Studies of Universality in Strongly Interacting $^6$Li Fermi Gases with Bragg Spectroscopy

A thesis submitted for the degree of Doctor of Philosophy

by

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June 15, 2011
Declaration

I, Eva Dorothy Kuhnle, declare that this thesis entitled:

“Studies of Universality in Strongly Interacting $^6$Li Fermi Gases with Bragg Spectroscopy”

is my own work and has not been submitted previously, in whole or in part, in respect of any other academic award.

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Abstract

Universal relations for dilute, strongly interacting Fermi systems can be studied in ultracold fermionic $^6\text{Li}$ quantum gases using Bragg spectroscopy. Standard techniques of laser trapping and cooling of atoms are applied to evaporate fermionic gases below the critical temperature for superfluidity, $T_C$. The atoms are prepared to equally populate the lowest two spin states and the interaction between atoms of opposite spin is precisely tunable via a Feshbach resonance. A unitary Fermi gas represents a special case where the interactions are categorised as strong, that is, the range of interaction exceeds the range of the interatomic potential. Elastic collisions in the gas become unitarity limited and independent of details of the atomic properties. This universality is a property of unitary Fermi gases and the universal relations adequately describe the thermodynamic behaviour of these gases. The universal contact parameter is a central quantity that encapsulates the microscopic details of the system and varies with the temperature and interaction strength.

The principal topic of this thesis is the use of Bragg spectroscopy as a tool to measure the universal contact in trapped Fermi gases. The contact parameter quantifies the short-range pair correlation function according to a universal law. Inelastic Bragg scattering of photons allows one to measure the static structure factor, which is by definition the Fourier transform of the pair correlation function. Due to this well defined relation between the contact and Bragg spectra, the universal relation for the static structure factor is experimentally verified for a range of transferred momenta, $k/k_F = 3.5 - 9.1$, in agreement with the theoretical predictions. The contact in the zero-temperature limit at different interaction strengths as well as in the unitarity limit at different temperatures agrees well with the calculations. The contact at unitarity decreases monotonically for $T/T_F = 0 - 1$ but has a non-zero value well above the critical temperature $T_C \approx 0.2 T_F$. The contact parameter may offer new insights into criticality or complex superfluid pairing mechanisms such as pseudogap-pairing.
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Introduction

One of the most fundamental problems in physics is the many-body problem due to its relevance to a diverse range of systems. Microscopic details are the origin of bulk properties and the question is how these details influence the bulk properties. The many-body problem involves studies of the mutual interactions between particles in a dense system and how they contrast with the behaviour of isolated, noninteracting, and statistically distributed particles \[1\]. The resulting correlations between interacting particles lead to collective modes whose significance is due to the contribution of many particles.

Triggered by the discovery of superconducting mercury in 1911 \[2\], there has been considerable interest in fermionic superfluidity and superconductivity, an effect arising from many-body correlations. During the last 100 years, models of strongly correlated systems have been developed that have shaped our modern understanding of, for instance, the high-density electron gas found in solid-state devices \[3, 4\], Bardeen-Cooper-Schrieffer (BCS) superconductivity \[5\], neutron stars and nuclear structure (e.g. \[6–8\]), Bose-Einstein condensation \[9–11\], and dilute fermionic gases with arbitrary interactions of finite range \[12–16\]. Dilute Fermi gases with strong interactions are of broad interest, since their pairing behaviour forms a widely applicable paradigm.

The basic system considered here is a two-component Fermi gas of particles with opposite spin, interacting only through a short-range potential. As long as the gas is dilute and thermal, particles rarely collide and their motion is dictated by their kinetic energy. The macroscopic behaviour is then classical and may be described by classical gas laws found in standard textbooks. To reach quantum degeneracy the temperature has to be reduced below a critical temperature where the Fermi-Dirac statistics become pronounced \[17\]. The system would smoothly cross over from a classical gas to an ideal quantum gas if there was no interaction present. In practice, the cooling mechanism of the gas involves adiabatic rethermalisation through collisional processes for the particles in the two different quantum states. However, due to the Pauli exclusion principle the single state occupation number
in a single-component Fermi gas is restricted to one particle per spin state and the collisional cross section for particles with the same spin is strongly suppressed. Higher order collisional processes are also frozen out due to the low temperatures; thus only the lowest order collisional process for particles with different spin, the so-called s-wave scattering, is relevant. The pursuit of fermionic quantum degeneracy effects has led to the implementation of magnetic and optical traps that allow Fermi gases to be cooled by evaporation of atoms in two different spin states \[18\], or as two different isotopes \[19,20\] or as a mixture with Bose gases as refrigerants \[21,22\].

As a consequence of cooling, the kinetic energy diminishes and pairing effects start to play a significant role; however, the superfluid phase transition occurs only in the presence of interactions between spin-up and spin-down particles and the interaction energy facilitates the pairing of fermions of opposite spin. Well known examples of low temperature fermionic quantum superfluids are fermionic \(^3\)He \[23\], neutron stars \[8\] and superconductors \[5\]. In ultracold atomic gases, the scattering length, and hence the atomic interaction, can be tuned and enhanced with the help of Feshbach resonances \[24,25\]. Feshbach resonances are characterised by the two-body interaction and permit one to change the magnitude as well as the sign of the scattering length by simply varying an external magnetic field. Bosonic systems at a large scattering length are accompanied by inelastic processes and subsequent loss of atoms \[26\]; however, inelastic processes due to three-body losses are prohibited in fermionic systems by the Pauli principle leading to a greater stability and lifetime of the gas \[27–29\]. This advantage provides a testbed for investigating the variety of pairing processes in the well-known crossover from fermionic superfluidity, where the scattering length is small and negative \[30,31\], to the (molecular) Bose-Einstein condensation of pairs, where the scattering length is small and positive \[32–36\]. The scattering length diverges in the strongly interacting regime \[37,38\], often referred to as the unitarity regime, where elastic collisions are quantum mechanically limited. Experiments in the crossover region have been performed in which characteristic quantities \[35,39\] and signatures of superfluidity such as collective properties \[37,40,41\] and vortices \[42\] have been exploited. Since the first experimental investigations in this regime in 2004 \[31,35,36,41,43–45\], progress has been extremely rapid with studies of collective oscillations \[40,46,47\], universal behaviour \[48–52\], superfluidity \[42,53–56\], polarised Fermi gases \[52,57–61\] and the speed of sound \[62\].

The present work focuses on the resonant regime at unitarity rather than the whole crossover region. Strong interactions induce strong correlations of particles in this many-body system. Many theoretical methods break down when dealing with such strong correlations, as it is difficult to identify a small parameter appropriate
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for a perturbation analysis. However, the universality hypothesis assumes that the relevant length scale in the ground state at unitarity is the interparticle spacing $l = n^{-1/3}$, which is related to the density $n$ and is much larger than the range of the interatomic potential, $l \gg r_0$. Interactions at a short distance and with short-time dynamics dominate over microscopic details. For example, at unitarity ($a \to \infty$) the cross section reaches a constant value of $4\pi/k^2$, where $k$ is the relative momentum of the scattered atoms. Here, the many-body system becomes universal. This means in turn that all dilute fermionic systems with sufficiently strong interactions behave identically. For precisely this situation, exact universal relations have been derived that accurately describe the behaviour of the system in any state: few-body or many-body ground state, zero or nonzero temperature, homogeneous or inhomogeneous gas, normal or superfluid states, balanced or imbalanced spin states. A number of these relations were presented by Shina Tan but efforts have since been devoted to deriving these relations from other theoretical models or to deriving new relations. Tan showed that, in principle, the problem can be described by modifying the many-body Schrödinger wave function for the case of an ideal gas with an approximated contact interaction parameter. At the heart of these relations is a quantity, the so-called contact, $C$, which is a measure of the number of closely spaced fermions in two different spin states. The contact enters various properties such as thermodynamic variables or large-momentum and high-frequency tails of correlation functions. The contact is a key parameter which quantifies physical properties in the phase diagram of the BEC-BCS crossover; therefore measurements of the coupling and temperature dependence of the contact could be used to verify the Tan relations.

In this thesis, Tan’s pair-correlation function between spin-up ($\uparrow$) and spin-down ($\downarrow$) atoms plays a central role. It diverges as $C/r^2$ at short distances, $r_0 \ll r < 1/k_F$, where $k_F$ is the magnitude of the Fermi wave vector. Correlation functions are difficult to measure directly in ultracold gases; however, it is possible to measure macroscopic quantities which depend on correlation functions in a well defined way. By considering the pair-correlation function in Fourier space, one has two advantages: (1) The macroscopic measurable quantity is the static structure factor, $S(k)$, which is simply given by the Fourier transform of the pair-correlation function, and (2) pair-correlations in momentum space can be probed by Bragg spectroscopy. Inelastic scattering is a well established technique to probe both the dynamic and static structure factors of many-body quantum systems. Ultra-cold atoms are highly amenable to inelastic scattering through Bragg spectroscopy which has previously been used to determine both the dynamic and static structure factors of atomic Bose-Einstein condensates. In ultracold Fermi
gases Bragg spectroscopy has been used by our group to determine both the dynamic and static structure factors over the BEC-BCS crossover, albeit at a single momentum \[ k_0 \]. The inverse healing length determines the border between the high momentum regime of single-particle excitations and the low momentum regime of collective excitations, such as phonons or the Bogoliubov-Anderson mode \[ \text{[81]} \]. Relevant to the Tan relations is the high momentum limit \( k \gg k_F \), where the pair momentum distribution is inevitably linked to the contact \( n_{\uparrow\downarrow}(k) \rightarrow C/k^4 \) and the static structure factor becomes \[ \text{[82]} \]

\[
S_{\uparrow\downarrow}(k \gg k_F) = \frac{C}{nk_F} \left[ 1 - \frac{4}{\pi k_F a} \right].
\]  

(1)

The experimental verification of this exact and universal relation is the subject of this thesis. It enables one to show the interaction dependence of the contact. In addition, for the special case at unitarity, \( a \rightarrow \infty \), the temperature dependence of the contact is determined. The measurements are compared to new calculations of the contact based on strong coupling theory \[ \text{[83]-[85]} \]. The ability to vary the momentum over a wide range differentiates Bragg spectroscopy from radio-frequency spectroscopy, thus providing access to a broad range of the excitation spectrum and avoiding final state interaction effects as no third atomic state is involved \[ \text{[56],[86]} \].

**Thesis outline**

Understanding unitary Fermi gases requires knowledge of the mechanisms causing the strong interactions as well as the associated thermodynamics. Therefore, starting with some theoretical background, chapter 1 recalls the basic scattering physics required to understand the role of strong interactions in ultracold Fermi gases. The BEC-BCS crossover provides a testbed to study pairing mechanisms. The thermodynamics in this regime are dominated by the statistical nature of Fermi gases and the characteristic Fermi-Dirac distribution determines the length and energy scales of the system.

Chapter 2 is devoted to the universal relations. Starting with an emphasis on universality in Fermi gases, the contact parameter and the Tan relations are introduced as pioneering work. Their ability to explain the thermodynamic relations is a powerful property, and in this chapter the temperature dependent contact at unitarity is reviewed.

The experimental tool of choice to measure short-range correlations is Bragg spectroscopy. In order to provide motivation for the use of this method an introduction on linear response theory is given in chapter 3. The dynamic and static
structure factors represent the measurable quantities provided by Bragg spectra, and can be extracted from the centre of mass displacement as well as from the width of the atomic distribution. In order to determine the absolute value of the static structure factor from Bragg spectra, sum rules are necessary.

The experimental apparatus is described in chapter 4. Most importantly, in order to conduct the following experiments precise control is required over the Fermi momentum and hence the trap frequencies. Imaging is carefully adjusted as obtaining good signal-to-noise is crucial in the Bragg spectra as well as for the determination of the temperature of the Fermi gases.

Chapter 5 describes the temperature determination of Fermi gases at unitarity. This topic is still a major challenge in current research requiring careful discussion, and a full chapter is devoted to this. The determination of the temperature is relevant for the results in the final experimental chapter.

The verification of the universal law for the static structure factor, $S(k)$, versus momentum transfer and its experimental procedure are the subject of chapter 6. The construction of Bragg spectra and their analysis are described. Having developed a well defined procedure to determine the absolute static structure factor, the universal relation is used to show the coupling dependence of the contact for a zero-temperature approximation.

The final chapter 7 combines previously addressed theoretical knowledge and experimental techniques to measure the temperature dependence of the contact at unitarity. Bragg spectra of strongly interacting Fermi gases are taken at increasing temperatures. Two comparative methods are used to obtain these spectra and the resulting values of the contact obtained from the static structure factors are compared with the theoretical predictions.
Chapter 1

BEC-BCS crossover physics

Ultracold strongly interacting Fermi gases provide a paradigm to investigate phenomena such as superfluidity and universality. In the crossover region, pairing mechanisms change from fully spatially correlated to fully momentum correlated, which is represented in the temperature-coupling phase diagram where Bose-Einstein condensates (BEC) change to Bardeen-Cooper-Schrieffer superfluids (BCS). In the unitarity regime, both the spatial and momentum correlations are comparable. This characteristic length scale of the system is smaller than the zero-energy scattering length and larger than the potential range of the interparticle interaction. Then, this principle of a dilute and strongly interacting Fermi gas is a model applicable to a broad range of physical systems like neutron stars or solid state physics.

1.1 Introduction

An important goal in ultracold quantum gases is to find novel macroscopic quantum states to investigate superfluidity and universality. In the following we consider a gas of fermions with an equal number of spin-up and spin-down particles. The two-body problem involves interaction between two particles of opposite spin. The degree of correlation of these pairs will then influence the interparticle collisions and will therefore characterise the macroscopic properties of the gas. The relevant quantities that modify these correlations are the temperature, $T/T_F$, in terms of the Fermi temperature, $T_F$, and interaction strength, $1/(k_F a)$. The latter is a quantity given by the Fermi wave vector, $k_F$, and the so-called s-wave scattering length, $a$. In the scattering problem at low temperatures only the lowest partial wave survives and $a$ becomes the quantity of interest to describe two-body interactions. The interaction strength $1/(k_F a)$ is sometimes referred to as the coupling constant. Depending on the temperature and scattering length, the macroscopic character of the gas changes
CHAPTER 1. BEC-BCS CROSSOVER PHYSICS

Figure 1.1: Sketch of the phase diagram as a function of the temperature and interaction strength. Pairs of composite fermions change their correlation range throughout the Bose-Einstein condensate (BEC) to Bardeen-Cooper-Schrieffer (BCS) crossover non-trivially from strong (light copper) to weak (dark copper). The dashed line indicates the onset of pairing, $T^*$. The solid line represents the critical temperature, $T_C$.

drastically. Figure 1.1 illustrates the temperature-coupling phase diagram. In the limit of a small and positive scattering length, $a \to +0$, tightly bound pairs are highly spatially correlated. They attain a bosonic character and can undergo Bose-Einstein condensation below a critical temperature. For a small and negative scattering length, $a \to -0$, the gas becomes a Fermi liquid described by the Bardeen-Cooper-Schrieffer theory for superfluids. Momentum correlated atoms in the two spin states are then also known as Cooper pairs. The mechanism for superfluidity evolves smoothly from the BEC side to the BCS side. At zero temperature, the ground state of a balanced gas is always superfluid. In the region where the scattering length diverges the interactions are the strongest and quantum-mechanically limited. This unitarity regime obeys universal relations and aroused considerable interest in atomic physics. The critical temperature, $T_C$, for fermionic superfluidity in this limit is about $0.2 T/T_F$, and is many orders of magnitude higher than in the non-interacting limits, $a \to \pm 0$. Also, the critical velocity, $v_C$, is much higher. Both effects allow superfluidity to be investigated away from the ground state.

This chapter reviews the influence of the interaction strength and temperature on the pairing mechanisms in Fermi gases throughout the crossover regime from the
limiting cases of spatially correlated pairs to momentum correlated pairs. Since the temperature and coupling strength form a two-fold parameter space, the structure of this chapter starts with the introduction of the scattering length, $a$, in section 1.2, which dominates the collisional properties of degenerate quantum gases at ultra-low temperatures. The maximum of the s-wave scattering amplitude and a change of the sign of the phase occurs at the Feshbach resonance, which is explained in section 1.3. Therefore, the unitarity regime can be realised with Feshbach resonances. These Feshbach resonances are a physical effect that allow control over the magnitude and sign of $1/(k_Fa)$ in terms of the scattering length by varying the external magnetic field. The isotope $^6$Li, which is used in this work, is a promising candidate due to its large and negative background scattering length. $^6$Li provides an exceptionally broad Feshbach resonance; hence the magnetic field can be used to precisely manipulate ultracold collisions and to investigate the whole BEC-BCS crossover. Once the theoretical background for the unitarity regime is built, the thermodynamic aspects for this regime are summarised in section 1.4.

In unitary Fermi gases, a clear definition of the length scales is important. For the remainder of this thesis, the following definitions apply for the scale of the characteristic length, $r$, and momentum, $k$, where $r \propto 1/k$:

- The Fermi gas is ultracold and $r$ must be smaller than the thermal deBroglie wavelength, $\lambda_{dB} = \sqrt{\hbar^2/(2\pi mk_B T)}$, with mass $m$, Boltzmann constant $k_B$ at a temperature $T$.

