions is also an important length scale. The approach discussed in chapters 6 and 7 is only valid when it is possible to average the interactions in space, especially in the saddle-point approximation. When the interactions between particles at large distances have an important effect, density differences over that length scale may significantly influence the phase of the system. LDA is only applicable when the range of the interactions is sufficiently small with respect to the length scales of the density variations. This is a potentially important limit to the applicability of the results obtained in chapter 7 for itinerant ferromagnetism.

LDA also fails when the number of particles becomes very small, but in that case also the theoretical assumption that the gas is uniform is no longer valid.

8.4 The choice of the channel

When constructing a Hubbard-Stratonovich transformation, there are three possible ways or channels to pair the four fermionic fields in the interaction term of the action (8.1) [92]:

- 1. Bogoliubov: $\bar{\psi}_{\sigma_1,\mathbf{x},\tau}\bar{\psi}_{\sigma_2,\mathbf{x}',\tau}$ and $\psi_{\sigma_1,\mathbf{x},\tau}\psi_{\sigma_2,\mathbf{x}',\tau}$
- 2. Hartree: $\bar{\psi}_{\sigma_1,\mathbf{x},\tau}\psi_{\sigma_1,\mathbf{x},\tau}$ and $\bar{\psi}_{\sigma_2,\mathbf{x}',\tau}\psi_{\sigma_2,\mathbf{x}',\tau}$
- 3. Fock: $\bar{\psi}_{\sigma_1,\mathbf{x},\tau}\psi_{\sigma_2,\mathbf{x}',\tau}$ and $\bar{\psi}_{\sigma_2,\mathbf{x}',\tau}\psi_{\sigma_1,\mathbf{x},\tau}$

The Hubbard-Stratonovich transformation is exact, as it is derived from an algebraic property of a bosonic path integral (as discussed in Sec. 4.2 and Sec. 6.2). However, the bosonic path integral cannot be calculated exactly for a general case. In most approximations, the interaction part of the action is expanded in terms of the bosonic field and its derivatives with respect to time and position. This approximation is only valid when the considered pairings of the fermionic fields dominate the physics of the system. Consequently, the choice of the channel determines the physics that is included after approximating the bosonic path integral.

The Bogoliubov channel is most suitable for describing superfluid pairing [25], while the Hartree channel is most suitable for describing the (density-density) interactions in the normal and itinerant ferromagnetic state [94,95]. The Fock channel is a special case.

For interactions between particles with opposite spin states, the Fock channel is often used in combination with the Hartree channel. The expectation value of the spin at each position can be expressed as a vector with a fixed length. In that view, the Hartree channel is used to describe the magnetization along the z-axis (or the population of the up and down spin states) and the Fock channel is used to describe the magnetization in the plane perpendicular to the z-axis. When combining the Hartree and Fock channels, the Hubbard-Stratonovich transformation can be rewritten in terms of a bosonic field ρ (corresponding to the total density) and a bosonic vector field ϕ (corresponding to the expectation value of the spin) [94–96]. In a true spin-1/2 Fermi gas (e.g. a free electron gas), this is a useful description. However, in ultracold atomic gases σ_1 and σ_2 are only pseudospin states: \uparrow and \downarrow are used as a label for the two different components of the gas. Furthermore, the number of atoms in each pseudospin state can usually be considered to be fixed for the duration of the experiment. Consequently, in the context of ultracold atomic gases polarization along the perpendicular plane is not as relevant as for electrons in a material.

For particles of the same spin state, the Hartree and Fock channels both describe the same densitydensity interactions between particles of the same spin state. This clearly shows that the names Hartree and Fock are used differently here than in the usual Hartree-Fock treatment. In that treatment, the Hartree contribution corresponds to the direct interactions and the Fock contribution to the exchange interactions. In this dissertation, Hartree and Fock are used to denote two different channels of the Hubbard-Stratonovich transformation, which initially contain the same information (before the approximation of the bosonic path integral). The Hartree and Fock channel contain both direct and exchange interactions. Coincidentally, without the modified interaction potential the Hartree channel does correspond to the direct interactions in the saddle-point approximation. However, the Fock channel does not correspond to the exchange contribution in the saddle-point approximation and it suffers from the same potential loss of the exchange interactions when approximating the bosonic path integral.

In conclusion, in the context of ultracold atomic gases the Bogoliubov and Hartree channels are most relevant, although the Fock channel could be used to further improve the description of the interactions between particles of different spin states. In this dissertation on itinerant ferromagnetism only the Hartree channel was studied. However, it is known that superfluid pairing also plays a very important role, as it will compete with magnetic domain formation. In the future, it would be interesting to combine the Hartree and Bogoliubov channels.

Because all channels initially contain the same physical information, it is a very difficult and dangerous undertaking to combine more than one channel. Great care has to be taken to avoid double counting when approximating the bosonic path integrals. That is the main reason why this combination of channels has not been attempted here.

8.5 The choice of the basis: position vs. momentum space

In Sec. 6.2, I proposed a new method to enforce the Pauli exclusion principle explicitly through a modification of the interaction potential. The Hubbard-Stratonovich transformation with this new modified interaction potential remains exact, and the modified interaction potential ensures that also in the saddle-point approximation the exchange is properly taken into account. The final question that remains is the following: is this new method exact or approximate?

Intuitively, the answer would be that it is exact, as the Hubbard-Stratonovich transformation is exact and the parts of the interaction potential that are modified only affect parts of the action that are excluded by the exchange interactions. However, in reality it is not exact: the exchange interactions cannot be described by an interaction potential. This is related to the fact that both behave differently under a Fourier transform. In order to demonstrate this fact, I will define a second modified interaction potential in the momentum basis and compare the results to the original results obtained in the position basis (see chapter 6 and 7).

Using definitions (4.15) and (6.5) for the Fourier transformed fermionic fields and interaction potentials, the original action (6.1) can be rewritten in the momentum basis as

$$S\left[\bar{\psi}_{\sigma},\psi_{\sigma}\right] = \sum_{\sigma=\uparrow,\downarrow}\sum_{k}\bar{\psi}_{\sigma,k}\left(-i\omega_{n}+\mathbf{k}^{2}-\mu_{\sigma}\right)\psi_{\sigma,k} + \frac{1}{2}\frac{1}{\beta\sqrt{V}}\sum_{k,k',Q}\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow}g_{\sigma_{1}\sigma_{2}}\left(\mathbf{Q}\right)\bar{\psi}_{\sigma_{1},k}\psi_{\sigma_{1},k-Q}\bar{\psi}_{\sigma_{2},k'}\psi_{\sigma_{2},k'+Q}$$
(8.3)

with $k = (\mathbf{k}, \omega_n)$, $k' = (\mathbf{k}', \omega_{n'})$ and $Q = (\mathbf{Q}, \Omega_m)$. The antisymmetry properties of the Grassmann numbers exclude terms where the two incoming or outgoing fermions are in the same quantum state:

1.
$$k = k'$$
, and
2. $k - Q = k' + Q \Leftrightarrow Q = (k - k')/2$.