- The s-wave scattering length at the broad Feshbach resonance, $|a_0| \equiv a$, is larger than $r$, see section 1.3.

- The interparticle distance, $l$, is larger than $r$.

- The inter-fermionic potential range, $r_0$, is smaller than $r$.

Therefore, the restrictions on the length scales are $r_0 \ll k^{-1} \ll l \ll \lambda_{dB} \ll a$.

### 1.2 Low temperature scattering

The interactions in a many-body system are determined by the scattering behaviour. Scattered particles not only give information about the inner structure of materials, see for instance chapter 3, but also are responsible for establishing the equilibrium state of the system through elastic and inelastic collisions; for example, rethermalisation during the evaporative cooling process is a collisional process. These collisions...
have a different influence on the dynamics of the gas depending on the involved particles (bosons or fermions). Here, only the two-body interactions are discussed because in a many-body system they provide the essential properties and any further change can be covered by a perturbation from the mean field of the many-body background. In this section, the relevant quantities in scattering events are recalled. Detailed discussions can be found in textbooks, e.g. [87].

1.2.1 Scattering cross section and partial wave amplitude

The scattering process will hitherto be described by the potential $V(x)$ and is located in the centre of the coordinate system. Two-body scattering problems are commonly described in the centre of mass frame as only the relative motion is relevant reducing the degrees of freedom from six to three. Let us consider the collision between two identical particles. At $t_0$, the incoming wave is a plane wave, or a particle with momentum, $\hbar k$, and reduced mass, $m$. The outgoing wave function consists of an unscattered part and a scattered part. The exact eigenstates, $\psi_k(x)$, after the scattering event have to obey the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(x)\right] \psi_k(x) = E_k \psi_k(x),$$

with the potential $V(x)$ and kinetic energy

$$E_k = \frac{\hbar^2 k^2}{2m} \geq 0.$$  \hfill (1.2)

Solutions with $E < 0$ support discrete bound states with a binding energy, $E_B$. The formal solution of the general structure of the stationary states $\psi_k(x)$ leads after some calculation to

$$\psi_k(x) = \psi_{k,\text{in}}(x) + \psi_{k,\text{sc}}(x) = e^{ik\cdot x} + \frac{e^{ikr}}{r} f_k(\theta, \phi).$$

The scattering amplitude, $f_k$, depends on the scattering angle $\theta$ but not on the distance and has the dimension of length. The total cross section is the integration over all solid angles $\Omega$

$$\sigma = \int d\Omega \left| f_k(\theta, \phi) \right|^2.$$  \hfill (1.4)

The scattering amplitude can be simplified by expanding the plane wave in partial waves and using symmetry arguments, i.e. considering the spherical symmetry of the problem and hence the independence of $\phi$. Then, the scattering amplitude
may be written as

\[ f_k(\theta) \equiv f(k, \theta) = \sum_{l=0}^{\infty} (2l + 1) f_l(k) P_l(\cos(\theta)). \] (1.5)

The expansion coefficients \( f_l \) are called the partial wave amplitudes which are given by the phase shift \( \delta_l(k) \) for the \( l \)th partial wave

\[ f_l(k) = e^{i\delta_l(k)} \frac{\sin(\delta_l(k))}{k}. \] (1.6)

Using the optical theorem, the scattering amplitude can be written as

\[ f_l(k) = \frac{1}{k \cot(\delta_l(k)) - ik}. \] (1.7)

Expansion in terms of the effective range, \( r_l \), and the scattering length, \( a_l \), leads to

\[ k \cot(\delta_l(k)) = -\frac{1}{a_l} + \frac{r_l}{2} k^2 + O(k^4). \] (1.8)

Each partial wave follows from equations 1.4, 1.5 and 1.6 as

\[ \sigma_l(k) = \frac{4\pi}{k^2} (2l + 1) \sin^2(\delta_l(k)). \] (1.9)

Since the cross section is additive, the total cross section can be calculated from

\[ \sigma = \sum_l \sigma_l. \]

### 1.2.2 Low energy s-wave scattering with interactions

The above scattering expressions can be modified for ultracold gases. The kinetic energy is low, thus \( k \to 0 \). The phase shift approximates \( \delta_l(k) \propto k^{2l+1} \) modulo \( \pi \) and all partial waves with \( l \neq 0 \) have a vanishing cross section according to \( \sigma_l(k) \propto k^{4l} \). Phenomenologically, this is due to a reflection of the free wave function from an additional centrifugal barrier in the effective scattering potential. For \( l = 0 \), the phase shift must be \( \delta_0(k) = -ka_0 \) and the cross section is dominated by pure, isotropic s-wave scattering. For the remainder of this thesis, the s-wave scattering length is denoted as \( a_0 \equiv a \).

In the Schrödinger equation of a many-particle system, an effective potential for the interactions can be expressed by a zero-range contact potential introduced
by Lee, Yang and Huang \[90\]

\[
V_{eff}(r) = \frac{2\pi a^2}{m} \delta (r) \frac{\partial}{\partial r} r.
\] (1.10)

This condition is sometimes contrasted with the Bethe-Peierls boundary condition \[91\]

\[
\left[ \frac{1}{r \psi} \frac{d (r \psi)}{dr} \right]_{r=0} = \frac{1}{a}.
\] (1.11)

Both equations constrain the wave function properly in the zero-range limit. This aspect is important when two fermions are close enough to each other to interact or form a dimer, depending on the sign of the scattering length. Under these assumptions, the right hand side of equation \[1.8\] reduces to \(-1/a_0 = -1/a\) in the zero range limit and equation \[1.7\] becomes

\[
f_0(k) = -\frac{a}{1 + ika}.
\] (1.12)

Poles occur for the condition \(-1/a_l = ik\), in general. The real part of \(-f_0(k)\) is sometimes denoted as the effective scattering length, \(a_{eff} = a/(1 + k^2 a^2)\). The scattering length follows as

\[
a = -\lim_{k \to 0} \frac{\tan (\delta_0 (k))}{k}.
\] (1.13)

The total cross section for two identical particles is obtained from

\[
\sigma = \frac{4\pi a^2}{1 + k^2 a^2}.
\] (1.14)

For the weakly interacting limit, \(ka \ll 1\), the cross section reads

\[
\sigma (k \to 0) = 4\pi a^2,
\] (1.15)

which is four times the classical scattering cross section and equal to the surface area of the sphere, i.e. scattering occurs from the entire surface. Equation \[1.13\] also shows that the low-energy scattering process does not depend on the details of the microscopic potential. In the strongly interacting limit, \(ka \gg 1\), the scattering cross section becomes independent of the scattering length giving the maximum possible cross section for s-wave collisions

\[
\sigma (a \to \infty) = \frac{4\pi}{k^2}.
\] (1.16)
This is the unitarity regime which can be realised in a Fermi gas at the BEC-BCS crossover.

1.3 The broad Feshbach resonance in Lithium-6

The broad s-wave Feshbach resonance in $^6\text{Li}$ at 834 G forms a rich testbed for the investigation of correlated fermions [12]. Broad s-wave Feshbach resonances have been subject to several experiments using either $^6\text{Li}$ [11, 12, 13, 14, 15] or $^{40}\text{K}$ [13]. These were initially studied in nuclear scattering mechanisms. The terms ‘open’, ‘closed channel’ were introduced and used to describe the picture of an effective potential [93, 94] as well as the resonances between discrete states coupled to a manifold of scattering states [95]. Originally proposed for hydrogen [96], the idea was extended to ultracold alkali atoms [97]. Early interest concerned the modification of elastic and inelastic atomic collisions [24, 25, 98]. The observed strong loss mechanisms in Bose gases [25, 26] were explained with the creation of large ultracold diatomic molecules [99–101] having a size of the order 1000 $a_0$. For fermionic gases, the collisional relaxation into deeply bound states is suppressed by the Pauli exclusion principle despite their highly excited vibrational state [27]. Consequently, a fermionic gas is stable close to a Feshbach resonance [102–105]. Important experiments to understand pairing mechanisms have been performed in the vicinity of a Feshbach resonance, for instance the formation of stable diatomic molecules [18, 28–30, 37, 38, 43, 106, 107] and the condensation of molecules [32–34]. The first production of cold dimers was demonstrated by photo-associating cold atoms [108]. After considering the possibility to create ultracold molecules near Feshbach resonances [109], the first signature of molecules created near a Feshbach resonance were seen through Ramsey fringes between molecules and atoms [112] and directly in $^{40}\text{K}$ after adiabatically sweeping across a Feshbach resonance [41]. Molecule creation with $^6\text{Li}$ followed in the same year [18, 28, 29]. Nowadays, it has become common to cool and evaporate close to the Feshbach resonance to generate a molecular BEC through weakly bound diatomic molecules of two fermions. More details can be found in review articles about Feshbach resonances, e.g. [110].

1.3.1 Scattering resonance

In this context, the Feshbach resonance is understood as a scattering resonance. We consider two free atoms in an arbitrary state. Their interatomic potential curve is shown in figure [12]. The open channel refers to the interatomic potential of the two
Figure 1.2: The Feshbach resonance results from tuning the potential curve for two interacting atoms in the open channel into resonance with the potential curve in the closed channel.

free atoms at large atomic distances ($R = \infty$). If the two states (molecule and two free atoms) have a different magnetic (electric) dipole moment, $\mu_{\text{molecule}} \neq \mu_{\text{2atoms}}$, an external magnetic (electric) field, $B$, can be used to detune the interatomic potential, $\Delta E \propto \Delta \mu B$. Then, the closed channel represents the energy-detuned potential such that the highest lying bound state is in resonance with the energy of the two free atoms. That is the threshold energy of the colliding atoms in an open channel becomes equal to a bound energy state in the closed channel. The molecular state exists for a limited lifetime. The scattering length of such a resonance depends on the applied external magnetic field, $B$, and is generally given by

$$a = a_{bg} a_0 \left(1 + \frac{\Delta B}{B - B_0}\right) \left(1 + \alpha (B - B_0)\right) \quad (1.17)$$

with the background scattering length of the open channel $a_{bg}$ in units of the Bohr radius $a_0 = 5.292 \times 10^{-11}$, the width of the resonance $\Delta B$, which depends on the magnetic moments of the closed and open channels, and the resonant magnetic field $B_0$ as well as the correction factor $\alpha$. 
1.3 THE BROAD FESHBACH RESONANCE IN LITHIUM-6

1.3.2 Situation in lithium

Lithium is an alkali element with a single valence electron in its ground state ($S = 1/2$ and $L = 0$, i.e. $J = S + L = 1/2$). The fermionic isotope $^{6}$Li has a nuclear spin of $I = 1$, leading to a total angular momentum $F = I \pm J$, which is $F = 1/2$ and $F = 3/2$. The hyperfine states split at high magnetic fields (Paschen-Back regime) depending on the projection quantum numbers $m_F$. The broad resonance occurs for an interatomic potential between the substates $|F, m\rangle = |1/2, 1/2\rangle$ and $|1/2, -1/2\rangle$ (triplet state $S = 1$). The exact resonance position is $B_0 = 834.15$ G (predicted by \[110\]) with a width of $\Delta B \approx 300$ G \[39\]. Another narrow resonance is found at 543 G and is $\approx 100$ mG wide (singlet state $S = 0$ \[106\]. Here, $k_F |r_0| \geq 1$, the effective range of interactions, $r_0$, is dominating \[92\]. The background scattering length for the broad resonance is $a_{bg} \approx -1405 a_0$ and $a_{bg} \approx -2100 a_0$ (triplet scattering length) at high fields. This is very unusual compared to other alkali elements where $a_{bg} \leq 100 a_0$. The large background scattering length modifies the continuum states such that two colliding atoms are likely to be found close together and leads to a large Franck-Condon factor (good overlap of the free continuum state and the closed channel bound state). In this experiment, a magnetic field is generated by a pair of Helmholtz coils and is used to precisely control the scattering length across the Feshbach resonance according to the relation equation \[1.17\]. Figure.13 sketches the scattering length versus magnetic field. Although not shown, the scattering length starts off near zero in zero magnetic field. With increasing magnetic field the scattering length decreases to a local minimum of $-300 a_0$ at 325 G before crossing zero at 530 G. The correction factor in equation \[1.17\] is $\alpha = 0.0004$ for $^{6}$Li.

1.3.3 Bound states

Feshbach bound states for a three-dimensional Fermi gas exist only for repulsive interactions, $ka > 0$. As discussed above, if the magnetic moment of a close channel is different from the open channel, these can be tuned into resonance by the magnetic field, where the resonance interaction is given by the scattering length $a$ \[30\]. As found by Petrov, the characteristic size of a Feshbach dimer is the scattering length $a$ \[27\]. The relaxation into a deeply bound molecular state requires three fermions within a distance $r_0$ to collide. As two of these three fermions must have the same spin, the relative wave function has to be antisymmetric; thus in the node where $r = 0$, the wave functions scales as $kr$, where $r$ is small and the relative momentum $k \propto 1/a$ goes with the inverse of the scattering length. Within the conditions of a zero-range model, see equations \[1.10\] and \[1.11\], and a positive scattering length, the
Figure 1.3: Broad s-wave Feshbach resonance at 834 G in $^6$Li. The scattering length diverges over a broad range and can therefore be precisely tuned with the magnetic field. This opens a way to investigate the BEC-BCS crossover.

The wave function of the bound state is

$$\Psi_b = \frac{e^{-r/a}}{\sqrt{2\pi ar}}. \quad (1.18)$$

The binding energy, $E_b$, of the dimer does not depend on the short-range details of the potential

$$E_b = -\frac{\hbar^2}{2ma^2}, \quad (1.19)$$

where $m$ is the mass in the centre of mass framework. The smaller the binding energy, the larger the dimer. Several collisional processes between a combination of dimers and atoms can take place once the molecular state is populated. On the one hand, when the scattering length approaches resonance, $1/a \to 0$, the binding energy vanishes. Due to the Pauli principle, elastic collisions dominate. On the other, for very deep binding energies, $ka \to +\infty$, and a molecular state far below the atomic continuum, a loss channel opens for atom-dimer collisions. It has been shown that the scattering length for dimer-dimer collisions $a_{dd} = 0.6a$ and dimer-atom collisions $a_{ad} = 1.2a$ can be related to the atom-atom scattering length $a$ [27,111]. But the rate constant of inelastic atom-dimer collisions is $\alpha_{ad} \propto (r_0/a)^{3.33}$, while for dimer-dimer collisions it is $\alpha_{dd} \propto (r_0/a)^{2.55}$. Nevertheless, as $r_0/a \to 0$, the dimer-dimer collision rate exceeds the atom-dimer collisions, allowing efficient cooling of dimers.
1.4 Thermodynamics of Fermi gases

The next sections discuss the basic thermodynamic quantities required to understand the physics occurring in degenerate Fermi gases. Many textbooks (e.g. [112]) provide detailed discussions, derivations, and relations for Fermi gases; to quote these is beyond the scope of this thesis and only a summary is given. As opposed to textbooks, the details on the Fermi-Dirac statistics are introduced only now, because the dependence on the temperature introduces another parameter in the problem. A spin balanced Fermi gas is considered unless stated differently. A set of equivalent, fundamental relations between energy, temperature and interaction shall describe the phase diagram and is given by \( E/N_\epsilon_F(T/T_F, 1/(k_F a)) \), see figure [1.1]. Energy and temperature are obviously macroscopic quantities. Though the interaction strength is a two-body quantity, in the many-body problem one can treat the two-body effects as central mechanisms which are weakly perturbed by the mean field. The Fermi-Dirac distribution enters thermodynamic equations including their derivations, see section [1.4.1], and the Fermi energy sets the relevant energy scale.

First, the ideal gas case is considered in the homogeneous case and the trapped case, in section [1.4.2] and [1.4.3], respectively, since this marks a reference point in contrast with the interacting cases, in section [1.4.4]. Then the ideal (non-interacting) trapped case is reviewed. The ideal case can often be used to describe the weakly interacting regime (BCS side) of the crossover. The thermodynamic quantities in the ideal gas case are valid for the equilibrium state and collisions are responsible for rethermalisation. The Fermi gas at zero temperature is not superfluid until interactions are included. It is peculiar that the unitarity regime shows the same behaviour as the ideal case within a rescaling. The chapter ends with a discussion of hydrodynamic expansion as shown by time-of-flight experiments, section [1.4.5].

1.4.1 Fermi distribution

Thermodynamics studies the macroscopic behaviour of gases in the thermodynamic limit, i.e. \( N \gg 1 \). At large \( N \) the fluctuations \( \Delta N \) are small and a statistical description becomes increasingly exact. The replacement of the temporal progression of the microscopic details in the gas with the parallel existence of all possible states is formulated in the ergodicity hypothesis; thus thermodynamics becomes thermostatistics. Extensive and intensive thermodynamic potentials such as entropy, tem-
perature, internal energy etc. describe the state of the gas macroscopically and their first and second derivatives are linked (Maxwell relations) such that the potentials can be re-constructed from each other. The information about the macroscopic state is stored in the grand partition function in either the micro-canonical, canonical or grand-canonical case, i.e. depending on a connection to an outer thermodynamic environment which would allow temperature and/or particle exchange. In the grand-canonical case of Fermi gases the grand partition function $Z$ is a product state that obeys asymmetry rules and the Pauli principle

$$Z_{FD} = (1 + f_1) (1 + f_2) ... (1 + f_k) ... = \prod_{i=1}^{\infty} (1 + f_i)$$  \hspace{1cm} (1.20)$$

with $f_i = e^{(\mu - \epsilon_i)/(k_B T)}$. The grand potential can be obtained from

$$\Omega_{FD} = -k_B T \ln Z_{FD} = -k_B T \sum_{i=1}^{\infty} \ln \left(1 + e^{(\mu - \epsilon_i)/(k_B T)}\right)$$  \hspace{1cm} (1.21)$$

and the occupation number of the energy levels is

$$f_{FD}^k = \frac{\partial \Omega_{FD}}{\partial \epsilon_k} = \frac{1}{e^{(\epsilon_k - \mu)/(k_B T)} + 1}$$  \hspace{1cm} (1.22)$$

known as the famous Fermi-Dirac distribution. This is the signature to all mechanisms in Fermi gases.

### 1.4.2 The non-interacting homogeneous case

In an ideal Fermi gas the number of states can be obtained by counting the states in an octant of the momentum sphere with radius $k(\epsilon) = \sqrt{2m \epsilon/\hbar^2}$, spin degree of freedom 2, and volume $4\pi/3 (\pi/L)^3$ (length $L$). Deriving this with respect to the energy limit $\epsilon$ gives the density of states

$$D(\epsilon) = \frac{2V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{\epsilon}. \hspace{1cm} (1.23)$$

When integrating over all energy states the Fermi distribution in equation\(1.22\) becomes

$$f(\epsilon, T, \mu) = \frac{1}{e^{(\epsilon - \mu)/(k_B T)} + 1}.$$  \hspace{1cm} (1.24)$$
1.4 THERMODYNAMICS OF FERMI GASES

Using equation (1.21) the grand potential is

\[
\Omega = -k_B T \int_0^\infty \ln \left(1 + e^{(\mu - \epsilon)/k_B T}\right) D(\epsilon)
\]

\[
= -k_B T \frac{2V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty \ln \left(1 + e^{(\mu - \epsilon)/k_B T}\right) \sqrt{\epsilon},
\]

which is unfortunately not analytically solvable. The atom number arises from

\[
N = - \left(\frac{\partial \Omega}{\partial \mu}\right)_{T,V} = \int_0^\infty f(\epsilon, T, \mu) D(\epsilon) d\epsilon \quad (1.26)
\]

The internal energy is

\[
U = \int_0^\infty \epsilon f(\epsilon, T, \mu) D(\epsilon) d\epsilon \quad (1.27)
\]

\[
U = \frac{2V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{\epsilon^{3/2}}{1 + e^{(\mu - \epsilon)/k_B T}} d\epsilon.
\]

A partial derivation shows \( \Omega = -\frac{2}{3}U = -PV \) and therefore the equation of state of a Fermi gas is

\[
P = \frac{2U}{3V} \quad (1.28)
\]

For high temperatures or low particle densities, the fugacity is \( \exp(\mu/(k_B T)) \ll 1 \) and equation (1.24) reduces to the classical Boltzmann statistics as the exponential term in the denominator exceeds the contribution +1:

\[
f(\epsilon, T, \mu) e^{(\mu/(k_B T))} \ll 1 \quad e^{(\epsilon - \mu)/(k_B T)}
\]

If the term ‘\( \exp(\mu/(k_B T)) \)’ is of the order of 1, quantum effects come into play. For \( T \leq 1 \text{ mK} \) the deBroglie wavelength \( \lambda_{dB} = \sqrt{2\pi \hbar^2/(mk_B T)} \) becomes comparable to the interparticle spacing, where \( m \) is the mass of the particle at temperature \( T \), and the phase space density \( D = n\lambda_{dB}^3 \) depends on the particle density. When the temperature approaches \( T = 0 \) the Fermi distribution becomes more and more similar to a step function, i.e. the occupation of available phase space cells smoothly
approaches unity
\[
f(\epsilon, T, \mu) = \frac{1}{e^{(\epsilon-\mu)/(k_B T)} + 1} \rightarrow \begin{cases} 
1 & \text{for } \epsilon \leq \mu \text{ and } T \to 0, \\
0 & \text{for } \epsilon \geq \mu \text{ and } T \to 0 
\end{cases}.
\]
(1.30)

The chemical potential is then a temperature dependent quantity. The particle number is
\[
N = \frac{2V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_{0}^{\mu_0} \sqrt{\epsilon} d\epsilon = \frac{V}{3\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \mu_0^{3/2}.
\]
(1.31)

The chemical potential is for a given particle number density-dependent
\[
\mu_0 \equiv \epsilon_F \equiv k_B T_F = \frac{\hbar^2}{2m} \left(3\pi^2 n\right)^{2/3} \propto n^{2/3}
\]
(1.32)
So, at zero temperature, \(\mu\) is the energy of the highest occupied state of the non-interacting Fermi gas and equals the Fermi energy \(\epsilon_F\). This is referred to as the ground state of the system where the lowest single particle states are filled up gapless and successively up to the Fermi energy \(\epsilon_F\). Any excitations into a higher lying state makes the step function smoother by creating a ‘particle-hole’ relation. Consequently, the width of the step increases at higher temperatures. The width is set by the temperature, \(\Delta \epsilon_F = 2k_B T\). The ground state energy of the system is
\[
E(T = 0) = \int_{0}^{\mu_0} \epsilon D(\epsilon) d\epsilon = \frac{3}{5} N\mu_0 = \frac{3}{5} N\epsilon_F
\]
(1.33)

Therefore, in the homogeneous case the mean energy per particle at \(T = 0\) is
\[
\frac{E}{N} = \frac{3}{5}\epsilon_F
\]
(1.34)
which is different from the classical gas case, where \(E = 3k_B T/2\) and would be zero at \(T = 0\). However, the classical gas case is not valid at arbitrary low temperatures.

In Fermi systems, thermodynamic quantities depend weakly on the temperature, because of the Pauli principle. The low lying states \(|\sigma_{\pm 1/2}, \mathbf{k}\rangle\) with small wave vectors are only occupied once and many particles have to sit in higher energetic states. For temperatures \(0 \leq T \ll T_F\), the step function becomes continuously a smoother transition between 0 and 1.
1.4.3 The non-interacting trapped case

Let us consider an ultracold Fermi gas of \( N = N/2 \) spin polarised fermions in a harmonic trapping potential

\[
V = \frac{1}{2} m \omega_x^2 x^2 + \frac{1}{2} m \omega_y^2 y^2 + \frac{1}{2} m \omega_z^2 z^2
\]

with a mean trapping frequency \( \bar{\omega} = (\omega_x \omega_y \omega_z)^{1/3} \) and, according to equation (1.24), a semiclassical (spatial and momentum) distribution function given by the occupation number for single states

\[
f(\epsilon (r, p), \rho) = f(r, p) = \frac{1}{e^{(\epsilon^2/2m + V(r) - \mu)/(k_B T)} + 1}.
\]

Since the density of states in a harmonic trap is \( g(\epsilon) = \epsilon^2 / (2 (\hbar \bar{\omega})^3) \), the atom number and total energy can be calculated using equations (1.27) and (1.28), respectively. Similarly to equation (1.31) the spatial distribution becomes for \( T \to 0 \) and \( \mu_0 = \epsilon_F \)

\[
n(r) = \int \frac{d^3p}{(2\pi \hbar)^3} f(r, p) \to \int_{\{|p|<\sqrt{2m(\epsilon_F-V(r))}/(2\pi \hbar)^3\}} \frac{d^3p}{(2\pi \hbar)^3}.
\]

The Fermi momentum lies on a sphere of radius \( \hbar k_F(r) \) with unit spacing \( (2\pi \hbar)^3 \). The spatial density distribution of a zero temperature non-interacting Fermi gas is thus

\[
n(r) = \frac{1}{6\pi^2} \left[ \frac{2m}{\hbar^2} (\epsilon_F - V(r)) \right]^{3/2}.
\]

The globally largest momentum is the Fermi momentum \( p_F \equiv h k_F \equiv \sqrt{2m\epsilon_F} \). In the Thomas-Fermi approximation \( (k_B T \gg \hbar \bar{\omega}) \), the Fermi momentum and energy at each point of the trap \( r \) are approximated by a uniform gas such that

\[
p_F(r) = \hbar k_F(r) = \sqrt{2m\epsilon_F(r)} = \hbar \left( 6\pi^2 n(r) \right)^{1/3}
\]

\[
\epsilon_F(r) = \mu(r, T=0) = \epsilon_F - V(r)
\]

At \( T = 0 \), equation (1.27) and (1.28) may be written as

\[
N_\uparrow = \int d^3r n(r) = \frac{1}{6} \left( \frac{\epsilon_F}{\hbar \bar{\omega}} \right)^3
\]

\[
\epsilon_F = \hbar \bar{\omega} \left( 6N_\uparrow \right)^{1/3} = k_B T_F.
\]
CHAPTER 1. BEC-BCS CROSSOVER PHYSICS

From the condition that the profile vanishes for $V(r) \geq \epsilon_F$, the Fermi radius $R_{F,i}$ in each direction $i = x, y, z$ is calculated from $V(R_{F,i}) = \epsilon_F$ as

$$R_{F,i} = \sqrt{\frac{2\epsilon_F}{m\omega_i^2}}. \quad (1.43)$$

Explicitly, the distribution function reads

$$n(r) = \frac{8 N_{\uparrow}}{\pi^2 R_{F,x} R_{F,y} R_{F,z}} \left[ 1 - \left( \frac{x}{R_{F,x}} \right)^2 - \left( \frac{y}{R_{F,y}} \right)^2 - \left( \frac{z}{R_{F,z}} \right)^2 \right]^{3/2} \quad (1.44)$$

and the mean energy per particle is readily found from the ratio of equation (1.27) and (1.28) at $T = 0$,

$$\frac{E}{N} = \frac{3}{4} \epsilon_F. \quad (1.45)$$

As per equation (1.29), for $k_B T \gg \epsilon_F (r)$ the gas shows a classical (Boltzmann) density distribution $n(r) \propto \exp(-V(r)/(k_B T))$. However, for $k_B T \ll \epsilon_F (r)$, the density profile characteristically approaches $n(r) \propto (\epsilon_F - V(r))^{3/2}$.

1.4.4 The interacting trapped case

Interactions are responsible for the pairing mechanisms between fermions of opposite spin. In an ultracold gas with a balanced mixture of $N_{\uparrow}$ and $N_{\downarrow}$ fermions in two different hyperfine states, interaction is allowed by lowest order collisions (s-wave collisions). At $T = 0$, the Fermi momentum, $k_F$, and the scattering length, $a$, can be expressed as a dimensionless parameter, $1/(k_F a)$, to quantify the strength and sign of the interactions. They also determine the many-body properties. The ground state in the BCS limit is reached for $1/(k_F a) \to -\infty$ because for weakly attractive interactions composite fermions are always unstable against pairing but simultaneously have to obey the Pauli principle; thus the density distribution is close to an ideal Fermi gas. Weak repulsive interactions lead to the BEC limit, $1/(k_F a) \to +\infty$, where a tightly bound state exists to create molecules of mass $M = 2m$. The Pauli principle is now a weak restriction on the bosonic character and molecules can accumulate closer to each other. Maximum interaction strength is reached for the unitarity limit, $1/(k_F a) \to 0$, as the scattering length diverges $a \to \pm\infty$ even at high temperatures. Here, the ground state is neither a BEC nor a BCS because it is neither a bound state nor a Cooper pair defined. But the ground state is always superfluid.
The following sections review the consequences on the density distributions and thermodynamic quantities in the limiting cases. In general, the spatial distribution of the clouds shrinks from the BCS side to BEC side due to the increasing interaction strength.

1.4.4.1 BEC limit

When the scattering length is small and positive $a > 0$ and $1/(k_F a) \to +\infty$, fermions will form bound dimers, see section 1.3.3, and acquire a bosonic character. These dimers obey Bose-Einstein statistics. Thermal molecules can be cooled to molecular Bose-Einstein condensates. For a trapping potential for molecules, $V_M (r)$, and intermolecular interactions $g = 4\pi \hbar^2 a_M / M$, the many-body wave function $\Psi (r)$ can be described by the Gross-Pitaevskii equation

$$
\left( -\frac{\hbar^2 \nabla^2}{2m} + V_M (r) + g |\Psi (r, t)|^2 \right) \Psi (r, t) = i\hbar \frac{\partial}{\partial t} \Psi (r, t). \quad (1.46)
$$

$|\Psi (r, t)|^2$ is the condensate density $n_C$, which for weak interactions and zero temperature equals the density of molecules $n_M$. For the ground state in equilibrium one can use the ground state energy given by the molecular chemical potential $\mu_M$. The wave function is then replaced by $\Psi (r, t) = \exp (-i\mu_M t / \hbar) \Psi (r)$. When the interactions dominate the kinetic energy of the condensate wave function, $g n_C \gg \hbar \omega_i$, the Thomas-Fermi approximation yields the condensate density

$$
n_C (r) = |\Psi (r)|^2 = \max \left( \frac{\mu_M - V_M (r)}{g}, 0 \right) \quad (1.47)
$$

which is also the order parameter. The chemical potential is again determined by the molecule number $N_M = (N_+ + N_-)/2 = \int d^3r n_C (r)$. The trap for molecules is twice as deep as for atoms, $V_M (r) = 2V (r)$, which changes the density profile to

$$
n_C (r) = \frac{15}{8\pi} \frac{N_M}{R_x R_y R_z} \max \left( 1 - \sum \frac{x_i^2}{R_i^2}, 0 \right). \quad (1.48)
$$

The Thomas-Fermi radius is given by $\sqrt{2\mu_M / M \omega_i}$. Bose condensed clouds still show a clear difference in the distribution compared to the thermal cloud.

1.4.4.2 BCS limit

In the BCS limit of weak attractive interactions, the scattering length is small and negative $a < 0$ and $1/((k_F a)) \to -\infty$. Compared to the ideal gas case, the density
profile is marginally influenced by the interactions or pairing behaviour because the sharp Fermi surface in $k$-space at $k_F$ is modified only in an exponentially narrow region of width $k_F \exp(-\pi/2k_F |a|)$. The density distribution is of the form given in equation (1.44) and the Fermi energy for $N/2 = N_\uparrow$ becomes $\epsilon_F = \hbar \tilde{\omega} (6N_\uparrow)^{1/3} = \hbar \tilde{\omega} (3N)^{1/3}$. Very low temperatures are necessary to observe the characteristic Fermi profile. For this case ($k_F |a| \ll 1$), the many-body problem can be solved both at $T = 0$ and at finite temperature using BCS theory, which describes superconductivity in metals [38]. The ground state is described by creation and annihilation operators $c_{k,\sigma}^\dagger$ and $c_{k,\sigma}$ for fermions of momentum $k$ and spin $\sigma = \uparrow, \downarrow$

$$\Psi_0 = \prod_k (u_k + v_k c_{k,\uparrow}^\dagger c_{-k,\downarrow}) |0\rangle. \quad (1.49)$$

$u_k$ and $v_k$ are the probability amplitudes. The chemical potential of the pairs in the ground state and the temperature dependent pairing gap $\Delta (T)$ are the characteristic quantities. The pairing gap is also the order parameter of the system. Since the interactions have a small influence on the density distribution, the Thomas-Fermi radius is taken for a non-interacting Fermi gas and compressed by a first-order correction, so

$$R_i = \sqrt{\frac{2\mu_0}{m\omega_i^2}} = R_{F,i} \left(1 - \frac{256}{315\pi^2}k_F |a| \right) \quad (1.50)$$

where $k_F$ is the Fermi wave vector of a non-interacting gas. If $k_F |a| \ll 1$, then the Thomas-Fermi radius becomes equal to the radius of a non-interacting gas

$$R_{F,i} = \sqrt{\frac{2k_R T_F}{m\omega_i^2}} \quad (1.51)$$

and the density distribution is given by

$$n (r) = \frac{4N}{\pi^2 R_{F,x}^2 R_{F,y}^2 R_{F,z}^2} \left[ 1 - \left( \frac{x}{R_{F,x}} \right)^2 - \left( \frac{y}{R_{F,y}} \right)^2 - \left( \frac{z}{R_{F,z}} \right)^2 \right]^{3/2} \quad (1.52)$$

The equation of state is approximated by that of an ideal Fermi gas, that is

$$\mu (n) = \frac{\hbar^2}{2m} (3\pi n)^{2/3}. \quad (1.53)$$
1.4.4.3 Unitarity regime

In the limit of strong interactions, the scattering length diverges \( a \to \pm \infty \) and \( k_F |a| \to 0 \). It follows that the interparticle distance, \( l = n^{1/3} \propto 1/k_F \), is the only relevant length scale and the Fermi energy is the only relevant energy scale \( \epsilon_F = \hbar^2 k_F^2 / (2m) \). For example, the scattering cross section maximises \( \sigma = 4\pi/k_F^2 \).