Note that interaction terms with k' = k and Q = 0 are excluded by both conditions. In order to enforce the Pauli exclusion principle, a new modified interaction potential $g'_{\sigma_1\sigma_2}(\mathbf{Q})$ has to be defined in a similar way as in eq. (6.34) for the transformation in position space:

$$g_{\sigma_{1}\sigma_{2}}'\left(Q,k,k'\right) = g_{\sigma_{1}\sigma_{2}}\left(\mathbf{Q}\right)\left\{1 - \delta_{\sigma_{1},\sigma_{2}}\left[\delta_{1}\left(k-k'\right) + \delta_{1}\left(Q - \frac{k-k'}{2}\right)\right] - \delta_{1}\left(k-k'\right)\delta_{1}\left(Q - \frac{k-k'}{2}\right)\right\}.$$

$$(8.4)$$

Next, the behavior of the modified interaction term under an inverse Fourier transform will be studied. The inverse Fourier transform is defined as

$$\begin{cases} \psi_{\sigma,\mathbf{k},n} = \frac{1}{\sqrt{\beta V}} \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \exp\left(-i\mathbf{k}\cdot\mathbf{x} + i\omega_{n}\tau\right)\psi_{\sigma,\mathbf{x},\tau} \\ \bar{\psi}_{\sigma,\mathbf{k},n} = \frac{1}{\sqrt{\beta V}} \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \exp\left(i\mathbf{k}\cdot\mathbf{x} - i\omega_{n}\tau\right)\bar{\psi}_{\sigma,\mathbf{x},\tau} \end{cases}, \tag{8.5}$$

$$g_{\sigma_1 \sigma_2} \left(\mathbf{Q} \right) = \frac{1}{\sqrt{V}} \int_{V} d\left(\mathbf{\Delta} \mathbf{x} \right) \exp\left(-i\mathbf{Q} \cdot \mathbf{\Delta} \mathbf{x} \right) g_{\sigma_1 \sigma_2} \left(\mathbf{\Delta} \mathbf{x} \right).$$
(8.6)

The modified interaction term can be split into four parts according to the four terms of the modified interaction potential (8.4),

$$\frac{1}{2} \frac{1}{\beta\sqrt{V}} \sum_{k,k',Q} \sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow} g_{\sigma_{1}\sigma_{2}}'(Q,k,k') \bar{\psi}_{\sigma_{1},k}\psi_{\sigma_{1},k-Q}\bar{\psi}_{\sigma_{2},k'}\psi_{\sigma_{2},k'+Q} \\
= \frac{1}{2} \frac{1}{\beta\sqrt{V}} \sum_{k,k',Q} \sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow} g_{\sigma_{1}\sigma_{2}}(\mathbf{Q}) \bar{\psi}_{\sigma_{1},k}\psi_{\sigma_{1},k-Q}\bar{\psi}_{\sigma_{2},k'}\psi_{\sigma_{2},k'+Q} \\
- \frac{1}{2} \frac{1}{\beta\sqrt{V}} \sum_{k,Q} \sum_{\sigma=\uparrow,\downarrow} g_{\sigma\sigma}(\mathbf{Q}) \bar{\psi}_{\sigma,k}\psi_{\sigma,k-Q}\bar{\psi}_{\sigma,k}\psi_{\sigma,k+Q} \\
- \frac{1}{2} \frac{1}{\beta\sqrt{V}} \sum_{k,k'} \sum_{\sigma=\uparrow,\downarrow} g_{\sigma\sigma}\left(\frac{\mathbf{k}-\mathbf{k}'}{2}\right) \bar{\psi}_{\sigma,k}\psi_{\sigma,\frac{k+k'}{2}}\bar{\psi}_{\sigma,k'}\psi_{\sigma,\frac{k+k'}{2}} \\
+ \frac{1}{2} \frac{1}{\beta\sqrt{V}} \sum_{k} \sum_{\sigma=\uparrow,\downarrow} g_{\sigma\sigma}(\mathbf{0}) \bar{\psi}_{\sigma,k}\psi_{\sigma,k}\bar{\psi}_{\sigma,k}\psi_{\sigma,k}.$$
(8.7)

Each term is inverse Fourier transformed separately and the result is given by

$$\frac{1}{2} \frac{1}{\beta\sqrt{V}} \sum_{k,k',Q} \sum_{\sigma_1,\sigma_2=\uparrow,\downarrow} g_{\sigma_1\sigma_2}'(Q,k,k') \bar{\psi}_{\sigma_1,k} \psi_{\sigma_1,k-Q} \bar{\psi}_{\sigma_2,k'} \psi_{\sigma_2,k'+Q} \\
= \frac{1}{2} \sum_{\sigma=\uparrow,\downarrow} \int_{V} d\left(\Delta \mathbf{x}\right) \int_{0}^{\beta} d\tau_1 \int_{V} d\mathbf{x}_1 \int_{0}^{\beta} d\tau_2 \int_{V} d\mathbf{x}_2 \int_{0}^{\beta} d\tau_3 \int_{V} d\mathbf{x}_3 \int_{0}^{\beta} d\tau_4 \int_{V} d\mathbf{x}_4 \\
\times \left[\delta\left(-\mathbf{x}_1 + \mathbf{x}_2\right) \delta\left(-\mathbf{x}_3 + \mathbf{x}_4\right) \delta\left(\Delta \mathbf{x} - \mathbf{x}_2 + \mathbf{x}_4\right) \delta\left(-\tau_1 + \tau_2\right) \delta\left(-\tau_3 + \tau_4\right) \delta\left(-\tau_2 + \tau_4\right) \\
- \frac{1}{\beta V} \delta\left(-\mathbf{x}_1 + \mathbf{x}_2 - \mathbf{x}_3 + \mathbf{x}_4\right) \delta\left(\Delta \mathbf{x} - \mathbf{x}_2 + \mathbf{x}_4\right) \delta\left(-\tau_1 + \tau_2 - \tau_3 + \tau_4\right) \delta\left(-\tau_2 + \tau_4\right) \\
- \frac{1}{\beta V} \delta\left(\frac{\mathbf{x}_2 + \mathbf{x}_4 + \Delta \mathbf{x}}{2} - \mathbf{x}_1\right) \delta\left(\frac{\mathbf{x}_2 + \mathbf{x}_4 - \Delta \mathbf{x}}{2} - \mathbf{x}_3\right) \delta\left(-\tau_1 + \frac{\tau_2 + \tau_4}{2}\right) \delta\left(\frac{\tau_2 + \tau_4}{2} - \tau_3\right) \\
+ \frac{1}{(\beta V)^2} \delta\left(-\mathbf{x}_1 + \mathbf{x}_2 - \mathbf{x}_3 + \mathbf{x}_4\right) \delta\left(-\tau_1 + \tau_2 - \tau_3 + \tau_4\right) \right] \\
\times g_{\sigma_1 \sigma_2} \left(\Delta \mathbf{x}\right) \bar{\psi}_{\sigma_1, \mathbf{x}_1, \tau_1} \psi_{\sigma_1, \mathbf{x}_2, \tau_2} \bar{\psi}_{\sigma_2, \mathbf{x}_3, \tau_3} \psi_{\sigma_2, \mathbf{x}_4, \tau_4}.$$
(8.8)