Due to the independence of microscopic details, this model is applicable to any other strongly interacting fermionic system where the scattering length diverges. This property is called universality. The chemical potential reduces by a universal parameter \( \xi = 1 + \beta \), so \( \mu = \xi \epsilon_F = (1 + \beta) (\hbar^2/(2m)) (3\pi n)^{2/3} \). Using the local density approximation, in which the gas is regarded as homogeneous in a small sphere, the chemical potential is \( \mu \propto n^{2/3} \). One thus has direct experimental access to the universal constant \( \xi \) by measuring the size of the cloud at unitarity although the universal constant has only a very weak dependence on the radius. At a present understanding, an exact solution of the many-body problem for \( k_F |a| \gg 1 \) is given by the relations outlined in chapter 2.

1.4.5 Hydrodynamic expansion of clouds

For this thesis, ultracold atomic samples are prepared and imaged in-situ or after release at and only at unitarity in the residual curvature of the high magnetic field. In
chapter\footnote{2} the imaging of atomic distributions at different temperatures is carefully
studied. The temperature of the coldest clouds are measured down to $(0.09 \pm 0.01)\ T/\T_F$, which is well below the critical temperature of $0.2\ T/\T_F$, creating therefore
superfluids. For increasing temperatures the normal phase contributes more and more. For a gas in this regime the dynamics are well described by the Boltzmann equation. But anisotropic expansion of a cold Fermi gas was measured at higher
temperatures (on the order $T \approx \T_F$), where the gas is not a superfluid, and found
to exhibit a similar hydrodynamic behaviour \cite{37}.

Hence, when unitary atomic distributions are released, one can assign hydro-
dynamic expansion laws. In general, these aspects can be very complex in different
crossover regime. Nevertheless, the discussion here is restricted to the unitarity
regimes, where the scattering length is large and the mean free path of the atoms
is on the order of the interatomic distances, $1/k \sim l$. The strong interactions raise
not only the critical temperature but also the critical velocity, compared to the limits $k_F a \rightarrow \pm \infty$. Therefore, the hydrodynamic expansion laws can be extended to
higher temperatures at unitarity.

Hydrodynamic equations as well as the collisional and collisionless regimes are
usually discussed in the context of macroscopic phenomena characterised by long-
wave excitations, where collective oscillations are precisely measurable and exhibit
collective features unambiguously, e.g. see \cite{92}. Hydrodynamic equations have been
used to describe the dynamics of BECs but it was suggested to extend them to
explain Fermi gases \cite{113}.

At $T = 0$, the macroscopic behaviour of a neutral superfluid is governed by the
Landau equations of irrotational hydrodynamics. The condition of irrotationality is
a consequence of the occurrence of off-diagonal long-range order, characterised by the
order parameter \cite{92}. The hydrodynamic equations of superfluids consist of coupled
and closed equations for the density and the velocity field \cite{114}. Derivations and
discussions on hydrodynamics of superfluids can be found elsewhere, e.g. \cite{92,112}.

For the released clouds collisions during the expansion cannot be neglected
as for ballistic expansion. Hence, it is not possible here to extract the original
momentum distribution of the particles from the density distribution after the trap
is switched off. Instead, as the collision rate is higher than the largest trapping
frequency, clouds are imaged in the hydrodynamic regime. In fact, the expansion
occurs into an inhomogeneous magnetic field with a saddle potential

\[
V (r, t > 0) = \frac{1}{2} m \left( \omega_{S_x}^2 x^2 + \omega_{S_y}^2 y^2 + \omega_{S_z}^2 z^2 \right) \tag{1.57}
\]
1.5 SUMMARY

with real and imaginary frequencies $\omega_S$. The chemical potential, $\mu$, has the power-law dependence on the superfluid density, $n(r,t)$, thus $\mu \propto n^\gamma$, where $\gamma = 2/3$ is exact at unitarity and in the BCS limit. Hence the scaling ansatz

$$n(r,t) = \frac{1}{b_x(t) b_y(t) b_z(t)} n\left( \frac{x}{b_x(t)}, \frac{y}{b_y(t)}, \frac{z}{b_z(t)}; t = 0 \right)$$ (1.58)

provides the exact solution. The scaling parameters $b_i$ follow the time-dependent equations

$$\ddot{b}_i = -\omega_{S_i}^2 b_i + \frac{\omega_i^2(0)}{b_x(t) b_y(t) b_z(t)}$$ (1.59)

which can be solved numerically. Here, $\omega_i$ is the initial trapping frequency.

1.5 Summary

The study of strongly interacting Fermi gases forms a rich testbed to investigate pair correlations. Previous experimental as well as theoretical work has paved the way to understand new effects in unitary Fermi gases. Collisions in low temperature Fermi gases are dominated by the two-body s-wave scattering length, $a$. In the vicinity of a broad Feshbach resonance, the scattering length can be tuned via an external magnetic field over a wide range. $^6$Li provides a very broad Feshbach resonance at 834 G and constitutes a good candidate to investigate the BEC-BCS crossover. The unitarity regime is of special interest, since universal relations in dilute and strongly interacting Fermi gases provide new, general insights into strongly correlated Fermi systems. The interactions modify the thermodynamics of the Fermi gas dissimilarly over the whole crossover region. The basic equations for the unitarity and ideal case are introduced which are used for this thesis. Hydrodynamic equations characterise the dynamic behaviour of unitarity-limited Fermi gases.
Chapter 2

Universal relations

The unitarity regime forms the physical setting for studying universal properties of strongly interacting Fermi gases. The strong interactions make it difficult to apply standard perturbation theories as it is difficult to define a small parameter. New models are necessary leading to strong coupling theories or improved quantum Monte-Carlo simulations. The Tan relations marked a major development in describing the resonance regime: the simplification of the problem created analytical expressions and the characteristic contact parameter, $C$. Universal relations and properties are valid throughout the BEC and BCS regimes as well as for zero and finite temperatures, any spin imbalance and few- or many-body systems. In this chapter, we revisit the problem of the unitarity regime and describe how the Tan relations forge ahead.

2.1 Introduction

The superfluid transition in ultracold Fermi systems presupposes interparticle interactions and strongly interacting Fermi gases facilitate the investigation of resonant superfluidity. The interaction strength is quantified by the Fermi wave vector $k_F$ and the two-body scattering length $|a|$ and is considered to be strong when $1/k_F |a| \to 0$ and weak when $1/k_F |a| \to \pm \infty$. In the latter case, $|a|$ represents a small parameter and standard perturbation theory is applicable. Unitary Fermi gases are both dilute, that is, the range of the interatomic potential is much smaller than the interparticle distance, and strongly interacting, because the magnitude of the zero-energy scattering length $|a|$ exceeds the interparticle distance. Elastic collisions are responsible for the energy distribution giving the scattering length and sign a key role in the many-body problem [14]. The question arose whether all strongly interacting Fermi systems share the same features. Coming from nuclear physics
Heiselberg \[115\] compared Fermi systems with large scattering lengths in different density regions to point out the relevance of dilute degenerate Fermi gases for nuclear and neutron star matter and, vice versa, the relevance of models for high energy neutron stars to the first magnetically trapped Fermi gas \[17\]. Ho introduced the term ‘universal properties’ for degenerate quantum gases \[63\] in the unitary limit where the cross section reaches independently of \(|a|\) a maximum value \(4\pi/k^2\), \(k\) being the relative momentum of the scattering atoms. In fact, this independence of any features of atomic potentials poses a challenging many-body problem as there are no small parameters anymore. Simplification is achieved by the so-called ‘universal hypothesis’, an assumption that the only relevant length scale in the ground state at unitarity is the interparticle spacing \(n^{-1/3}\), which is related to the particle density \(n\). For unitarity limited, dilute Fermi gases (for which the interaction range is finite as well as larger than interparticle distances) the microscopic details of the interaction potential become indistinct and universality becomes a property of the many-body system. This means in turn that all dilute systems with sufficiently strong interaction behave identically except for a scaling parameter. Ho also considered universality for higher temperatures \[116\] inspired by the early work near the Feshbach resonance. Ergo, universality is a property of strongly interacting Fermi gases \[63, 115, 117\] and one can therefore study universal properties in ultracold atomic gases to help understand other strongly interacting Fermi superfluids, e.g. neutron matter \[118, 119\]. The principle of universality is studied in other research areas, such as for phase transitions in general thermostatistics \[120\] or the \(\beta\)-decay in nuclear physics \[121–124\].

Universal relations in ultracold Fermi gases represent a major breakthrough in understanding highly correlated ensembles and their importance is to date only just being established \[125\]. One of the first results on universality was the derivation and measurement of the virial theorem for unitary Fermi gases together with a universal expression for the hydrodynamic expansion under isentropic conditions \[119\]. The Tan relations, being exact and widely applicable, had an avalanche effect on the investigation of universal properties in strongly interacting Fermi gases \[64–66\]. Tan exploited the fact that in the zero-range limit a well quantified parameter reciprocal to the two-body interaction strength (scattering length), can enter the many-body Schrödinger wave function of a non-interacting gas as a single, characteristic parameter. The so-called ‘contact’, \(C\), specifies the likelihood of finding two composite fermions close enough to interact with each other in a certain integration volume. Stemming from the strong correlations, the number of pairs counted in this volume appears to be higher compared to the number derived from a downscaling of
macroscopic considerations; hence, an enhancement of collective effects occurs due to the energy carried by every pair. The contact encapsulates all of the information required to determine the many-body properties and depends on the $s$-wave scattering length (interaction strength), spin compositions and temperature of the system. The validity of the contact on a short interparticle range, $1/|a| \ll k \ll 1/r_0$, implies the effectiveness of the contact for large momenta and, furthermore, in the high momentum limit of the density distribution of the gas.

Exact universal relations can shed light on new aspects of strongly interacting Fermi systems and are relevant to research areas dealing with dilute Fermi systems with strong interactions. Usually, theoretical models for ideal cases can be found [126]. However, when interactions are switched on, methods like perturbation theory are necessary to describe the system [127–129]. The odd thing about the unitarity regime is that on the one hand the interactions become too strong, such that exactly these models, such as perturbation theory, fail. On the other, these strong interactions and correlations cause effects which must lead to a nonperturbative model (as everything is only depending on the scattering length and which falls out of the problem) and hence analytic expressions become available again.

Triggered by the Tan relations, further theoretical work has strived towards rederivations of some Tan relations within other theoretical models and derivations of new universal relations [68, 71–73]. Within a quantum field theory, universal relations follow from renormalisation and from the operator product expansion [67]. Such a framework allows the derivation of additional universal relations and the systematic inclusion of corrections associated with the nonzero range of interactions. Also, the ‘contact density’ appears in the short-distance expansion for the correlator of the quantum field operators that create and annihilate the atoms.

In this chapter, the general idea of universal relations is discussed. It is necessary to distinguish the contact for the homogeneous and trapped case. The relevant definitions are introduced in section 2.2. The contact appears in a number of universal relations. However, in section 2.3, we revisit only a selection of relations, which are the pair-correlation, the adiabatic sweep and the generalised virial theorem. Section 2.4 discusses briefly the contact in the crossover region in regard of chapter 6. In order to provide an understanding for the remainder of this thesis, different theories on the universal contact of strongly interacting fermions at finite temperatures are compared in section 2.5.
2.2 Definitions of the contact

Several presentations of the contact are circulating in the literature. The contact can be locally defined, denoted as $C(r)$, and is therefore sometimes called the contact density. In a homogeneous system with volume $V$, one can use the average contact, $VC$. Note that the contact of the uniform gas is also solely determined by the equation of state, as experiments have shown $\text{[130]}$. From a comparison of the prediction with the measured large momentum part, one could find out whether a particular equation of state is correct. In this way, the experimental data in the large momentum part give details about the equation of state of the uniform gas.

In order to predict $VC$ for a trapped cloud, the local density approximation (LDA) is used to calculate the local contact $C(r)$ from the locally uniform gas. In a trapped Fermi gas, the Thomas-Fermi approximation can be used to obtain locally a uniform gas with enough atoms to satisfy the validity of the thermodynamic limit and the thermodynamic quantities. Then, the local contact $C(r)$ is still an exact concept, the reason being that there is a negligible contribution to $C(r)/k^4$ for a small change of $\delta k \ll 1$. Using the Thomas-Fermi approximation, the spatial contact can be considered in a trapped gas as

$$\int C(r) d^3 r \equiv I. \quad (2.1)$$

Note that if the momentum distribution $n_\sigma(k)$ for a spin state $\sigma$ is normalised to the particle number, $N_\sigma = \int d^3 k / (2\pi)^3 n_\sigma(k)$, then $C$ is an extensive quantity with dimensions of a momentum. It is therefore conventional to consider $C$ in units of the Fermi momentum, $k_F$, divided by the total number of particles, $N = N_\uparrow + N_\downarrow$. For the remainder of this thesis, the notation of the contact reads for the homogeneous and trapped case, respectively,

$$\frac{C}{nk_F} \quad \text{(homogeneous)} \quad (2.2)$$

$$\frac{I}{Nk_F} \quad \text{(trapped)}. \quad (2.3)$$

2.3 The contact and universal theorems

The contact enters several relations and properties for strongly interacting Fermi gases. Some of those which have been experimentally accessible are discussed in the following. In order to introduce the Tan relations, the physical scenario and the
relevant length scales are outlined first. A non-interacting two-component Fermi gas is described by a wave vector \( \mathbf{k} \), spin \( \sigma = \uparrow, \downarrow \) and Fermi wave number \( k_F \). The energy for a noninteracting gas, \( E_{\text{non-int}} = \sum_{k\sigma} \epsilon_k n_{\sigma}(k) \), depends on its momentum distribution, \( n_{\sigma}(k) \equiv \langle c_{\sigma}^\dagger(k) c_\sigma(k) \rangle \), which is built up from annihilation (creation) operators \( c_{\sigma}(k) \) on the momentum states per spin. The potential range of the interaction is labelled \( r_0 \) and the mean interparticle distance is denoted as \( l = n^{-1/3} \).

The Fermi gas in the BEC-BCS crossover has additionally a large scattering length \( |a| \). To study short-range physics, the characteristic length scale, \( r \propto 1/k \), must be larger than the interatomic distance, \( r \gg r_0 \), but smaller than the other length scales, i.e. the system is dilute \( r \ll l \), strongly interacting \( r \ll |a| \) and ultracold \( r \ll \lambda_{dB} \) where \( \lambda_{dB} \) is the deBroglie wave length; actually, \( r_0 \ll 1/k \ll l \ll \lambda_{dB} \ll a \).

Equations [1.10] and [1.11] already pointed out constraints for the zero-range limit. This model simplifies the description of universal properties of a general model with strong interactions, since the scattering length is the only quantity that arises from interactions. Despite this interpretation, the disadvantage of the zero-range limitations are divergences of some observables, see below, and singularities in intermediate steps of the derivations of the universal relations.

The zero-range model enters the Schrödinger equation for non-interacting particles by considering the boundary conditions given by equation [1.11]. The \( N_1 \) particles in state \( |\uparrow\rangle \) and \( N_2 \) particles in state \( |\downarrow\rangle \) form a wave function, \( \Psi(r_1, \ldots, r_{N_1}; r'_1, \ldots, r'_{N_2}) \), which is according to the Pauli principle totally antisymmetric in the first \( N_1 \) positions, \( r_1, \ldots, r_{N_1} \), as well as the last \( N_2 \) positions, \( r'_1, \ldots, r'_{N_2} \). This wave function diverges for \( r_1 = r'_1 \) for any pair of fermions with different spin. When \( r_1 \) and \( r'_1 \) are
nearly equal, the wave function takes the form

\[ \Psi \left( R + \frac{1}{2} r, r_2, ..., r_{N_1}; R - \frac{1}{2} r, r'_2, ..., r'_{N_2} \right) \rightarrow \phi (r) \Phi (r_2, ..., r_{N_1}; r'_2, ..., r'_{N_2}; R) \]  

(2.4)

\( \Phi (R) \) is a smooth function, where \( R \) is the centre of mass position of the pair. Note that \( r \) is the general space coordinate and not assigned to any particle. \( \phi (r) \) is the zero-scattering wave function for two particles. In order to investigate correlations, it is obvious to consider the relative wave function between composite spins, which behaves like

\[ \phi_{\uparrow \downarrow} (r) = \left( \frac{1}{r} - \frac{1}{a} \right) \Phi (r_2, ..., R) + O (r). \]  

(2.5)

In the limit of closely spaced counterparts, i.e. short spacing \( r \), the interaction is understood as a contact interaction. The resulting interaction energy, \( E_{\text{int}} \), due to the large scattering length modifies the total energy of the system. The expectation value of the total energy of the system is the sum of the internal and potential energy, \( E_{\text{tot}} = E_{\text{int}} + E_{\text{pot}} = E_{\text{ia}} + E_{\text{kin}} + E_{\text{pot}} \). Both the kinetic energy, \( E_{\text{kin}} \), and the interparticle interaction, \( E_{\text{ia}} \), depend each sensitively on the short scale physics, or equivalently their large momentum physics \( k \to \infty \) in the limit of \( r_0 \to 0 \). It is necessary to cut off at a range such that the kinetic energy \( E_{\text{kin}} \) behaves \( \propto 1/r_0 \) for \( r_0 \to 0 \). Then, the momentum distribution decays like \( 1/k^4 \) at large \( k \).