The first term is the original interaction term in position space,

$$\frac{1}{2} \sum_{\sigma=\uparrow,\downarrow} \int_{V} d\left(\mathbf{\Delta}\mathbf{x}\right) \int_{0}^{\beta} d\tau_{1} \int_{V} d\mathbf{x}_{1} \int_{0}^{\beta} d\tau_{2} \int_{V} d\mathbf{x}_{2} \int_{0}^{\beta} d\tau_{3} \int_{V} d\mathbf{x}_{3} \int_{0}^{\beta} d\tau_{4} \int_{V} d\mathbf{x}_{4}$$

$$\times \delta\left(-\mathbf{x}_{1} + \mathbf{x}_{2}\right) \delta\left(-\mathbf{x}_{3} + \mathbf{x}_{4}\right) \delta\left(\mathbf{\Delta}\mathbf{x} - \mathbf{x}_{2} + \mathbf{x}_{4}\right) \delta\left(-\tau_{1} + \tau_{2}\right) \delta\left(-\tau_{3} + \tau_{4}\right) \delta\left(-\tau_{2} + \tau_{4}\right)$$

$$\times g_{\sigma_{1}\sigma_{2}}\left(\mathbf{\Delta}\mathbf{x}\right) \bar{\psi}_{\sigma_{1},\mathbf{x}_{1},\tau_{1}} \psi_{\sigma_{1},\mathbf{x}_{2},\tau_{2}} \bar{\psi}_{\sigma_{2},\mathbf{x}_{3},\tau_{3}} \psi_{\sigma_{2},\mathbf{x}_{4},\tau_{4}}$$

$$= \frac{1}{2} \sum_{\sigma=\uparrow,\downarrow} \int_{0}^{\beta} d\tau \int_{V} d\mathbf{x} \int_{V} d\mathbf{x}' g_{\sigma_{1}\sigma_{2}}\left(\mathbf{x} - \mathbf{x}'\right) \bar{\psi}_{\sigma_{1},\mathbf{x},\tau} \psi_{\sigma_{1},\mathbf{x},\tau} \bar{\psi}_{\sigma_{2},\mathbf{x}',\tau} \psi_{\sigma_{2},\mathbf{x}',\tau}, \qquad (8.9)$$

but there is a series of extra terms that was not present in the original interaction term:

$$\frac{1}{2} \sum_{\sigma=\uparrow,\downarrow} \int_{V} d\left(\mathbf{\Delta}\mathbf{x}\right) \int_{0}^{\beta} d\tau_{1} \int_{V} d\mathbf{x}_{1} \int_{0}^{\beta} d\tau_{2} \int_{V} d\mathbf{x}_{2} \int_{0}^{\beta} d\tau_{3} \int_{V} d\mathbf{x}_{3} \int_{0}^{\beta} d\tau_{4} \int_{V} d\mathbf{x}_{4} \qquad (8.10)$$

$$\left[-\frac{1}{\beta V} \delta\left(-\mathbf{x}_{1} + \mathbf{x}_{2} - \mathbf{x}_{3} + \mathbf{x}_{4}\right) \delta\left(\mathbf{\Delta}\mathbf{x} - \mathbf{x}_{2} + \mathbf{x}_{4}\right) \delta\left(-\tau_{1} + \tau_{2} - \tau_{3} + \tau_{4}\right) \delta\left(-\tau_{2} + \tau_{4}\right) - \frac{1}{\beta V} \delta\left(\frac{\mathbf{x}_{2} + \mathbf{x}_{4} + \mathbf{\Delta}\mathbf{x}}{2} - \mathbf{x}_{1}\right) \delta\left(\frac{\mathbf{x}_{2} + \mathbf{x}_{4} - \mathbf{\Delta}\mathbf{x}}{2} - \mathbf{x}_{3}\right) \delta\left(-\tau_{1} + \frac{\tau_{2} + \tau_{4}}{2}\right) \delta\left(\frac{\tau_{2} + \tau_{4}}{2} - \tau_{3}\right) + \frac{1}{(\beta V)^{2}} \delta\left(-\mathbf{x}_{1} + \mathbf{x}_{2} - \mathbf{x}_{3} + \mathbf{x}_{4}\right) \delta\left(-\tau_{1} + \tau_{2} - \tau_{3} + \tau_{4}\right) \right]$$

$$g_{\sigma_{1}\sigma_{2}}\left(\mathbf{\Delta}\mathbf{x}\right) \bar{\psi}_{\sigma_{1},\mathbf{x}_{1},\tau_{1}} \psi_{\sigma_{1},\mathbf{x}_{2},\tau_{2}} \bar{\psi}_{\sigma_{2},\mathbf{x}_{3},\tau_{3}} \psi_{\sigma_{2},\mathbf{x}_{4},\tau_{4}}.$$

$$(8.11)$$

Each additional delta function (or restriction) in momentum space results in a reduction in the number of delta functions (so in an extra degree of freedom) in the corresponding term in position space. This is because a delta function Fourier transforms into a constant function, instead of into another delta function.

A peculiar property of the Grassmann algebra is the fact that a restriction imposed by the Pauli exclusion principle in position space Fourier transforms into a restriction imposed by the Pauli exclusion principle in momentum space and vice versa. For real and complex functions (e.g. interaction potentials), a restriction in position space Fourier transforms into an extra freedom in momentum space and vice versa.

The results of this reasoning imply that the use of a modified interaction potential instead of the real interaction potential affects the physics of the system, even when only terms affected by the exchange interactions in position or momentum space are excluded. The only true way forward in the implementation of the exchange interactions is the treatment of the full fourth order interaction term. However, the fact that the full fermionic path integral cannot (yet) be performed exactly remains a problem. Another possibility for improving the results is to search for an approximation of the bosonic path integral where all "forbidden terms" that are taken into account cancel each other.

At this moment, the use of a modified interaction potential is the best solution available for including the exchange interactions when approximating the bosonic path integral after the Hubbard-Stratonovich transformation for a general interaction potential. Even though it is not exact, it is still possible that this treatment is a reasonably good approximation to the physics of the system. This can only be revealed by comparison with future experimental results.

The agreement between theory and experiment may depend on the basis used in the analysis. In position space, particles are regarded as perfectly localized. In momentum space, particles are regarded as unlocalized waves. As the de Broglie wavelength λ_{dB} is relatively large in experiments with ultracold atomic gases, it may be more accurate to consider the particles as waves in momentum space. A starting point for such an analysis is given in appendix A.

Part IV Conclusion

Chapter 9

Conclusion

The goal of this dissertation was to improve the theoretical description of itinerant ferromagnetism in the context of ultracold atomic gases. This goal was met in several steps.

In **part II**, itinerant ferromagnetism is studied in a two-component or (pseudo)spin-1/2 Fermi gas with contact interactions.

In **chapter 4**, the thermodynamic grand potential of a two-component Fermi gas with contact interactions was calculated in the saddle-point approximation of the path-integral formalism. Central to this description is the Hubbard-Stratonovich transformation, which is used to convert the fourthorder interaction term into terms of second order in the fermionic fields, at the cost of introducing an extra path integral over an auxiliary bosonic field. The choice of this bosonic field determines the physics included in the saddle-point approximation. In order to describe itinerant ferromagnetism, the Hartree channel was chosen and two density fields (one for each component) were introduced in the transformation. In the saddle-point approximation, the bosonic fields are assumed to be constant and their value is determined by extremizing the thermodynamic grand potential. Finally, it was shown in the zero-temperature limit that the results of the mean-field Stoner model are recovered.

In chapter 5, it was shown that none of the solutions to the saddle-point equations are minima of the thermodynamic grand potential, meaning that they are unstable to small density fluctuations. However, the meaning of this instability was still unclear.

In **part III**, itinerant ferromagnetism is studied in a two-component or (pseudo)spin-1/2 Fermi gas with a general form of the interaction potentials.

In chapter 6, the thermodynamic grand potential of a two-component Fermi gas with general interaction potentials was calculated in the saddle-point approximation of the path-integral formalism. Three different interaction potentials were used: one for interactions between two particles of opposite (pseudo)spin states and two for interactions between particles of the same (pseudo)spin state. In analogy to the calculation for contact interactions in chapter 4, two density fields (one for each component) were used to construct a Hubbard-Stratonovich transformation for the interaction terms. Before the transformation, the Pauli exclusion principle is automatically included in the symmetry properties of the product of four Grassmann variables. I showed that after the transformation, terms forbidden by the Pauli principle do contribute to the bosonic path integral. The Pauli exclusion principle remains valid due to the fact that these "forbidden terms" cancel each other when taking the full bosonic path integral. However, the bosonic path integral cannot be calculated exactly for a general case and it is no longer guaranteed that the Pauli exclusion principle will be included when the bosonic path integral is approximated. In order to ensure that the "forbidden" terms do not contribute to the approximated bosonic path integral, I proposed to explicitly enforce the Pauli exclusion principle through a modification of the interaction potential. In the saddle-point approximation, only three relevant interaction parameters remain: one for each interaction potential, each one equal to the corresponding modified interaction potential integrated over the volume.

In chapter 7, a stability analysis of the solutions to the saddle-point equations was performed in the example most relevant to itinerant ferromagnetism: equal chemical potentials and equal intracomponent interaction potentials in 3D. When the interactions become too strong, all saddle points become unstable to density fluctuations. This strongly limits the itinerant ferromagnetic region in the phase diagram. Furthermore, mid-to-long ranged net attractive intracomponent interactions are needed in order to dynamically stabilize the gas.

In chapter 8, implicit assumptions and approximations made in the choice of the action, the choice of the density fluctuations, the choice of the ensemble, the choice of the channel in the Hubbard-Stratonovich transformation and the choice of the basis (e.g. the position or momentum basis) were discussed, with special attention to the implications for the validity of the results from chapters 6 and 7. The main result is that the newly proposed method for implementing the Pauli exclusion principle in the Hubbard-Stratonovich transformation is not exact, as an interaction potential does not Fourier transform in the same way as a product of fermionic Grassmann fields. The use of the modified interaction potential still has to be validated by comparison with future experiments.

To summarize, there are four important results of this dissertation:

- 1. When approximating the bosonic path integral after the Hubbard-Stratonovich transformation, it is no longer guaranteed that the Pauli exclusion principle is correctly included.
- 2. A new approximate method was proposed, in order to enforce the Pauli exclusion principle explicitly through a modification of the interaction potential.
- 3. The results obtained with this new method in the saddle-point approximation suggest that stability against density fluctuations is an important factor to take into account when studying itinerant ferromagnetism, as it greatly limits the itinerant ferromagnetic region in the phase diagram. This may help explain why itinerant ferromagnetism is so notoriously hard to find experimentally.
- 4. The use of a modified interaction potential is not an exact implementation of the Pauli exclusion principle.

Furthermore, in the conditions where itinerant ferromagnetism is expected to occur (strong repulsive intercomponent interactions at low temperatures) many different physical effects compete (e.g. magnetic domain formation, superfluid pairing, crystallization,...), which makes itinerant ferromagnetism very sensitive to modeling bias. That is why the model proposed in this dissertation is by no means final, but only a first step in the creation of better models for itinerant ferromagnetism in particular and the exchange interactions in general.

Publications

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Appendix A

Saddle-point grand potential in momentum space

A.1 The Hubbard-Stratonovich transformation

Expressed in the momentum basis, the action (6.1) is given by eq. (8.3),

$$S\left[\bar{\psi}_{\sigma},\psi_{\sigma}\right] = \sum_{\sigma=\uparrow,\downarrow} \sum_{k} \bar{\psi}_{\sigma,k} \left(-i\omega_{n} + \mathbf{k}^{2} - \mu_{\sigma}\right) \psi_{\sigma,k} + \frac{1}{2} \frac{1}{\beta\sqrt{V}} \sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow} \sum_{k,k',Q} g_{\sigma_{1}\sigma_{2}}\left(\mathbf{Q}\right) \bar{\psi}_{\sigma_{1},k} \psi_{\sigma_{1},k-Q} \bar{\psi}_{\sigma_{2},k'} \psi_{\sigma_{2},k'+Q}.$$
(A.1)

In the momentum basis, a Hubbard-Stratonovich transformation can be constructed in the Hartree channel using $\bar{\psi}_{\sigma_1,k}\psi_{\sigma_1,k-Q}$ and $\bar{\psi}_{\sigma_2,k'}\psi_{\sigma_2,k'+Q}$ as reference fields (in analogy to the construction of the Hubbard-Stratonovich transformation in the position basis in Sec. 4.2 and Sec. 6.2). Because these reference fields are not equal to their complex conjugates, it is no longer possible to use real (instead of complex) bosonic fields. The resulting transformation is given by

$$\exp\left[-\frac{1}{2}\frac{1}{\beta\sqrt{V}}\sum_{k,k',Q}\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow}g_{\sigma_{1}\sigma_{2}}\left(\mathbf{Q}\right)\bar{\psi}_{\sigma_{1},k}\psi_{\sigma_{1},k-Q}\bar{\psi}_{\sigma_{2},k'}\psi_{\sigma_{2},k'+Q}\right]$$

$$=\frac{1}{Z_{\rho}}\left(\prod_{\sigma}\int \mathcal{D}\bar{\rho}_{\sigma}\int \mathcal{D}\rho_{\sigma}\right)\exp\left(\frac{1}{\beta\sqrt{V}}\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow}\sum_{k,k',Q}\frac{g_{\sigma_{1}\sigma_{2}}'\left(Q,k,k'\right)}{4}\right)$$

$$\times\left\{\bar{\rho}_{\sigma_{1}}\left(k-Q,k\right)\rho_{\sigma_{2}}\left(k',k'+Q\right)+\rho_{\sigma_{1}}\left(k,k-Q\right)\bar{\rho}_{\sigma_{2}}\left(k'+Q,k'\right)\right)$$

$$-\left[\bar{\rho}_{\sigma_{1}}\left(k-Q,k\right)\rho_{\sigma_{1}}\left(k,k-Q\right)\right]\bar{\psi}_{\sigma_{2},k'}\psi_{\sigma_{2},k'+Q}$$

$$-\bar{\psi}_{\sigma_{1},k}\psi_{\sigma_{1},k-Q}\left[\bar{\rho}_{\sigma_{2}}\left(k'+Q,k'\right)+\rho_{\sigma_{2}}\left(k',k'+Q\right)\right]\right\}\right),$$
(A.2)

where $g'_{\sigma_1\sigma_2}(Q,k,k')$ is the modified interaction potential as defined in eq. (8.4),

$$g_{\sigma_{1}\sigma_{2}}'\left(Q,k,k'\right) = g_{\sigma_{1}\sigma_{2}}\left(\mathbf{Q}\right)\left\{1 - \delta_{\sigma_{1},\sigma_{2}}\left[\delta_{1}\left(k-k'\right) + \delta_{1}\left(Q - \frac{k-k'}{2}\right)\right] - \delta_{1}\left(k-k'\right)\delta_{1}\left(Q - \frac{k-k'}{2}\right)\right]\right\}.$$
(A.3)

In contrast to position space where only one position coordinate suffices, two momentum coordinates remain in the definition of ρ_{\uparrow} and ρ_{\downarrow} in momentum space. Due to this fact, the bosonic fields ρ_{\uparrow} , $\bar{\rho}_{\uparrow}$, ρ_{\downarrow} and $\bar{\rho}_{\downarrow}$ from eq. (A.2) can no longer be interpreted as density fields. They are closer related to first order correlation functions, which express the likelihood of a particle to propagate from one state to another.