Tan reformulated the integral representation of this famous s-wave contact interaction problem to relate the energy and momentum distribution to the contact. Tan showed that the sum of the two energies \( (E_{\text{int}} = E_{\text{kin}} + E_{\text{ia}}) \) is independent of the details of the short-distance physics. The simple relation between the energy and the momentum distribution, where the only microscopic parameter is the scattering length \( a \), may be written as

\[ E_{\text{int}} = E_{\text{ia}} + E_{\text{kin}} = \frac{\hbar^2 V C}{4\pi a m} + \lim_{k \to \infty} \sum_{k < k, \sigma} \frac{\hbar^2 k^2}{2m} \left( n_{\sigma} (k) - C k^4 \right). \]  

(2.6)

The summation over momentum is \( \sum_k \equiv V \int d^3 k / (2\pi)^3 \). The contact is defined as

\[ C \equiv \lim_{k \to \infty} k^4 n_{\downarrow} (k) \equiv \lim_{k \to \infty} k^4 n_{\uparrow} (k). \]  

(2.7)

The mathematical proof is elegant but lengthy and necessitates functional expressions much like generalised delta distributions. Therefore the interested reader is referred to the original literature or the review article.
Both equations 2.6 and 2.7 are Tan relations. In equation 2.7, $C$ is the same for both spin states. Equation 2.6 holds for any finite-energy states, few-body or many-body, equilibrium or nonequilibrium, zero temperature or finite temperature, superfluid state or normal state, and any (im)balanced spin population.

### 2.3.1 Pair-correlation function

In this thesis, the contact is experimentally determined via the definition of the short-range pair correlation function between fermions with opposite spins. Details on the measurement of the pair-correlation function and the contact can be found in chapters 6 and 7 of this thesis. The link to the pair correlations is probably the most intuitive interpretation of the contact. Taking equation 2.4 for the wave function for one fermionic pair of composite spin, one can express the spin-antiparallel pair correlation function as

$$g^{(2)}_{\uparrow\downarrow}(R) \equiv \int dR \langle \hat{n}_{\uparrow}(R - \frac{r}{2}) \hat{n}_{\downarrow}(R + \frac{r}{2}) \rangle.$$  (2.8)

where $\hat{n}_{\uparrow}$ and $\hat{n}_{\downarrow}$ are the number densities. Short-range ($R \to 0$) structure in a quantum fluid depends upon the relative wave function of the interacting fermions in different spin states, $\phi_{\uparrow\downarrow}(r) \propto 1/r - 1/a$, see equation 2.3. The contact parameter appears as a prefactor

$$g^{(2)}_{\uparrow\downarrow}(R \to 0) \approx \frac{C}{16\pi^2} \left( \frac{1}{r^2} - \frac{2}{ar} \right).$$  (2.9)

at small $r$. This means that the correlation between the number densities for the two spin states at points separated by a small distance $r$ diverge as $1/r^2$ and the coefficient of the divergence is proportional to the contact. Sometimes it is convenient to work in Fourier space, for instance, when probing the correlation function with Bragg spectroscopy. The Fourier transform of equation 2.9 is

$$\phi(k) = \frac{4\pi}{k^2} - \frac{(2\pi)^2}{a} \delta^3(k).$$  (2.10)

From equation 2.11 and 2.9 it follows that the expectation of the number of pairs of fermions with diameters smaller than a small distance $s \gg r_0$ or in a certain volume element $d^3r$ is

$$dN_{\text{pair}} = \frac{C(r)}{4\pi} d^3r \to \frac{s^4}{4} C(r).$$  (2.11)
The volume is $V = (4\pi/3)s^3$ and the number of pairs is $N_{\text{pair}} = N_i N_j$. Hence, the contact measures the number of pairs and fermions with different spin states that have a small separation. The $s^4$-scaling has a so-called anomalous scaling dimension, as it is not $s^6$, due to the strong correlations. The contact density corresponds to the local pair density when the range of interactions is similar to the interparticle distance, $1/k \sim l$. This is not to be confused with Cooper pairs which are totally dominated by a correlation of momentum, $1/k \gg l$.

### 2.3.2 Adiabatic sweep theorem

Another way the contact can be determined is via the adiabatic sweep theorem. The high-momentum tail of the momentum distribution of the gas determines the number of large momentum fermions (on average), see equation 2.7, $N_{k \to \infty} = VC/\pi^2 k$ plus higher order corrections which are negligible at large $k$. By tuning the inverse scattering length adiabatically while keeping the confinement potential fixed, the total energy $E$ of the gas will change. The adiabatic derivative of energy, expressed as $dE/d(1/a)$, and the contact for the magnitude of the $1/k^4$ tail are two independent quantities. Tan derived the simple, exact, and universal relation

$$\frac{\hbar^2 VC}{4\pi m} = \frac{dE}{d(-1/a)}$$

(2.12)

which is called the adiabatic sweep theorem. The rate of change of energy due to a small change of the inverse scattering length is proportional to the contact, for fixed entropy and particle numbers. The definitive form of equation 2.12 is not obvious. In other words, equation 2.12 gives the magnitude of the large momentum part, i.e. the contact density $C$, when the derivative of the energy with respect to $-1/a$ is taken. A small and slow change in the reciprocal of the scattering length is equivalently treated with quantum mechanical first-order perturbation theory which determines the amount of energy level shift. In the limit of a zero effective interaction radius, two fermions in opposite spin states only interact if they appear at the same position, so the energy shift should be proportional to the probability that this occurs. Then their momenta are large and nearly opposite and $VC$ a characteristic quantity. If one substitutes the energy with the free energy $F = E - TS$ in equation 2.12, then this expression determines the thermodynamics of the system, as $F$ enters all other thermodynamic functions. When changing the scattering length suddenly, the energy shift is also proportional to the contact. Tan also proposed that a sudden change in the scattering length could help to detect dissociation of a fermionic dimer.
2.3.3 Generalised virial theorem

A virial theorem has been shown in the unitarity limit stating that the total energy is twice the potential energy \( E = 2E_{\text{pot}} \), but theoretical calculations were restricted to \( 1/(k_F a) \equiv 0 \) and the local density approximation [19]. In chapter 4, this relation is used to calculate the temperature from the energy per particle at unitarity. Tan generalised the virial theorem to finite scattering lengths. Let us consider the general confinement potential \( V(\mathbf{r}) = r^\beta f(\mathbf{r}) \) where \( \beta > -2 \), \( \beta \neq 0 \) and \( \beta f(\mathbf{r}) > 0 \). \( f(\mathbf{r}) \) is a smooth function. Then the generalised virial theorem is

\[
E_{\text{tot}} - \frac{\beta + 2}{2} E_{\text{pot}} = -\frac{\hbar^2 C}{8\pi am}.
\]  

(2.13)

For harmonic trapping potentials, \( (m/2)\bar{\omega}^2 r^2 \), it follows \( \beta = 2 \) and

\[
E_{\text{kin}} + E_{\text{ia}} - E_{\text{pot}} = -\frac{\hbar^2 C}{8\pi am}
\]  

(2.14)

since \( E_{\text{tot}} = E_{\text{kin}} + E_{\text{ia}} + E_{\text{pot}} \). For a small and negative scattering length, \( a \to 0^- \), as in the deep BCS limit, the ratio behaves like \( C \propto a^2 \) and the virial theorem for the noninteracting Fermi gas is recovered. The unitarity case, \( a \to \infty \), and a trap confinement \( \beta = 2 \) lead to \( E = 2E_{\text{pot}} \). For large atom numbers \( N_\uparrow = N_\downarrow \gg 1 \) and a small and positive scattering length, \( a \to 0^+ \), the system approaches in the zero temperature limit a BEC of tightly bound molecules, so the above expression approaches the virial theorem for the Gross-Pitaevskii equation for these bosonic molecules [134] with scattering length \( a_m \approx 0.6a \) [27]. In equation 2.13, the details of the statistical distribution of the energy levels are unimportant, as long as the statistical weight decays sufficiently fast at large energy and the average value of \( C \) for the individual energy levels can be applied. Thus, this expression is valid for any finite temperature states in the canonical or grand canonical ensemble, as well as the ground state.

2.4 Contact in the BEC-BCS crossover

The contact parameter plays a part in setting the many-body properties and thermodynamic quantities in the phase diagram, as shown in figure 1.1. In the zero temperature limit, the contact has been calculated [84, 131, 132, 135] and measured with several experimental techniques [70, 132, 136], as shown in figure 6.7a in chapter 6. The contact will be adequate in the crossover region if it recovers the known results in both the BEC and BCS limits. The analytic expression of the ground
state energy is known in these limits. Using for instance the adiabatic sweep theorem equation \ref{2.12}, the contact is definable. In the following, the particle density is denoted as \( n = k_F^3 / (3\pi^2) \).

**Contact in the BEC limit**

In the BEC limit the ground state is expanded in terms of the Bose gas parameter \( n_d a_{dd}^3 \), where the dimer-dimer scattering length is given by \( a_{dd} = 0.6a \).

\[
E_V = n_d E_d + \frac{2\pi \hbar^2 n_d^2 a_{dd}}{m_d} \left( 1 + \frac{128}{15\sqrt{\pi}} \sqrt{n_d a_{dd}^3} + \ldots \right)
\]  

(2.15)

where \( n_d / 2 \) is the dimer density and \( m_d = 2m \) is the dimer mass. \( E_d = -\hbar^2 / (ma^2) \) is the energy of an isolated dimer at rest. The second term considers the mean-field energy of a BEC of dimers. For \( 1 / (k_F a) \to +\infty \) the contact becomes \( C \to 4\pi n / a \) from equation \ref{2.12} and \ref{2.15}.

**Contact in the unitarity limit**

In the unitarity limit, the expansion is

\[
E_V = 3\frac{\hbar^2 k_F^2 n}{5 \cdot 2m} \left( \xi - \frac{\zeta}{k_F a} - \frac{5\nu}{3(k_F a)^2} + \ldots \right)
\]  

(2.16)

The universal numerical constant, \( \xi \approx 0.42 \pm 0.01 \), is used in this work to calculate the true temperature. The parameters \( \zeta \approx 1 \) and \( \nu \approx 1 \) were originally extracted with Quantum Monte-Carlo calculations, but more recently \( \zeta \) was measured to be \( \zeta \approx 0.91 \). Also, \( \zeta \approx 0.95 \) from equation \ref{2.12} and \( \xi \approx 0.383(1), \zeta \approx 0.901(2), \nu \approx 0.49(2) \) from QMC calculations. After applying equation \ref{2.10} and \ref{2.12} the contact is of the form \( C \to k_F^4 2\zeta / (5\pi) \). This dependence on \( k_F^4 \) is on dimensional grounds as the interaction does not provide a length scale at \( 1 / (k_F a) = 0 \).

**Contact in the BCS limit**

In the BCS limit, the ground state energy is expandable in terms of the interaction parameter \( 1 / (k_F a) \) and may be written as

\[
E_V = 3\frac{\epsilon_F n}{5} \left( 1 + v_{BCS,1} (k_F a)^1 + v_{BCS,2} (k_F a)^2 + v_{BCS,3} (k_F a)^3 + \ldots \right)
\]  

(2.17)
where the coefficients $v_{BCS,1} = 10/(9\pi)$ and $v_{BCS,2} = 4(11 - 2\ln 2)/(21\pi^2)$ are exact \[137\] but $v_{BCS,3} = 0.030(5)$ is numerical \[137\]. Consequently, the contact follows from equations 2.17 and 2.12 and approaches in the BCS limit $C \to 4\pi^2 n^2 a^2$ and the contact density decreases to 0 as $a \to 0^-$ with an $a^2$-dependence. In contrast, the BCS superfluid energy has an exponential character, $\propto \exp(-\pi/2k_F |a|)$ for $a \to 0^-$. While Cooper pairs can be explained with standard BCS equations, the BCS theory does not predict the correct value of $C$ in the BCS limit \[65\].

### Verifications of the contact in the BEC-BCS crossover

The contact can be inferred from different definitions, which makes the contact so powerful and reflects its versatility, and its values can be taken from different kinds of experiments. Experimental verifications showed the monotonic decrease of the contact from the BEC to BCS limit. In this work, Bragg spectroscopy is used to extract the behaviour of the pair-correlation function at high momenta, \[26, 75, 148\] and is presented in chapter 6.

The contact was first extracted with photo-association \[70\]. The excitation rate $\Gamma = \Omega^2 R/\gamma N_{mol}$ depends on in the Rabi frequency $\Omega_R$, the line width $\gamma$ and the number of photo-associated molecules $N_{mol}$.

The contact is directly accessible by using equation 2.7 and measuring the large momentum tail of the radial momentum distribution $n(k)$ \[133\]. The external interactions are switched off through fast ramps of the magnetic field such that the scattering length vanishes. The radial momentum distribution is taken from an absorption image of a ballistically expanded cloud and an Abel transform. Then, the momentum distribution is totally determined by the kinetic energy. The measurement will exhibit a curve like that shown in figure 2.1. While the cloud is always imaged at zero-scattering length, the cloud can be prepared at different initial scattering lengths (magnetic fields); therefore this method allows the contact to be measured across the BEC-BCS crossover. This method depends on the speed of the magnetic field ramp to zero-scattering length and good image qualities.

Radio-frequency (rf) and photo-emission spectroscopy (PES) measure the bulk spectral function of an ultracold gas. The rf-transition rate $\Gamma(\nu)$ for an excitation frequency $\nu$ shows at high frequencies a $\nu^{-3/2}$-dependence such that $\Gamma(\nu) \to C/(2^{5/2}\pi^2\nu^{3/2})$ \[133, 151\]. The rf-transition between two (hyperfine) states selects the contact between atoms in these two (hyperfine) states, given final state effects are small. Similarly, PES can also couple out atoms from a certain state \[133\]. Angle-resolved PES (ARPES) can additionally measure excitation spectra depend-
ing on the transferred momentum, such that one obtains information about the total momentum distribution \( n(k, \nu) \). After frequency integration and using again equation 2.7, the contact can be extracted.

Equation 2.12 has also been measured since adiabatic sweeps are controllable with adiabatic magnetic field ramps [133]. Tan suggested an experimental sequence to directly test the adiabatic sweep theorem in a trap at any temperature [64]. Also, in an adiabatic sweep the entropy is conserved. The experimental verification is reported in [133]. The total energy of a cloud can be measured with the mean square size, \( \sigma^2 \), \( E_{\text{int}} = E_{\text{kin}} + E_{\text{ia}} = (2/\epsilon_F)(m/2)\omega^2\sigma^2 \) in terms of the Fermi energy, \( \epsilon_F \). By measuring the mean square size with and without the external potential and comparing images at zero- and finite scattering length, the contact can be extracted from equation 2.14. For different starting scattering lengths, the contact across the BEC-BCS crossover is obtained.

The homogeneous contact may be extracted from the equation of state [130].

### 2.5 Universal contact at finite temperatures

The contact is an important quantity for characterising many-body properties and phases in strongly interacting Fermi gases. The contact \( C \) depends on the temperature \( T/T_F \) (relative to the Fermi temperature \( T_F = \hbar^2 k_F^2 / (2m k_B) \)) and can be used to study the complete momentum distribution in the entire \((-1/\langle k_F a \rangle, T/T_F)\)-plane (for balanced populations of the two spin states). There remain open questions about the details of the nature of unitary-limited Fermi gases and measurements of the contact may help to clarify the mysterious pseudogap. The determination of the temperature of a strongly interacting Fermi gas is complicated and will be discussed in chapter 5. In the next sections, the contact is briefly reviewed in relation to finite temperatures, because the experimental results are compared to the different calculations for the trapped case in chapter 4. Different theoretical models describe the zero-temperature coupling as well as the temperature dependent contact at unitarity, which are characterised by the contact, in the temperature-coupling phase diagram.

The contact parameter describes how the short-range (high-momentum) physics impacts on the bulk properties of the system. In contrast, it is not clear if the contact can be related to the low-energy properties of the system, where so far the so-called ‘Bertsch parameter’ and the pairing gap are characteristic features [92, 182, 183]. Although only the trapped case is measured in this work, it is necessary to mention also the homogeneous case to understand where the physical signatures find their origin. The accuracy of the theoretical models can be quantified by their predictions.
for the contact.

2.5.1 Thermodynamic contact from the entropy

Tan suggested the determination of the temperature in the unitarity regime with the frequently used projection of the temperature to the weakly interacting regime (BCS side) and then using the adiabatic sweep theorem, equation $f_{2.12}$. The entropy is preferred over the reduced temperature $T/T_F$ due to its invariance under adiabatic sweeps. Since the contact depends on the temperature, the determination of the contact from the entropy and inverse scattering length would represent an indirect temperature measurement. Starting from the BCS side and tuning the inverse scattering length adiabatically into unitarity regime, or vice versa, one knows the entropy of the final state from that of the well-known initial state. For various initial entropies the derivative of energy with respect to entropy can be calculated at any scattering length to obtain the temperature of the gas $f_{2.18}$. This principle has the advantage of being model-independent, since almost no theoretical approximations are involved.