A.2 Fermionic path integral

After the Hubbard-Stratonovich transformation, the partition sum can be rewritten in terms of an effective action,

$$\mathcal{Z} = \left(\prod_{\sigma=\uparrow,\downarrow} \int \mathcal{D}\bar{\psi}_{\sigma} \int \mathcal{D}\psi_{\sigma} \int \mathcal{D}\bar{\rho}_{\sigma} \int \mathcal{D}\rho_{\sigma}\right) \exp\left(-S_{eff}\left[\bar{\psi}_{\sigma},\psi_{\sigma},\bar{\rho}_{\sigma},\rho_{\sigma}\right]\right),\tag{A.4}$$

$$S_{eff} \left[\bar{\psi}_{\sigma}, \psi_{\sigma}, \bar{\rho}_{\sigma}, \rho_{\sigma} \right] = \sum_{\sigma=\uparrow,\downarrow} \sum_{k} \bar{\psi}_{\sigma,k} \left(-i\omega_{n} + \mathbf{k}^{2} - \mu_{\sigma} \right) \psi_{\sigma,k} - \frac{1}{\beta\sqrt{V}} \sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow} \sum_{k,k',Q} \frac{g'_{\sigma_{1}\sigma_{2}}(Q,k,k')}{4} \bar{\rho}_{\sigma_{1}} \left(k - Q,k \right) \rho_{\sigma_{2}} \left(k',k' + Q \right) - \frac{1}{\beta\sqrt{V}} \sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow} \sum_{k,k',Q} \frac{g'_{\sigma_{1}\sigma_{2}}(Q,k,k')}{4} \rho_{\sigma_{1}} \left(k,k-Q \right) \bar{\rho}_{\sigma_{2}} \left(k' + Q,k' \right) + \frac{1}{\beta\sqrt{V}} \sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow} \sum_{k,k',Q} \frac{g'_{\sigma_{1}\sigma_{2}}(Q,k,k')}{4} \left[\bar{\rho}_{\sigma_{1}} \left(k - Q,k \right) + \rho_{\sigma_{1}} \left(k,k-Q \right) \right] \bar{\psi}_{\sigma_{2},k'}\psi_{\sigma_{2},k'} + Q + \frac{1}{\beta\sqrt{V}} \sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow} \sum_{k,k',Q} \frac{g'_{\sigma_{1}\sigma_{2}}(Q,k,k')}{4} \bar{\psi}_{\sigma_{1},k}\psi_{\sigma_{1},k-Q} \left[\bar{\rho}_{\sigma_{2}} \left(k' + Q,k' \right) + \rho_{\sigma_{2}} \left(k',k' + Q \right) \right].$$
(A.5)

In order to perform the fermionic path integral, the effective action still needs to be rewritten. The second term of (A.5) can be shown to be equal to the third term using $\sigma_1 \leftrightarrow \sigma_2$, $k \leftrightarrow k'$, $Q \rightarrow -Q$ and $g'_{\sigma_1\sigma_2}(-Q,k,k') = g'_{\sigma_1\sigma_2}(Q,k,k')$. With the same coordinate transformation, it can be shown that the fourth term of (A.5) is equal to the fifth term. Finally, all terms can be rewritten using the coordinate transformation $k_1 = k$, $k_2 = k - Q$ and $k_3 = k'$. The effective action is then given by

$$S_{eff} \left[\bar{\psi}_{\sigma}, \psi_{\sigma}, \bar{\rho}_{\sigma}, \rho_{\sigma} \right] = \sum_{\sigma_{1}=\uparrow,\downarrow} \sum_{k_{1},k_{2}} \bar{\psi}_{\sigma_{1},k_{1}} \left[-G_{\sigma_{1}}^{-1} \left(k_{1}, k_{2} \right) \right] \psi_{\sigma_{1},k_{2}}$$

$$- \frac{1}{\beta \sqrt{V}} \sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow} \sum_{k_{1},k_{2},k_{3}} \frac{g_{\sigma_{1}\sigma_{2}}' \left(\Delta k, k_{1}, k_{3} \right)}{2} \bar{\rho}_{\sigma_{1}} \left(k_{2}, k_{1} \right) \rho_{\sigma_{2}} \left(k_{3}, k_{3} + \Delta k \right)$$
(A.6)

with $\Delta k = k_1 - k_2$ and

$$-G_{\sigma_{1}}^{-1}(k_{1},k_{2}) = \left(-i\omega_{n_{1}} + \mathbf{k}_{1}^{2} - \mu_{\sigma_{1}}\right)\delta\left(\Delta k\right)$$

$$+\sum_{\sigma_{2}=\uparrow,\downarrow}\sum_{k_{3}}\frac{1}{\beta\sqrt{V}}\frac{g_{\sigma_{1}\sigma_{2}}'\left(\Delta k,k_{1},k_{3}\right)}{2}\left[\bar{\rho}_{\sigma_{2}}\left(k_{3}+\Delta k,k_{3}\right) + \rho_{\sigma_{2}}\left(k_{3},k_{3}+\Delta k\right)\right].$$
(A.7)

After performing the fermionic path integral, the partition sum becomes

$$\mathcal{Z} = \prod_{\sigma=\uparrow,\downarrow} \left(\int \mathcal{D}\bar{\rho}_{\sigma} \int \mathcal{D}\rho_{\sigma} \right) \exp\left(\sum_{\sigma_{1}=\uparrow,\downarrow} \operatorname{Tr}_{k_{1},k_{2}} \left\{ \ln\left[-G_{\sigma_{1}}^{-1}\left(k_{1},k_{2}\right) \right] \right\} + \frac{1}{\beta V} \sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow} \sum_{k_{1},k_{2},k_{3}} \frac{\sqrt{V}g_{\sigma_{1}\sigma_{2}}'\left(\Delta k,k_{1},k_{3}\right)}{2} \bar{\rho}_{\sigma_{1}}\left(k_{2},k_{1}\right) \rho_{\sigma_{2}}\left(k_{3},k_{3}+\Delta k\right) \right).$$
(A.8)

A.3 Saddle-point approximation

The bosonic path integral in eq. (A.8) has to be approximated. In this case, I choose a saddle-point approximation within the assumption that only interactions with $\Delta k = Q = 0$ contribute,

$$\begin{cases} \bar{\rho}_{\sigma}(k,k') = \beta V \delta_{k,k'} \rho_{\sigma}^{*}(k) \\ \rho_{\sigma}(k,k') = \beta V \delta_{k,k'} \rho_{\sigma}(k) \end{cases}$$
(A.9)

This is a reasonable approximation in ultracold atomic gases, where interactions with low momentum exchange are dominant. Note that the function $\rho_{\sigma}(k)$ is not equal to the Fourier transformed density function in position space from chapter 6. Here, $\rho_{\sigma}(k)$ corresponds to a density in momentum space. After the saddle-point approximation, the thermodynamic grand potential is given by

$$\Omega_{sp} \left[\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\uparrow}\left(k\right), \rho_{\downarrow}\left(k\right)\right] = -\sum_{\sigma_{1}, \sigma_{2}=\uparrow, \downarrow} \sum_{k_{1}, k_{3}} \frac{\sqrt{V}g_{\sigma_{1}\sigma_{2}}\left(\mathbf{0}\right) \left[1 - \delta_{\sigma_{1}, \sigma_{2}}\delta_{1}\left(k_{1} - k_{3}\right)\right]}{2} \rho_{\sigma_{1}}^{*}\left(k_{1}\right) \rho_{\sigma_{2}}\left(k_{3}\right) \\
- \frac{1}{\beta V} \sum_{k_{1}} \ln \left\{-i\omega_{n_{1}} + \mathbf{k}_{1}^{2} - \mu_{\sigma_{1}} + \sum_{\sigma_{2}=\uparrow, \downarrow} \sum_{k_{3}} \sqrt{V}g_{\sigma_{1}\sigma_{2}}'\left(0, k_{1}, k_{3}\right) \operatorname{Re}\left[\rho_{\sigma_{2}}\left(k_{3}\right)\right]\right\}, \quad (A.10)$$

$$g_{\sigma_{1}\sigma_{2}}'\left(0, k_{1}, k_{3}\right) = g_{\sigma_{1}\sigma_{2}}\left(\mathbf{0}\right) \left[1 - \delta_{\sigma_{1}, \sigma_{2}}\delta_{1}\left(k_{1} - k_{3}\right)\right]. \quad (A.11)$$

This can be rewritten using $g_{\sigma_1\sigma_2} = \sqrt{V} g_{\sigma_1\sigma_2}(\mathbf{0})$ and the fact that the total particle density ρ_{σ} of spin state σ is given by

$$\rho_{\sigma} = \sum_{k} \rho_{\sigma} \left(k \right) = \sum_{k} \rho_{\sigma}^{*} \left(k \right) = \sum_{k} \operatorname{Re} \left[\rho_{\sigma} \left(k \right) \right].$$
(A.12)

The result is given by

$$\Omega_{sp}\left[\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}\left(k\right),\rho_{\downarrow}\left(k\right)\right] = -\frac{1}{2}\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow}g_{\sigma_{1}\sigma_{2}}\rho_{\sigma_{1}}\rho_{\sigma_{2}} + \frac{1}{2}\sum_{\sigma=\uparrow,\downarrow}g_{\sigma\sigma}\left\{\sum_{k}\operatorname{Re}\left[\rho_{\sigma}\left(k\right)\right]^{2}\right\} + \frac{1}{2}\sum_{\sigma=\uparrow,\downarrow}g_{\sigma\sigma}\left\{\sum_{k}\operatorname{Im}\left[\rho_{\sigma}\left(k\right)\right]^{2}\right\} - \frac{1}{\beta V}\sum_{\sigma_{1}=\uparrow,\downarrow}\sum_{k}\ln\left\{-i\omega_{n}+\mathbf{k}^{2}+g_{\sigma_{1}\sigma_{1}}\operatorname{Re}\left[\rho_{\sigma_{1}}\left(k\right)\right]-\mu_{\sigma_{1}}'\right\}$$
(A.13)

with the effective chemical potential

$$\mu'_{\sigma_1} = \mu_{\sigma_1} - \sum_{\sigma_2 = \uparrow, \downarrow} g_{\sigma_1 \sigma_2} \rho_{\sigma_2} \tag{A.14}$$

defined in a similar way as in eq. (6.39). The imaginary parts of $\rho_{\sigma}(k)$ are isolated in a separate term of $\Omega_{sp}[\beta, \mu_{\uparrow}, \mu_{\downarrow}; \rho_{\uparrow}(k), \rho_{\downarrow}(k)]$, so they can be removed by shifting the zero point of the thermodynamic grand potential. If we rename Re $[\rho_{\sigma}(k)]$ to $\rho_{\sigma}(k)$, which are now real instead of complex functions of k,

$$\Omega_{sp}\left[\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}\left(k\right),\rho_{\downarrow}\left(k\right)\right] = -\frac{1}{2}\sum_{\sigma_{1},\sigma_{2}=\uparrow,\downarrow}g_{\sigma_{1}\sigma_{2}}\rho_{\sigma_{1}}\rho_{\sigma_{2}} + \frac{1}{2}\sum_{\sigma=\uparrow,\downarrow}g_{\sigma\sigma}\left[\sum_{k}\rho_{\sigma}^{2}\left(k\right)\right] \\ -\frac{1}{\beta V}\sum_{\sigma_{1}=\uparrow,\downarrow}\sum_{k}\ln\left[-i\omega_{n}+\mathbf{k}^{2}+g_{\sigma_{1}\sigma_{1}}\rho_{\sigma_{1}}\left(k\right)-\mu_{\sigma_{1}}'\right].$$
(A.15)

The saddle-point thermodynamic grand potential $\Omega_{sp}(\beta, \mu_{\uparrow}, \mu_{\downarrow})$ can then be found by solving the saddle-point equations

$$\frac{\partial\Omega_{sp}\left[\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\uparrow}\left(k\right),\rho_{\downarrow}\left(k\right)\right]}{\partial\rho_{\sigma}\left(k'\right)}\Big|_{\beta,\mu_{\uparrow},\mu_{\downarrow};\rho_{\sigma}\left(k\right) \text{ with } k\neq k',\rho_{-\sigma}\left(k\right)} = 0.$$
(A.16)

This is an infinite set of equations, with one equation for each value of k' per spin state σ . All these equations have to be solved self-consistently and together with the number equation for the total density $n = n_{\uparrow} + n_{\downarrow}$, with

$$n_{\sigma} = -\left. \frac{\partial \Omega_{sp} \left(\beta, \mu_{\uparrow}, \mu_{\downarrow}\right)}{\partial \mu_{\sigma}} \right|_{\beta, \mu_{-\sigma}}.$$
(A.17)

There are many similarities between the saddle-point thermodynamic grand potential (6.38) in position space and (A.15) in momentum space, but also several important differences. The terms with ρ_{σ} are identical in both expressions, apart from the fact that the interaction constants in eq. (A.15) are related to the true interaction potential, while the interaction constants in eq. (6.38) are related to the modified interaction potential in position space. Instead, in eq. (A.15) the exchange contributions appear as an extra term

$$\frac{1}{2} \sum_{\sigma=\uparrow,\downarrow} g_{\sigma\sigma} \left[\sum_{k} \rho_{\sigma}^{2} \left(k \right) \right]$$
(A.18)

in the interaction energy and a modification $g_{\sigma_1\sigma_1}\rho_{\sigma_1}(k)$ of the dispersion relation.

Due to the remaining k-dependence in $\rho_{\uparrow}(k)$ and $\rho_{\downarrow}(k)$, it becomes much harder to solve the saddle-point equations in momentum space than in position space (let alone study the stability of the saddle points). That is why this calculation has not been attempted in this dissertation, but it remains an interesting future research avenue.

Nederlandstalige samenvatting

Achtergrond

Itinerant ferromagnetisme is spontane polarisatie van niet-gelokaliseerde deeltjes, oftewel ferromagnetisme in een gas. In een spin-1/2 Fermi gas wordt het verwacht bij sterk repulsieve interacties tussen de deeltjes. Het Pauli uitsluitingsprincipe van de kwantummechanica stelt dat twee fermionen zich niet in dezelfde toestand kunnen bevinden. Door dit uitsluitingsprincipe kunnen deeltjes met dezelfde spintoestand "minder dicht" bij elkaar komen dan deeltjes met tegengestelde spintoestand. Indien de interacties op korte dracht repulsief zijn, is de interactie energie het laagst als alle deeltjes zich in dezelfde spintoestand bevinden. Dit kost echter kinetische energie, omdat dezelfde fermionen door het uitsluitingsprincipe in een spin-gepolariseerd gas in hogere energietoestanden gestapeld moeten worden dan in een ongepolariseerd gas. Indien de repulsieve interacties voldoende sterk zijn, treedt spontane polarisatie of itinerant ferromagnetisme op.

Itinerant ferromagnetisme werd voor het eerst voorgesteld door F. Bloch, die in 1929 aantoonde dat een vrij elektronengas (met homogene positieve achtergrond) bij grote dichtheden itinerant ferromagnetisch kan worden. Sindsdien is uitgebreid gezocht naar deze toestand, maar het blijkt onverwacht moeilijk om deze toestand experimenteel te realiseren. Itinerant ferromagnetisme komt voor in bepaalde ferromagnetische materialen waarvan de conductieband vlak genoeg is om de elektronen erin als vrij te beschouwen (bv. d-band transitiemetalen zoals ijzer, nikkel en kobalt). In deze materialen zijn er echter ook sterke aanwijzingen voor ferromagnetisme van gelokaliseerde elektronen.