2.5.2 Contact for the trapped case at zero temperature

The trapped contact at unitarity takes an analytic expression at $T = 0$ $f_{2.18}$

$$
\left( \frac{T}{Nk_F} \right) = \frac{256}{105\pi} \xi^{-1/4} \left( \frac{C}{nk_F} \right) = \frac{512\xi}{175\xi^{1/4}}.
$$

(2.18)

because the density profile, $n(r)$, is exactly known. The two universal parameters $\xi$ and $\zeta$ are related to the expansion of the ground state energy per volume of an interacting Fermi gas at unitarity, see equation $f_{2.18}$. They were measured to be $\xi \approx 0.41(1)$ and $\zeta \approx 0.93(5)$ in the ENS group $f_{2.18}$, however $\zeta \approx 0.90(1)$ from a Quantum Monte Carlo simulation $f_{2.18}$.

2.5.3 Below the critical temperature

Various strong coupling theories can be used to model strongly interacting Fermi gases beyond standard perturbative methods. The given strong interactions require assumptions in the fundamental equations (many-body Schrödinger equation, s-wave contact problem), which reduce the theoretical model of choice. The Feynman-diagrammatic structure in the $t$-matrix approximations needs an infinite ladder sum to solve the principal equations, which are the $t$-matrix, particle-particle propagator
and self-energy, depending on the Green’s function \[153, 155\]. These equations can be self-consistent (GG) \[156–158\], or non-self-consistent (G\(_0\)G\(_0\)) \[159–161\]. The Nozière-Schmitt-Rink procedure uses additional path integrals to include Gaussian (pair) fluctuations and is in the following referred to as the NSR or GPF method \[83, 146, 162–164\]. While this thesis was being written it was discussed which of the strong coupling theories is the most appropriate. The absence of a small parameter and the possibility to choose a particular approximation eventually prevent a common agreement on the prediction for the contact, especially in the critical temperature region. Details of these techniques can be found in \[135\]. Another possibility is provided by quantum Monte-Carlo simulations (QMC) \[131, 132\].

**Homogeneous case**

Due to the different approximations in the strong coupling models, the predictions deviate slightly and show discrepancies around the critical temperature, especially in the calculations for the homogeneous case. However, the result influences its interpretation. The entropy relation

\[
\left( \frac{\partial L}{\partial T} \right) = \frac{4\pi m}{\hbar^2} \left[ \frac{\partial S}{\partial (-1/a_s)} \right]_{T,\mu} \tag{2.19}
\]

allows the contact to be directly obtained by taking the temperature derivative in equation \[165\]. Similar to the suggestion of Tan, the temperature dependence of the contact is determined by the variation in the entropy with respect to the coupling constant. It has been argued that at low temperatures, phonon excitations contribute significantly with a maximum at \(\sim (0.5 \pm 0.1) \, T/T_F\), using the G\(_0\)G\(_0\)-method and ab-initio G\(_0\)G\(_0\)-method over the whole temperature range \[84, 85, 165\]. The interpretation is that the local order is established by pairing fluctuations around the critical temperature \[84\]. The contact is enhanced where pseudogap phenomena are maximal. Fluctuations above \(T_C\) strengthen the local pairing correlations in the absence of the long-range order. However, the contact is proportional to the two-body correlation function, which is affected by pairing fluctuations in the particle-particle channel. The definitions for the short-range boundary conditions need to be refined, i.e. to identify the approximate spatial boundary between short-range \((r \ll k_F^{-1})\) and medium-range \((r \approx k_F^{-1})\) physics. The characteristic moment \(k_c\) is introduced, such that \(1/k_c^3\) is the spatial range at which two-body physics interfaces with medium-range physics, and is of the size of the composite boson. It is an open question how the values of the contact are influenced by this medium-range physics and how the presence of a pseudogap connects to the single-particle excitation spectrum.
In the NSR (GPF) method the contact decreases monotonically without a maximum due to the break down of the strong coupling theories around the critical temperature \[135, 160, 167\]. Within the GPF-theory, the phonon excitations contribute in a temperature window \(T < 0.07 T_F \ll T_C\) \[135\]. Fermi liquid theory predicts a maximum, but its applicability is doubtful in the relevant short length scale \[135\].

In comparison with strong coupling theories, QMC simulations offer another way to access the contact \[131, 132\]. They seem to be especially useful due to their precision and freedom from uncontrolled approximations. One can derive Tan’s expression for the contact parameter using just the short-range behaviour of the ground-state many-body wave function and calculate the momentum distribution and contact density. Within QMC methods, extracting the contact from the equation of state is the simplest and most reliable way \[131\]. QMC simulations for the momentum distribution at different temperatures can also show that the contact may have a maximum at \(\sim 0.4 T/T_F\) supporting the phononic scenario where the contact increases with \(T/T_F\). However, problems may arise from low density edge effects in a trapped cloud.

All theories predict that the contact decays slowly at higher temperatures because it is weakly depending on the long-range order. Measuring the spatial contact in the homogeneous case provides more information compared to the contact in the trapped case, where the different shells in the energy distribution have different local \(T/T_F\). The result found for the universal homogeneous contact calculated with different approaches from strong-coupling theories can be briefly summarised: With the GPF theory \(C/(nk_F) = 3.34\) was found whereas \(C/(nk_F) = 3.02\) followed from GG calculation \[168\] and \(C/(nk_F) = 3.23\) resulted from the \(G_0G_0\) theory \[84\]. Experimental investigations showed \(C/(nk_F) = 3.51 \pm 0.19\) from the equation of state data at ENS \[130\]. QMC calculations have yielded \(C/(nk_F) = 3.40\) \[75\], \(C/(nk_F) = 3.39(6)\) \[131\] and \(C/(nk_F) = 2.95 \pm 0.1\) \[132\].

**Trapped case**

Compared to the homogeneous case, the contact is translated into the trapped case with a weighting of the energy shells, \(n(k)^{4/3}\). Experimental values for \(I/(Nk_F)\) were found to be \(3.4 \pm 0.18\) (ENS) and \(3.1 \pm 0.3\) (this work). The theoretical predictions for \(I/(Nk_F)\) are \(3.26\) (GPF), \(3.03\) (GG) and \(3.05\) (\(G_0G_0\)). Trap averaging washes out the maximum just below \(T_C\) \[51, 57\] and brings all predictions in qualitative agreement over the whole temperature range. The contact for an isotropic trap is derived from equation \[141\] and the LDA. The Fermi momentum is replaced by
CHAPTER 2. UNIVERSAL RELATIONS

\[ k_F^3 = n(r)3\pi^2 \] and the density, \( n(r) \), depends on the reduced temperature, \( T/T_F(r) \). The integral to obtain \( I/(Nk_F) \) is cumbersome and can be solved in different numerical ways. Due to the particular calculations with strong-coupling theories at low temperatures, \( T < 0.3 \, T_F \), the universal trapped contact spreads over the values mentioned above.

2.5.4 Above the critical temperature

Above the critical temperature the fugacity is a small parameter, \( z \equiv \exp(\mu/(k_B T)) \), and therefore quantities can be expanded as a function of the fugacity or inverse fugacity. The quantum virial expansion (QVE) has been shown to accurately describe the high-temperature range in strongly interacting Fermi gases [116, 149, 169–171]. For the contact calculations, either one can insert the expression of the temperature [165] into the QVE, or one can develop, analogously to the QVE of thermodynamic potentials [169], the contact in terms of universal temperature independent coefficients as a consequence of fermionic universality [135]. Thus the contact evolves in powers of the fugacity like \( C \propto [c_2 z^2 + \ldots + c_j z^j + \ldots] \). The contact coefficients, \( c_j = \partial \Delta b_j/\partial (\lambda_{dB}/a) \), include the \( j \)-th virial coefficient, \( \Delta b_j \), and the thermal deBroglie wave length \( \lambda_{dB} \). The first virial coefficients were predicted to be \( \Delta b_{2,\infty} = 1/\sqrt{2} \) [172] and \( \Delta b_{3,\infty} \approx -0.355 \) [169] and confirmed by the ENS group [173].

Homogeneous case

In the homogeneous case, the contact-QVE is valid down to \( T \sim T_F \) and one finds \( c_{2,\infty} = 1/\pi \) and \( c_{3,\infty} = -0.141 \) [135]. These enter the high-temperature dimensionless contact for the homogeneous gas as

\[
\frac{C}{nk_F} = 3\pi^2 \left( \frac{T}{T_F} \right)^2 [c_{2,\infty} z^2 + c_{3,\infty} z^3 + \ldots]
\]

(2.20)

where the fugacity \( z \) is determined by a number equation [171].

Trapped case

For an isotropic trap the contact-QVE works for temperatures down to 0.5 \( T/T_F \) because the contact coefficients are by a factor of \( j^{3/2} \) smaller than for harmonic traps, \( c_{j,\infty,T} = c_{j,\infty}/j^{3/2} \). As discussed before, for a harmonic trapping potential \( V_T(r) \) the LDA can be applied. This modifies the chemical potential \( \mu(r) = \mu - V_T(r) \) and the local fugacity \( z(r) = \exp(\mu(r)/(k_B T)) \equiv z \exp(-V_T/(k_B T)) \). The contact
coefficients are determined to be \( c_{2,\infty,T} \cong 1/(2\sqrt{2}\pi) \) and \( c_{3,\infty,T} \cong -0.0271 \) \cite{135}. The dimensionless contact depends on these as

\[
\frac{T}{Nk_F} = 24\pi^{3/2} \left( \frac{T}{T_F} \right)^{7/2} \left[ c_{2,\infty,T} z^2 + c_{3,\infty,T} z^3 + \ldots \right].
\]

This expression explicitly shows that the contact in harmonic traps decays much faster than in the homogeneous case. The reason is the reduction of the peak density at the trap centre at high temperatures.

### 2.6 Summary

In this chapter the problem of unitarity limited Fermi gases has been introduced. The lack of a small parameter complicates standard perturbation theories in this strongly interacting regime. Universal relations overcome this problem by examining the short-range structure, which is equivalent to characterising the problem in the high-momentum limit. Many important relations and thermodynamic quantities are related to the central parameter, the contact \( C \). For the spin-balanced gas, it is possible to measure the interaction and temperature dependence of the contact and compare the data to numerical and analytical models. Contact measurements are complementary to the measurements of the equation of state. The contact is proportional to the observed energy, and therefore it is a more sensitive test of theoretical predictions than a direct measurement of the thermodynamic quantity \( [135] \). Although there has been theoretical work on the temperature dependent contact, discrepancies at the critical temperatures need to be resolved by accurate experiments. Possible candidates are measurements of the homogeneous equation of state near unitarity, measurements of the tail of the spatially-resolved rf spectrum at unitarity, and measurements of the spatially-resolved Bragg scattering spectrum at unitarity.
Chapter 3

Structure factor of a Fermi gas

The strong correlations found in interacting Fermi gases at unitarity naturally lead one to the study of the spectrum of elementary excitations. In a measurement, they will respond linearly to an external probe if the interaction with the system is weak and the system behaves as if it was undepleted. In general, inelastic scattering of particles is a well established means of investigating correlation functions. Different energy ranges can be covered: in solid state physics, fast electrons are used to study charged Fermi liquids, inelastic scattering of slow neutrons measures correlations in $^4$He and superconductors, whereas Bragg scattering of photons can probe correlations in ultracold atomic quantum gases. In this chapter the theory and analysis of inelastic Bragg scattering is outlined to form the physical background for the experiments explained in detail later in the thesis.

3.1 Introduction

Linear response theory allows many-body problems to be addressed for interacting systems at all temperatures as long as the probe-coupling interaction is weak. The probe-system coupling can be treated as a weak perturbation and therefore many quantities can be derived accurately from first order perturbation theory, which exactly is the linear response of the system. Bragg scattering in the low momentum limit can reveal the collective behaviour of the system through macroscopic excitations. Excitations at high momenta reveal the momentum distribution or single-particle excitations of the system. A detailed discussion on the differences of high and low momentum Bragg spectroscopy of Bose-Einstein condensates is presented in [17], where the Bogoliubov theory is applied to explain the excitation spectra. Essential in linear response theory is the dynamic structure factor, $S(q, \omega)$, which encapsulates all information about correlations and obeys particle conservation as
well as sum rules. To measure \( S(q, \omega) \), linear response theory links it to a response function containing the system properties and therefore \( S(q, \omega) \) is a measurable quantity that probes the spectral properties of the system. The static structure factor, \( S(k) \), gives the net momentum transfer for the energy unresolved dynamic structure factor. It represents the Fourier transform of the two-body correlation function \( [1] \). Linear response theory covers a wide range of scenarios and detailed discussions can be found in various textbooks \([1, 76]\). However, for this thesis, it is sufficient to consider density-density correlations, i.e. the measured density profile is the response to a periodic perturbation of the probe density profile. Only the limit where the transferred momentum is much larger than the Fermi momentum \( |k| \gg k_F \) will be discussed here. Not included in these explanations is the low momentum limit which could disclose superfluid mechanisms due to collective behaviour.

It is common to define the dynamic structure factor either in terms of the momentum and energy, such that \( S(q, E) \), or in terms of the wave vector and frequency, thus \( S(k, \omega) \). In this chapter, a mixed notation is used due to convenience and the dynamic structure factor consists of the momentum and the frequency, \( S(q, \omega) \), while \( \hbar \) is inserted in the equations if necessary.

Beginning with the motivation of Bragg spectroscopy as a tool to investigate pair correlations, the principles and advantages are discussed in section 3.2. The spectral functions are related to the dynamic structure factor, as shown in section 3.3. Derived from these is the static structure factor, section 3.4, which is linked to the pair-correlations. In section 3.5 it will be pointed out that sum-rules provide a powerful constraint on the spectral function. The link to the linear response function is made in section 3.6 and the response at finite temperature is discussed in section 3.7, introducing the detailed balancing which arises from the fluctuation-dissipation theorem. An explanation on the acquisition of \( S(q, \omega) \) and \( S(q) \) from the measurements is the subject of section 3.8.

### 3.2 Bragg spectroscopy of pair-correlations

A direct measurement of pair-correlations in ultracold Fermi gases can be difficult because the spatial range of interest is usually much smaller than the resolution of typical imaging systems. Bragg spectroscopy offers a model-independent tool to probe pair-correlations in momentum space. The probe particles are photons provided by the Bragg laser beams. The total momentum and the energy of the photons have to be conserved in a photon absorption-emission process, where an
atom compensates the momentum and energy transfer. By measuring the change in the centre of mass or the energy of the atomic distribution after a short Bragg pulse, the spectral response becomes evident. This leads to the dynamic structure factor and the static structure factor, which is linked to the two-body correlation function and the contact, $C$, see chapters 2 and 6.

### 3.2.1 Principle of Bragg scattering

An ultracold quantum gas is illuminated with two low-power Bragg beams that intersect at an angle, $\theta$, and form a moving periodic potential. The wave vector, $k_L = 2\pi/\lambda_{Br}$, of the laser depends on the wave length, $\lambda_{Br}$. Absorption of $N$ photons from one laser beam and subsequent stimulated emission into the other imparts a momentum to a number of atoms where the order of the scattering process is $N$. The momentum transfer may be written as

$$ q = \hbar k = 2N\hbar k_L \sin \left( \frac{\theta}{2} \right). \tag{3.1} $$

The energy transfer to an atom with an initial momentum $k_{ini}$ is

$$ \hbar \omega \equiv E_n - E_0 = \frac{q^2}{2m} + \frac{\hbar k_{ini} \cdot q}{m}, \tag{3.2} $$

where $\omega$ denotes the frequency difference between the two Bragg beams. These two equations fulfill energy and momentum conservation. A resonance will occur when the momentum of the moving potential, $2\hbar k$, matches the momentum of the atom $mv$ with mass $m$. For single atoms this simplifies to the usual Bragg resonance frequency, $\omega_R = 2\hbar k^2/m$. The second term in equation 3.2 is related to the Doppler shift of the resonance and shows that Bragg scattering is a velocity-selective process. Energy and momentum can be decoupled if the angle between $k_{ini}$ and $q$ is small. The energy is varied by the frequency difference, $\omega$, between one beam, $c/\lambda_{Br}$, and the other, $(c/\lambda_{Br}) - \omega$, where $c$ is the speed of light. The Bragg scattering process is a two-photon process where fluctuations are caused by the time-varying electric field of the Bragg laser beams. Hence, the potential seen by the atoms oscillates with time and induces transitions of energy $\hbar \omega$.