Aangezien itinerant ferromagnetisme voor zover bekend niet in pure vorm voorkomt in de context van vastestoffysica, wordt er nu gezocht of deze toestand in andere systemen gerealiseerd kan worden. Ultrakoude atomaire gassen werden voorgesteld als een potentieel systeem voor de experimentele realisatie van itinerant ferromagnetisme. Ultrakoud betekent dat de atomen zodanig zijn afgekoeld dat hun *de Broglie* golflengte vergelijkbaar wordt met de interatomaire afstand. In dit regime worden kwantum effecten macroscopisch. De typische temperaturen waarbij de experimenten plaatsvinden zijn van de orde van μ K of 100 nK. Bij deze temperaturen moet het gas in een magnetische of optische val gevangen worden gehouden, omdat het drastisch zou opwarmen bij het raken van een wand.

Ultrakoude atomaire gassen hebben een aantal grote voordelen. Ze zijn experimenteel zeer goed te controleren: het aantal deeltjes per (pseudo)spintoestand, de geometrie van de opsluitingspotentiaal en de interactiesterkte kunnen nauwkeurig aangepast worden. In de context van itinerant ferromagnetisme zijn dat zeer belangrijke factoren. Ten eerste kan de aanwezigheid van een onderliggende periodische potentiaal uitgesloten worden, wat onmogelijk is in een conventionele vaste stof met kristalrooster. Ten tweede kan de interactiesterkte via Feshbach resonanties gewijzigd worden door de sterkte van een extern aangelegd homogeen magnetisch veld aan te passen. Hierdoor kan itinerant ferromagnetisme als functie van de interactiesterkte bestudeerd worden.

De aanpasbaarheid van de interacties heeft echter één groot nadeel: de repulsieve tak van de Feshbach resonantie is instabiel. Bij sterk repulsieve interacties worden drie-deeltjes interacties resonant versterkt. Deze interacties produceren diatomaire moleculen die uit de val kunnen ontsnappen, wat de levensduur van het experiment sterk beperkt.

In 2009 werden de sterke repulsieve interacties waarbij itinerant ferromagnetisme wordt verwacht voor het eerst experimenteel gerealiseerd door de onderzoeksgroep van Wolfgang Ketterle aan MIT (Cambridge, VS). Er werd echter geen itinerant ferromagnetisme gevonden: moleculaire paring domineerde het experiment en zorgde ervoor dat er geen evenwichtstoestand gevormd kon worden. Dit voorkwam dus ook de vorming van magnetische domeinen. Het feit dat itinerant ferromagnetisme tot nu toe nog niet experimenteel gerealiseerd werd is een belangrijke indicatie dat de theorie ervan verbeterd moet worden. Dat is dan ook de inspiratie en het doel van deze doctoraatsthesis: het verbeteren van de beschrijving van itinerant ferromagnetisme in de context van ultrakoude quantum gassen. Dit is een heel uitdagende opdracht, omdat itinerant ferromagnetisme gepaard gaat met sterke interacties en correlaties die zeer moeilijk theoretisch te beschrijven zijn.

Om dit probleem aan te pakken, ben ik terug gegaan naar de basistheorie van itinerant ferromagnetisme in het padintegraalformalisme. Meer specifiek heb ik bestudeerd hoe de interacties worden behandeld in de padintegraalbeschrijving van itinerant ferromagnetisme en hoe deze behandeling van de interacties verbeterd kan worden.

Contact interacties

In het eerste deel van mijn doctoraatsonderzoek heb ik gekeken naar de behandeling van contact interacties. Door de koude temperaturen is enkel de s-golf verstrooiingslengte tussen deeltjes met een verschillende (pseudo)spin toestand belangrijk in de meeste experimenten met ultrakoude gassen. Aangezien de dracht van de interatomaire (Van der Waals) interacties in ultrakoude gassen veel korter is dan de andere relevante lengteschalen in het experiment, is het vaak een goede aanname om de interatomaire potentiaal te beschrijven als een contact potentiaal met dezelfde s-golf verstrooiingslengte.

In hoofdstuk 4 heb ik de (groot-canonische) vrije energie van het gas in de zadelpuntsbenadering berekend. Om deze vrije energie te berekenen werd eerst de groot-canonische toestandssom van het gas bepaald, die in het padintegraal formalisme gelijk is aan een gewogen som over alle mogelijke configuraties van de fermionische velden. De gewichtsfactor is gerelateerd aan de klassieke actie van elke specifieke veldconfiguratie. De interactie term in de actie is van vierde orde in de fermionische velden, maar we kunnen enkel fermionische padintegralen met een actie van tweede orde in de fermionische velden exact uitrekenen. Om dit probleem te omzeilen, wordt de Hubbard-Stratonovich transformatie gebruikt.

De Hubbard-Stratonovich transformatie zet de vierde orde interactie term om in termen van tweede orde in de fermionische velden. De prijs die we hiervoor betalen is het invoeren van een extra padintegraal over een bosonisch hulpveld, dat als drager van de interacties optreedt. Na de transformatie kan de fermionische padintegraal exact uitgerekend worden. De bosonische padintegraal moet daarna echter nog benaderd worden. In deze thesis hebben we gekozen voor de zadelpuntsbenadering, waarbij we aanemen dat het bosonisch veld een constante waarde heeft. Deze waarde wordt bepaald door het zoeken van extrema (bij voorkeur minima) van de zadelpunt vrije energie.

Er zijn verschillende manieren om het bosonische veld in te voegen, die telkens na benadering een andere betekenis of interpretatie aan het bosonische veld geven. Om itinerant ferromagnetisme te beschrijven werd gebruik gemaakt van bosonische dichtheidsvelden (ook wel het Hartree kanaal genoemd). Dit resulteert in een extra interactieterm in de zadelpunt vrije energie en een verschuiving van de effectieve chemische potentiaal. Vervolgens werd aangetoond dat dit bij temperatuur nul leidt tot het gekende Stoner criterium $a_s k_F > \pi/2$ voor itinerant ferromagnetisme (met a_s de s-golf verstrooiingslengte en k_F de Fermi golfvector).

Tot slot heb ik in hoofdstuk 5 aangetoond dat geen van de extrema van de zadelpunt vrije energie minima zijn. Dit betekent dat deze extrema instabiel zijn t.o.v. dichtheidsfluctuaties en dat ze dus niet corresponderen met een metastabiele toestand van het gas. Het was echter nog onduidelijk wat deze instabiliteit betekent: is itinerant ferromagnetisme niet stabiel in een spin-1/2 Fermi gas met contact interacties? Of is er iets anders aan de hand? Is het gebruik van contact interacties wel een goede aanname bij het bestuderen van itinerant ferromagnetisme? Om deze vragen te beantwoorden heb ik het gebruikte formalisme in het volgende onderdeel van deze thesis uitgebreid naar algemene interactiepotentialen. Dit is extra relevant in het licht van de nieuwe interactiepotentialen die momenteel experimenteel verkend worden in ultrakoude gassen: dipool interacties en p-golf Feshbach resonanties.