The spatial period of the Bragg potential sets the momentum range being probed. In spin-balanced fermionic gases, two fermions may scatter as a single particle with mass $2m$ when the size of the pair is small compared to $1/k$, where $k = |k|$. Since the momentum range is freely selected, the relative probe momentum $k/k_F > 2$ allows the fraction of pairs to be mapped within a particular size range.
0 < r < λ_{Br}. A sketch of this scenario is presented in figure 3.1 in an energy-momentum diagram.

\[
\begin{align*}
\text{excited state} & \quad E \\
\text{ground state} & \quad \frac{\hbar q^2}{2m} \\
\end{align*}
\]

\[\Delta = 1.5 - 2.0 \text{ GHz}\]

\[\frac{c}{\lambda_{Br}} = 2\pi 446 \text{ THz}\]

\[\Omega = 0 - 500 \text{ kHz}\]

\[q = 2\hbar k\]

**Figure 3.1:** Principle of Bragg scattering sketched as energy versus momentum. The energy of the two-photon process between the ground and excited state lies on a \( q^2 \)-parabola. In \(^6\text{Li}\), it is the transition \(|2^2S_{1/2}, F = 1/2, m_F = -1/2\rangle \rightarrow |2^2P_{1/2}, F = 3/2, m_F = -1/2\rangle\). The detuning \(\Delta\) from the upper level is necessary to avoid spontaneous scattering. For a given momentum transfer, \(q\), there exists a resonance frequency \(\omega_R = 2\hbar k^2/m\). The laser frequency of the Bragg beams, \(c/\lambda_{Br}\), is given by the speed of light, \(c\), and the Bragg wave length, \(\lambda_{Br}\).

### 3.2.2 Advantages of Bragg spectroscopy

The concept of inelastic scattering is a traditional technique to probe many-body quantum systems [76], such as inelastic neutron scattering in superfluid helium or inelastic light scattering from ultracold Bose gases [176–179]. After the first steps in manipulating atomic samples with Bragg spectroscopy [180–182], its potential for the investigation of properties of ultracold quantum gases has been slowly appreciated [183]. In Bragg spectroscopy, two momentum states of the same internal atomic state are connected by a stimulated two-photon process: The stimulated process implies higher resolution and sensitivity in the measurement as the signal is background free. Compared to radio-frequency spectroscopy [56, 86] or Raman spectroscopy, Bragg scattering does not involve a third atomic state or an inter-
3.3 Dynamic structure factor

mediate metastable state and thus final state interaction effects are avoided. The momentum range is broad and easily selected for fermionic gases. The momentum transfer $q = \hbar k$ and energy transfer $\hbar \omega$ are predetermined by the laser beams and not postevaluated from the measurements. Bragg spectroscopy can probe density fluctuations and measures $S(q)$ which probes the two-body correlation function in a many-body system. Coherent properties and $S(q, \omega)$ have been measured in atomic Bose-Einstein condensates [26, 77] as well as the static structure factor [78, 79]. In the fermionic case, Bragg spectroscopy has been successfully used to determine the dynamic and static structure factors in the BEC-BCS crossover at a single momentum [80]. Bragg spectroscopy of atoms confined in periodic lattices aims to find effects similar to those found in solid state physics, for instance band structures and transitions from superfluid to Mott-insulator states [183, 187].

3.3 Dynamic structure factor

The Bragg spectra provide access to the dynamic structure factor, $S(q, \omega)$, which characterises the cross section for inelastic scattering. The momentum and energy transferred to the cloud lifts the ground state, $|0\rangle$, into an excited state, $|n\rangle$, according to equation (3.2), and the particle gains a momentum $q$. As mentioned above, this is a stimulated process. The many-body system is perturbed by the periodic potential, $V_r$, formed by the electric fields of the Bragg laser beams. The Fourier transform of the perturbing potential, $V_q = 2\hbar \Omega_R$, can be expressed in terms of the two-photon Rabi frequency, $\Omega_R$, which expresses the coupling strength between the atom and light field. Implicitly, it is assumed that at $t = -\infty$ the system is governed by the unperturbed Hamiltonian. The interaction between the atoms and the probe, $H_{int} = H_{Br}$, may be written as

$$H_{int} = \frac{V_q}{2} \left( \delta \rho_q^\dagger e^{-i\omega t} + \delta \rho_q e^{i\omega t} \right). \quad (3.3)$$

The Fourier transform of the particle density (operator) is defined as

$$\rho_q = \int d^3r \rho(r) e^{-iqr} = \sum_j \int d^3r \delta(r - r_j) e^{-iqr} = \sum_j e^{-iqr_j}. \quad (3.4)$$

The fluctuations generated by the external field of the particle density, $\delta \rho_q = \rho_q - \rho_0$, oscillate about the average value, $\rho_0$. Let $H_{int}$ couple weakly to the ground state of the fermionic cloud $|0\rangle$. This implies that the eigenstates are unperturbed before,
\[ |0, \mathbf{p}\rangle \), and after, \( \langle n, \mathbf{p} - \mathbf{q} | \), the scattering event. Hence, 

\[ \langle n, \mathbf{p} - \mathbf{q} | H_{\text{int}} | 0, \mathbf{p}\rangle = V_q \langle n | \delta \rho^\dagger_{\mathbf{q}} | 0 \rangle \equiv V_q \langle \delta \rho^\dagger_{\mathbf{q}} | n_0 \rangle. \]  (3.5)

The density fluctuations, \( \delta \rho^\dagger_{\mathbf{q}} \), depend on the matrix elements between the exact many-particle eigenstates in the absence of the Bragg pulse. The external particle thus probes the density fluctuations in the system. The probability, \( W(\mathbf{q}, \omega) \), of momentum and energy transfer per unit time is readily given by the golden rule of second order perturbation theory, i.e. the summation runs over all states, \( |n\rangle \), that are coupled to the ground state, \( |0\rangle \), by the density fluctuations \( \delta \rho^\dagger_{\mathbf{q}} \), so

\[ W(\mathbf{q}, \omega) = 2\pi |V_q|^2 S(\mathbf{q}, \omega) \]  (3.6)

with

\[ S(\mathbf{q}, \omega) = \hbar \sum_n \left| \langle \delta \rho^\dagger_{\mathbf{q}} | n_0 \rangle \right|^2 \delta (\omega - \omega_{n0}) \]  (3.7)

and \( \omega_{n0} = \omega_n - \omega_0 \). \( \omega \) and \( \mathbf{q} \) depend on each other as in equation 3.2. Thus \( S(\mathbf{q}, \omega) \) embodies all the properties of the many-body system that are relevant to the scattering of the Bragg photon and it represents the maximum information of the system behaviour that can be obtained in a particle scattering experiment. The distribution of squared matrix elements for each allowed transition reflects the excitation spectrum of the system. At \( T = 0 \), \( S(\mathbf{q}, \omega) \) is real and positive, i.e. \( S(\mathbf{q}, \omega \leq 0) = 0 \), since all excitation frequencies, \( \omega_{n0} \), are necessarily positive. The spectral density of the state \( \delta \rho^\dagger_{\mathbf{q}} | 0 \rangle \) corresponds to correlations between density fluctuations at different times. The correlation between a density fluctuation at time \( t = 0 \) and at time \( \tau \) is expressed by the correlation function, \( S(\mathbf{q}, \tau) \), which is the Fourier transform of \( S(\mathbf{q}, \omega) \) with respect to time. In the high momentum limit collective features are irrelevant, since the probe can directly scatter out individual constituents, but the momentum distribution \( n(\mathbf{p}) \) of the sample can be investigated. In Fermi gases the momentum distribution is a key quantity as it dominates the dynamics and properties. In the high momentum limit, \( S(\mathbf{q}, \omega) \) can be written as

\[ S_{\text{IA}}(\mathbf{q}, \omega) = \int d\mathbf{p} n(\mathbf{p}) \delta \left( \hbar \omega - \frac{(\mathbf{p} + \mathbf{q})^2}{2m} + \frac{\mathbf{p}^2}{2m} \right). \]  (3.8)

This impulse approximation is uniquely determined by the momentum distribution of the cloud \([188] \). From here, one can see that a resonance occurs at the recoil
3.3 Dynamic Structure Factor

frequency, \( \omega_R = \frac{\hbar q^2}{2m} \), when \( \mathbf{p} = 0 \). Note that for a noninteracting Fermi gas the spectral function of \( S(\mathbf{q}, \omega) \) reflects the particle density distribution, \( n^0(p) \), of an ideal Fermi gas \([80]\), see figure 3.2.

Figure 3.2: The dynamic structure factor for an ideal Fermi gas, \( S_{IA}^0(k, \omega) \), in the impulse approximation at \( T = 0 \) shows the momentum transferred with a Bragg pulse. The resonance occurs at \( \omega = \omega_R \).

For a non-interacting Fermi gas, an illustration is given by figure 3.3a. The ground state, \( |0\rangle \), consists of all plane waves filled up to the Fermi sphere with radius \( p_F \), or \( \hbar k_F \). When the operator \( \delta \rho^+_\mathbf{q} \) acts on the ground state, single-particle transitions are induced. A particle in state \( \mathbf{p} \) is annihilated, \( c_{\mathbf{p}} \), and in state \( \mathbf{p} + \mathbf{q} \) created, \( c^\dagger_{\mathbf{p} + \mathbf{q}} \), such that \( \delta \rho^+_\mathbf{q} = \sum_p c^\dagger_{\mathbf{p} + \mathbf{q}} c_\mathbf{p} \) for the wave vector \( \mathbf{p} \) and spin \( \sigma \), which is implicitly included in the summation. \( \rho^+_\mathbf{q} \) represents a superposition of particle-hole pairs each of net momentum \( \mathbf{q} \) since particle scattering is described equally well as creation of a particle-hole pair. Because of the exclusion principle, a given pair in the ground state can only be excited if the state \( \mathbf{p} \) is filled and the state \( \mathbf{p} + \mathbf{q} \) is empty. Hence, the allowed values of \( \mathbf{p} \) are located at the intersection between the ground state Fermi sphere with \( p_F \) and the sphere with \( p'_F \) of empty states which is displaced by an amount \( -\mathbf{q} \). If \( k < 2k_F \), the Pauli exclusion principle begins to reduce the number of available final states. The excitation spectrum of particle-hole
CHAPTER 3. STRUCTURE FACTOR OF A FERMI GAS

Figure 3.3: (a) Left: particle with Fermi surface at radius $p_F$. Right: the particle gains momentum $-q$. The fermionic character restricts scattering to particles which fulfill initial momentum states with $p < p_F$ as well as final states with $|p + q| > p'_F$. All of these excitations are represented by the grey shaded area. The closer the relative momentum transfer, $(q/p_F)$, is to unity, the more excitations can contribute as the probing wavelength becomes closer to the correlation length. In contrast, a large momentum transfer, $q/p_F \gg 1$ corresponds to excitations in the corners of the grey shaded area and the signal of correlated pairs is smaller. (b) Visualisation of particle-hole excitations for a non-interacting Fermi gas in time-of-flight. Atoms are excited when they are resonant with the Bragg momentum. The out-scattered atoms travel within a release time and leave a slice in the momentum distribution of the parent cloud [189].

Pairs with total momentum $q$ will form a continuum limited by

$$- \frac{q p_F}{m} + \frac{q^2}{2m} \leq \omega \leq \frac{q p_F}{m} + \frac{q^2}{2m} \quad \text{for} \quad k > k_F. \quad (3.9)$$

At $T = 0$, the dynamic structure factor in the ideal Fermi case, $S^0(q, \omega)$, vanishes outside this finite range, see figure 3.2. This feature changes for real Fermi liquids. For all values of $q$, $S^0(q, \omega) \to 0$ when $\omega \to 0$ due to the proportionality to $\omega$ (which is at the margins of the intersecting surfaces where the shifted Fermi sphere is not very different from the Fermi sphere of the ground state). Such behaviour is a direct consequence of the exclusion principle and of the corresponding scarcity of low-energy excitations as the number of available empty states is much smaller.
3.4 Static structure factor

With the simplification that the momentum transfer is essentially independent of the energy transfer, the probability to transfer energy and momentum to a particle, given by equation 3.6, can be integrated over all permissible frequencies

\[
\int_0^\infty d\omega W(\mathbf{q}, \omega) = 2\pi |V_\mathbf{q}|^2 NS_\mathbf{q}.
\]  

(3.10)

The definition of the static structure factor follows as

\[
S_\mathbf{q} = S(\mathbf{q}) = \frac{\hbar}{N} \int_0^\infty d\omega S(\mathbf{q}, \omega).
\]  

(3.11)

\(NS_\mathbf{q}\) is the non-energy-weighted moment and is governed by the momentum of the scattered particles. It is equal to the Fourier transform of \(S(\mathbf{q}, \tau)\) taken for \(t = 0\), so \(NS_\mathbf{q} = \langle 0 | \rho_\mathbf{q}^\dagger \rho_\mathbf{q} | 0 \rangle\). The static structure factor provides a measure of the instantaneous density correlations in the system or mean square density fluctuations at momentum \(\mathbf{q}\) and provides an integrated response of the equilibrium configuration of \(S(\mathbf{q}, \omega)\). If \(\hat{\psi}\) is the field operator, then \(S(k)\) is related to the two-body density matrix

\[
n^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = \left\langle \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) \hat{\psi}(\mathbf{r}_2) \right\rangle
\]  

(3.12)

by

\[
S(\mathbf{q}) = 1 + \frac{1}{N} \int d\mathbf{r}_1 d\mathbf{r}_2 \left[ n^{(2)}(\mathbf{r}_1, \mathbf{r}_2) - n(\mathbf{r}_1) n(\mathbf{r}_2) \right] e^{iq(\mathbf{r}_1 - \mathbf{r}_2)}.
\]  

(3.13)

As only the relative distance, \(s = \mathbf{r}_1 - \mathbf{r}_2\), is relevant in uniform systems

\[
S(\mathbf{q}) = 1 + n \int ds [g(s) - 1] e^{iq(s)}.
\]  

(3.14)

The pair correlation function, \(g(s) = n^{(2)}(s) / n^2\) is normalised to \(n = \left\langle \hat{\psi}^\dagger \hat{\psi} \right\rangle\) and is given through the Fourier transformation of the static structure factor

\[
g(s) = 1 + \frac{1}{n(2\pi)^3} \int d\mathbf{q} [S(\mathbf{q}) - 1] e^{-iq(s)}.
\]  

(3.15)

At high momenta, \(S(\mathbf{q} \to \infty)\) approaches unity because momentum states are uncorrelated such that \(g(s) \to 1\) and incoherent processes dominate. Mathematically speaking, only the diagonal elements in \(\rho_\mathbf{q}^\dagger \rho_\mathbf{q} = \sum_{ij} \exp[iq(\mathbf{r}_i - \mathbf{r}_j)]\) make the sig-
nificant contributions.

### 3.5 f-sum rule

Sum rules ensure that the many-particle systems converge in certain limits. In this context, particle conservation relates the scattered particles with the involved energy states through the f-sum rule. The derivation is outlined below. The strongly interacting Fermi gas can be regarded as an incompressible liquid as in the hydrodynamic picture. There, the fundamental equation of continuity guarantees particle conservation. In the Heisenberg picture this is

$$i\hbar \frac{d\rho_q}{dt} = [\rho_q, H].$$  \hfill (3.16)

The particle density, $\rho_q$, is described by equation 3.4 and has no time dependence. One needs to calculate $[\rho_q, H]$ with the Hamiltonian of the system

$$H = \sum_j \left[ \frac{p_j^2}{2m} + U(r_j) \right] + \frac{1}{2} \sum_{j \neq l} V_{rl}(r_j - r_l),$$  \hfill (3.17)

which has an external potential $U(r_j)$ and an interparticle potential $V_{rl}(r_j - r_l)$. Both potentials are independent of the velocity. As the particle density, $\rho_q$, is also only dependent on the position, it commutes with the potentials and the only contribution from $[\rho_q, H]$ stems from the kinetic energy term. In a detailed calculation one can use standard commutator relations to show that $[\rho_q, H]$ is equal to the scalar product, $\hbar (j_q \cdot q)$, of the current density fluctuation, $j_q$, and the wave vector, $q$. Its eigenvalues, $\hbar \omega_{n0}(\rho_q)_{n0} = \hbar (\rho_q \cdot q)_{n0}$, lead to the matrix elements between the eigenstates, $\hbar \omega_{n0}(\rho_q)_{n0}$, of the real system, which are the transitions from the ground state. As an interim result, particle conservation is linked to the permissible energy states, $n$, in the scattering event by

$$i\hbar \frac{d\rho_q}{dt} = [\rho_q, H] = \hbar \omega_{n0}(\rho_q)_{n0}. \hfill (3.18)$$

To calculate the energy-weighted momentum of $S(q, \omega)$, the double commutator is evaluated for the ground state, $\langle 0 \left| \left[ [\rho_q, H], \rho_q^\dagger \right] \right| 0 \rangle$. On the one hand, one obtains with equation 3.18

$$\langle 0 \left| \left[ [\rho_q, H], \rho_q^\dagger \right] \right| 0 \rangle = 2\hbar \sum_n \omega_{n0} \left( (\rho_q^\dagger)_{n0} \right)^2.$$

\hfill (3.19)
On the other, one can explicitly calculate the double commutator for the kinetic part of the Hamiltonian, equation (3.17), which may be written for \( N \) particles as
\[
\left[ [\rho_\mathbf{q}, H], \rho_\mathbf{q}^\dagger \right] = \frac{N q^2 \hbar^2}{m}.
\] (3.20)

The double commutator leads to
\[
\hbar \sum_n \omega_n \left| \left( \rho^\dagger_{\mathbf{q}n} \right) \right|^2 = \frac{N q^2 \hbar^2}{2m}.
\] (3.21)

Hence, the f-sum rule follows with equation (3.7) as
\[
\hbar^2 \int_0^\infty d\omega \omega S(\mathbf{q}, \omega) = \frac{N q^2 \hbar^2}{2m}.
\] (3.22)

It bears this name because the oscillator strength for each transition is defined as
\[
f_{0n} = \frac{(2m/q^2)}{2m} \sum_n \omega_n \left| \left( \rho^\dagger_{\mathbf{q}n} \right) \right|^2
\] such that \( \sum f_{0n} = N \), e.g. [4]. The strength of the f-sum rule lies in its validity for a wide range of interacting many-body systems, independent of statistics and temperature, and it is well-known in atomic physics. In the long wavelength limit, \( q \to 0 \), other sum rules also exist, for instance, the compressibility sum rule, which can be used to obtain the speed of sound.