Algemene interactiepotentialen

In hoofdstuk 6 werd het formalisme uit hoofdstuk 4 uitgebreid naar algemene interactiepotentialen. In de praktijk betekent dit dat er drie interactiepotentialen nodig zijn: één voor interacties tussen deeltjes van verschillende (pseudo)spintoestanden en twee voor interacties tussen deeltjes van dezelfde (pseudo)spintoestand (één per spintoestand). Bij het opstellen van de Hubbard-Stratonovich transformatie ontdekte ik dat het Pauli uitsluitingsprincipe niet meer in elke afzonderlijke term van de bosonische padintegraal voldaan is. Zolang de volledige bosonische padintegraal wordt genomen is er geen probleem, omdat de termen die geassocieerd zijn met interacties die verboden zijn door het Pauli uitsluitingsprincipe elkaar opheffen. Zodra de bosonische padintegraal benaderd wordt is het echter niet meer zeker dat het Pauli uitsluitingsprincipe nog voldaan is. Dit is een groot probleem bij het bestuderen van itinerant ferromagnetisme, waar het correct meenemen van het Pauli uitsluitingsprincipe essentieel is.

Om dit probleem op te lossen heb ik voorgesteld om de verboden termen artificieel uit te sluiten van de sommatie over de bosonische veldconfiguraties door het invoegen van een gemodificeerde interactiepotentiaal. Vervolgens heb ik deze methode gebruikt om de vrije energie te berekenen in de zadelpuntsbenadering. Analoog aan de resultaten in hoofdstuk 4, zorgden de interacties in het Hartree kanaal voor een extra interactieterm in de zadelpunt vrije energie en een verschuiving van de effectieve chemische potentiaal.

In de zadelpuntsbenadering zijn er slechts drie parameters nodig om het effect van de interacties te beschrijven: één per interactiepotentiaal. Voor interacties tussen deeltjes van verschillende spintoestanden is deze parameter gelijk aan de corresponderende interactiepotentiaal geïntegreerd over het volledige volume. Voor interacties tussen deeltjes van dezelfde spintoestand is deze parameter gelijk aan de corresponderende gemodificeerde interactiepotentiaal geïntegreerd over het volledige volume. Deze parameters houden dus rekening met de uitsluiting van bepaalde interacties tussen deeltjes van dezelfde spintoestand.

In hoofdstuk 7 werden de stabiliteit en de polarisatie van de extrema van de zadelpunt vrije energie geanalyseerd in de context van itinerant ferromagnetisme in 3D. Om polarisatie door andere oorzaken uit te sluiten, werden de twee interactieparameters voor interacties tussen deeltjes met dezelfde spintoestand gelijk gekozen. Verder werd ook de chemische potentiaal van de twee spintoestanden gelijk gekozen. Dit resulteerde in een aantal fasediagrammen bij verschillende temperaturen die als functie van de interactieparameters weergeven waar extrema met een bepaalde polarisatie stabiel zijn. Hieruit konden verschillende conclusies getrokken worden:

- Als de interacties te sterk zijn of als de effectieve interacties tussen deeltjes van dezelfde spintoestand repulsief zijn, worden dichtheidsfluctuaties belangrijk en zijn geen van de extrema van de zadelpunt vrije energie stabiel. In dat regime is de opgestelde beschrijving dus geen geldige beschrijving en daarom kunnen we binnen dit formalisme ook geen uitspraken doen over wat er daar gebeurt.
- Volledig gepolariseerde extrema kunnen enkel stabiel zijn bij temperatuur nul. Bij lage temperatuur is er echter nog altijd een vergelijkbaar gebied met bijna-volledige polarisatie.
- Als de temperatuur toeneemt, wordt het stabiliteitsgebied voor ongepolariseerde extrema groter. De stabiele gepolariseerde extrema worden met toenemende temperatuur steeds minder gepolariseerd, tot ze worden opgeslokt door het groeiende ongepolariseerde gebied. De maximale polarisatie van de stabiele toestanden neemt af als functie van de temperatuur.
- De stabiliteitsgebieden voor gedeeltelijk en volledig gepolariseerde extrema is kleiner dan verwacht aan de hand van het Stoner criterium. Het Stoner criterium gaat enkel uit van de vraag of de gepolariseerde toestand een lagere energie heeft dan de ongepolariseerde toestand, wat leidt tot een ondergrens op de interactieparameters. De eis dat de itinerant ferromagnetische toestand ook dynamisch stabiel moet zijn zorgt voor een bovengrens op de interactieparameters. De interactieparameter tussen deeltjes van gelijke spintoestanden is bovendien essentieel voor de stabiliteit van de toestand.

In hoofdstuk 8 werd bekeken welke impliciete aannames en benaderingen er gemaakt werden in de voorgaande hoofdstukken, en in hoeverre deze geldig zijn. De belangrijkste conclusie is dat het gebruik van de gemodificeerde interactiepotentiaal niet exact is, omdat restricties opgelegd via een interactiepotentiaal in de positiebasis Fourier transformeren in extra vrijheden in de reciproke ruimte. Een eigenaardige eigenschap van de fermionische velden en het Pauli uitsluitingsprincipe is het feit dat restricties opgesteld in de positiebasis Fourier transformeren in equivalente restricties in de reciproke ruimte en omgekeerd. Het Pauli uitsluitingsprincipe is dus niet gelijk aan of equivalent met een interactiepotentiaal!

In hoofdstuk 6 werden de restricties in de gemodificeerde interactiepotentiaal opgelegd in de positie basis. In appendix A wordt de zadelpunt vrije energie afgeleid met de equivalente restricties in de reciproke ruimte. Aangezien de *de Broglie* golflengte van de atomen in ultrakoude gassen relatief groot is, is het mogelijk dat een analyse met vlakke golven in de reciproke ruimte een preciezere voorspelling oplevert voor de situatie in ultrakoude gassen. De prijs die we hiervoor betalen is dat we niet meer met gewone deeltjesdichtheden kunnen werken. Dit compliceert de minimalisatie en interpretatie van de zadelpunt vrije energie. Daarom werd deze analyse niet verder uitgewerkt tot fasediagrammen.

Conclusie

In deze doctoraatsthesis wordt een nieuwe methode voorgesteld om het Pauli uitsluitingsbeginsel expliciet mee te nemen in de Hubbard-Stratonovich transformatie en de daarop volgende benaderingen binnen het padintegraal formalisme. Deze methode werd toegepast om de stabiliteit van itinerant ferromagnetisme in 3D te bestuderen. Stabiliteit tegen dichtheidsfluctuaties is een belangrijke factor om in rekening te brengen bij het bestuderen van itinerant ferromagnetisme. Sterk repulsieve interacties tussen deeltjes van verschillende spintoestanden zijn noodzakelijk om itinerant ferromagnetische domeinen te vormen, maar bij te sterke interacties wordt deze toestand instabiel tegen dichtheidsfluctuaties. Dit beperkt het gebied waar itinerant ferromagnetisme verwacht wordt in het fasediagram als functie van temperatuur en interactieparameters.

Als finale opmerking zou ik willen meegeven dat itinerant ferromagnetisme zeer gevoelig is voor "modeling bias": indien men een model opstelt voor itinerant ferromagnetisme zal men de effecten meenemen die zorgen voor itinerant ferromagnetisme, maar vaak andere effecten weglaten die itinerant ferromagnetisme tegenwerken. In het sterk interagerend regime waar itinerant ferromagnetisme verwacht wordt treden veel verschillende effecten met elkaar in competitie. In de context van ultrakoude gassen is superfluïde paarvorming het belangrijkste. De methode voorgesteld in deze doctoraatsthesis is dus geen eindpunt, maar een tussenstap in de creatie van geavanceerdere modellen die hier rekening mee houden.

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