### 3.6 Linear response function

In this work, the true linear response function is not explicitly calculated but its imaginary part is measured and linked to \( S(\mathbf{q}, \omega) \). For these experiments, the linear response is restricted to the density-density correlations. The idea is, as stated above, that the weak perturbation of the Bragg photons on the Fermi gas results in density fluctuations which are proportional to the linear response function and the general formalism is provided by first order perturbation theory. Amongst the phenomena of non-equilibrium dynamics, linear response theory is limited to small disturbances from the equilibrium state where the Born approximation is valid, that is, the many-body system is assumed to be undepleted by the scattering event. This is a widely applicable concept in natural systems. The standard linear response function, \( \chi(\mathbf{r}, t) \), is defined by
\[
\langle \rho(\mathbf{r}, t) \rangle = \int d^3 \mathbf{r}' \int dt' \chi(\mathbf{r} - \mathbf{r}', t - t') \phi(\mathbf{r}', t'),
\] (3.23)
where a fluctuation of the physical quantity \( \langle \rho(\mathbf{r}, t) \rangle \) is caused by an external potential \( \phi(\mathbf{r}', t') \). In Fourier space the expression is more compact through the replacement of space and time with momentum and frequency. The scalar potential is real, \( \phi(\mathbf{q}, \omega) = \phi^*(-\mathbf{q}, -\omega) \), and is part of the time dependent Hamiltonian. For the solution the Dirac picture is useful where the unperturbed part is given in the Schrödinger picture and the external perturbation, \( H_{\text{int}} \), follows the Heisenberg picture with time-dependent operators. All the transitions, \( \omega_{n0} \), from the ground state, \( |0\rangle \), to any excited state, \( |n\rangle \), are coupled by the density fluctuations. For Bragg scattering it follows that \( \phi(\mathbf{q}, \omega) \rightarrow V_{\mathbf{q}} \) and \( H_{\text{int}} \rightarrow H_{\text{Br}} \). In experiments, the atoms in the unperturbed system \( (t = -\infty) \) respond to the Bragg pulse, whose rising slope has a finite width. For the calculation of the response function, one needs adiabatic boundary conditions and causality, because a physical response to a perturbation happens only after the perturbation and the evolution of the system should not diverge after the perturbation. These conditions are governed by introducing a small parameter \( \eta \rightarrow 0 \). Independent of the details of the scattering potential and using again equation (3.7), the connection between the linear response and \( S(\mathbf{q}, \omega) \) is defined as

\[
\chi(\mathbf{q}, \omega) = \int_0^\infty d\omega' S(\mathbf{q}, \omega') \left\{ \frac{1}{\omega - \omega' + i\eta} - \frac{1}{\omega + \omega' + i\eta} \right\}.
\]  

(3.24)

The dynamic structure factor contains the spectral information on the density-density response function. The result gives the linear response function in terms of the true eigenstates of the system, \( \omega \). The symmetric notation is necessary to account for reversible excitations, where \( S(\mathbf{q}, \omega) \) is already symmetric. In the high-frequency limit equation (3.24) becomes

\[
\chi(\mathbf{q}, \omega) \rightarrow \frac{2}{\omega^2} \int_0^\infty d\omega' S(\mathbf{q}, \omega') = \frac{Nq^2}{m\omega^2} (\omega \rightarrow \infty)
\]  

(3.25)

and this asymptotic form of \( \chi(\mathbf{q}, \omega) \) is unaffected by the interaction between the system particles. The real and imaginary parts of the response function \( \chi = \chi' + i\chi'' \) are

\[
\chi'(\mathbf{q}, \omega) = \int_0^\infty d\omega' S(\mathbf{q}, \omega') P \left( \frac{2\omega'}{\omega^2 - \omega'^2} \right)
\]  

(3.26)

\[
\chi''(\mathbf{q}, \omega) = -\pi [S(\mathbf{q}, \omega) - S(-\mathbf{q}, -\omega)],
\]  

(3.27)
where $P$ is called the principal part, which is a mathematical residue from the Dirac relation when integrating in the limit of $\eta \to 0$. These equations are linked through the well-known Kramers-Kronig relations, [190, 191]. $S(q, \omega)$ provides a measure of the real transitions induced by the probe, i.e. of the energy transfer from the probe to the system. The imaginary part measures the inelastic cross section in the dissipative scattering event. $\chi(q, \omega)$ does not provide any more physical information than $S(q, \omega)$. At $T = 0$, the quantity which represents the physical information in the most compact form is $S(q, \omega)$; it gives the density fluctuation excitation spectrum as a positive definite function. But at finite temperatures the relation between $S(q, \omega)$ and $\chi''(q, \omega)$ is more complicated. Bragg spectra have been numerically calculated based on the linear response function, $\chi(q, \omega)$ [192]. In general, the formalism of the response function is applicable to any quantum liquid, whether Bose or Fermi, charged or neutral, normal or superfluid, and is a compact way to describe experimental measurements involving weakly coupled external probes. In the hydrodynamic regime, such as for a strongly interacting Fermi gas, the correlation functions need to be determined by macroscopic considerations, since details of the single particle excitation spectrum have been washed out by the collisions. Section 3.8 will focus on this.

### 3.7 Response at finite temperature

At finite temperatures, $T$, a statistical description is necessary to account for the thermal equilibrium of the initial ($t = -\infty$) configuration. In the canonical ensemble of statistical mechanics, the exact eigenstates $|m\rangle$ of the system Hamiltonian possess an energy $E_m$, and the probability of finding the system in state $|m\rangle$ is given by

$$W(m) = \frac{e^{-\frac{E_m}{k_B T}}}{Z}$$

where the partition function is $Z = \sum_m e^{-E_m/(k_B T)}$, i.e., in thermal equilibrium the probability of finding a particle in either of the two spin states is related to the Boltzmann factor. A consequence of the interaction between the Bragg pulse (a time-dependent external probe) and the fermionic many-particle system is the possibility of energy transfer to and from the probe. The principle of detailed balancing is used to link $S(q, \omega)$ with the imaginary part of the density-density response function $\chi''(q, \omega)$, so equation 3.27 is modified [76]. Unlike the general expressions in the previous section, at finite temperatures they are different as $S(q, \omega)$ is a direct measure of the fluctuations in the system, while $\chi''(q, \omega)$ describes the dissipative
part of the system response. The integrated form of detailed balancing is the well-known fluctuation-dissipation theorem [193, 194].

3.7.1 Consequences for the dynamic structure factor and the response

Within the Born approximation the dependence on the statistical weight, equation 3.28, enters the probability per unit time that a probe particle transfers momentum $q$ and energy $\omega$ to the system as

$$W(q, \omega) = 2\pi |V_q|^2 Z^{-1} \sum_{mn} e^{-\frac{E_m}{k_B T}} \left| (\delta \rho^\dagger_{q})_{nm} \right|^2 \delta (\omega - \omega_{nm}).$$ (3.29)

The result follows from second order perturbation theory for a transition from a given state $|m\rangle$ to another state $|n\rangle$. $\hbar \omega_{nm}$ is the exact energy difference, $E_n - E_m$.

For the density-density response function one finds

$$\chi(q, \omega) = Z^{-1} \sum_{mn} e^{-\frac{E_m}{k_B T}} \left[ \left| (\delta \rho^\dagger_{q})_{nm} \right|^2 \left\{ \frac{1}{\omega - \omega_{nm} + i\eta} - \frac{1}{\omega + \omega_{nm} + i\eta} \right\} \right].$$ (3.30)

$$\eta \rightarrow 0 Z^{-1} \sum_{mn} e^{-\frac{E_m}{k_B T}} \left| (\delta \rho^\dagger_{q})_{nm} \right|^2 \frac{2\omega_{nm}}{\omega^2 - \omega_{nm}^2}.$$

which was first stated by Kubo [195] for any linear operator. The spectral excitations are now thermally weighted, and therefore $S(q, \omega)$ must depend on the temperature, since it contains the properties of the many-particle system

$$S(q, \omega) = Z^{-1} \sum_{mn} e^{-\frac{E_m}{k_B T}} \left| (\rho^\dagger_{q})_{nm} \right|^2 \delta (\omega - \omega_{nm}).$$ (3.31)

Equation 3.7 is recovered for $T = 0$, where $S(q, \omega)$ identically vanishes for $\omega < 0$. The excitation energies $\omega_{n0}$ are always positive for a system in the ground state.

3.7.2 Detailed balancing

In general, if the system can undergo a transition from a state $m$ with equilibrium probability $\pi_m$ to a state $n$ with equilibrium probability $\pi_n$, the transition probability is $W_{mn}$ and its reciprocal transition is $W_{nm}$. Detailed balancing

$$\pi_m W_{mn} = \pi_n W_{nm},$$ (3.32)
states that in thermal equilibrium all microscopic processes are compensated for by their reciprocal processes. In this context, the equilibrium probabilities are given by the Boltzmann factors $\pi_m = \exp(-\hbar \omega_m / (k_B T))$ and $\pi_n = \exp(-\hbar \omega_n / (k_B T))$ at the thermal equilibrium temperature, $T$, and $\hbar \omega_{mn} = E_m - E_n$. Recalling equation (3.29) and that the probe can also absorb momentum $-q$ and energy $-\omega_{mn} = +\omega_{mn}$ from the system, the probability per unit time is written as

$$W(-q, -\omega) = 2\pi |V_q|^2 Z^{-1} \sum_{mn} e^{-\frac{E_m}{k_B T}} \left| (\rho_q^\dagger)_{nm} \right|^2 \delta(\omega + \omega_{nm})$$

(3.33)

and $S(q, \omega)$ is proportional to the transfer probability. In that case, the principle of detailed balancing states that

$$\frac{W(q, \omega)}{W(-q, -\omega)} = \frac{S(q, \omega)}{S(-q, -\omega)} = e^{\frac{\hbar \omega_{mn}}{k_B T}}$$

(3.34)

which is satisfied by equation (3.29) and equation (3.31). This can also be seen when interchanging indices in equation (3.31)

$$S(q, \omega) = Z^{-1} \sum_{mn} e^{-\frac{E_m}{k_B T}} \left| (\rho_q^\dagger)_{nm} \right|^2 \delta(\omega - \omega_{nm})$$

(3.35)

$$= Z^{-1} \sum_{nm} e^{-\frac{E_n}{k_B T}} \left| (\rho_q^\dagger)_{mn} \right|^2 \delta(\omega + \omega_{nm})$$

$$= Z^{-1} \sum_{nm} e^{-\frac{E_n - E_m}{k_B T}} e^{-\frac{E_m}{k_B T}} \left| (\rho_q)_{nm} \right|^2 \delta(\omega + \omega_{nm})$$

$$= e^{\frac{\hbar \omega_{mn}}{k_B T}} S(-q, -\omega).$$

Notice that if the system is in thermal equilibrium, and hence equation (3.34) holds, the total energy rate is always positive due to causality.

### 3.7.3 Fluctuation-dissipation theorem

The dynamic structure factor is related to the density response function through its imaginary (dissipative) part which specifies directly the steady state energy transfer from an oscillating probe (Bragg lattice) to the many-particle system (strongly interacting Fermi gas). At finite temperature, the imaginary part, equation (3.27), may be written explicitly as

$$\chi''(q, \omega) = -\pi \left[ 1 - e^{-\frac{\hbar \omega_{mn}}{k_B T}} \right] S(q, \omega)$$

(3.36)
which is known as the fluctuation-dissipation theorem \[193, 194\]. It is one of the most fundamental results of quantum statistics. The derivation is very arduous. In principle, a system in thermal equilibrium is considered, for which the theorem states that the reaction to a small external perturbation is the same as the reaction to spontaneous fluctuations and that the dissipative part is proportional to these fluctuations. With regard to \( S(q, \omega) \), one can find an explicit relation between the microscopic dynamics and macroscopic reactions to time-dependent perturbations. These dynamics are accessible with Bragg spectroscopy. In contrast, the dissipation-fluctuation theorem allows one to use microscopic models in a statistical equilibrium for predictions of macroscopic properties which might deviate from equilibrium. At finite temperatures, \( \chi''(q, \omega) \) and \( S(q, \omega) \) have a slightly different temperature dependence. The dynamic structure factor can be presented in a more symmetric way

\[
\tilde{S}(q, \omega) = S(q, \omega) + S(q, -\omega) = S(q, \omega) \left( 1 + e^{-\frac{\hbar \omega}{k_B T}} \right).
\] (3.37)

The dissipative part is introduced by equation (3.36) such that

\[
\tilde{S}(q, \omega) = \frac{-1}{2\pi} \chi''(q, \omega) \coth \left( \frac{1}{2} \frac{\hbar \omega}{k_B T} \right).
\] (3.38)

The mean square thermal fluctuations can be written as

\[
\langle \rho_q^\dagger \rho_q \rangle = NS_q = -\hbar \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \chi''(q, \omega) \coth \left( \frac{1}{2} \frac{\hbar \omega}{k_B T} \right).
\] (3.39)

This integrated form of the detailed balance is a form of the fluctuation-dissipation theorem. The sum rules for \( \chi''(q, \omega) \) and \( S(q, \omega) \), which were derived in the zero temperature case, are also applicable at finite temperatures. The f-sum rule can be rewritten as

\[
2\hbar^2 \int_{-\infty}^{\infty} d\omega \omega S(q, \omega) = -\frac{\hbar^2}{\pi} \int_{-\infty}^{\infty} d\omega \omega \chi''(q, \omega) = \frac{Nq^2\hbar^2}{m}.
\] (3.40)

The above considerations are particularly important at finite temperatures. In fact, at \( T = 0 \), \( \chi''(q, \omega) \) and \( S(q, \omega) \) coincide for positive \( \omega \) and only processes transferring energy to the system are allowed, while at finite temperatures the two functions differ significantly if \( \hbar \omega/(k_B T) \) is small. All temperature dependent Bragg spectra will be represented in terms of \( S(q, \omega) \) in the later chapters since the additional factor of \( (1 + \exp[-\hbar \omega/(k_B T)])/2 \) is very small in the applied temperature range and \( S(q, \omega) \)
is conventionally used in inelastic scattering experiments.

### 3.8 Dynamic structure factor from Bragg spectra

Bragg spectroscopy is a powerful tool to investigate the dynamics in ultracold gases. This section shows how the microscopic details of strongly interacting Fermi gases given by $S(q, \omega)$ can be measured under macroscopic considerations of an atomic distribution. All results for this thesis are extracted from absorption images. This technique is well understood and has been applied since the beginning of ultracold atomic gas experiments. Despite the convenience of gaussian fitting, which is often applied when the signal-to-noise drops, more careful methods are necessary to adapt to accurately fit the density profiles of Fermi clouds to determine their properties. A series of absorption images (time-of-flight technique) at different Bragg frequencies are recorded. The line profiles of each image are the basis to generate an energy resolved Bragg spectrum. As the sample is excited by a momentum kick, the response of the trapped cloud is manifested in a distortion of the cloud shape and the response is proportional to the number of scattered particles, $N_{sc}$. There are two possibilities to evaluate the response. One way is to look at the distribution shortly after the Bragg pulse. The integrated line profile is then asymmetric. Traditionally, the centre of mass displacement $\langle r \rangle$ or the number of optically excited atoms is considered and more recently the counted photons in the Bragg beams. The centre of mass displacement reflects the first moment of the line profile. However, also the second moment of the line profile contains valuable information. Another way is to apply a long hold time after the Bragg pulse, so that the scattered atoms in the trap reach energetic equilibrium. Then, the line profiles are symmetric and the information is linked to the change in the width of the cloud. The evaluation of the width, which is associated with the transferred energy, has been used in experiments with bosons in optical lattices. The details on the acquisition of Bragg spectra are described later as every experiment has an individually modified image process. In the following sections, it is important to make the connection between a spectrum and $S(q, \omega)$, and concentrate on the application of interdisciplinary sum-rules helping to distil physical information stored in a Bragg spectrum.

Note that atoms can scatter by absorbing a photon from either of the two laser beams, and that the response of the system measures the difference rather than $S(q, \omega)$ itself, as seen in equations

$$\chi''(q, \omega) = \pi [S(q, \omega) - S(-q, -\omega)] = \pi S(q, \omega) \left[ 1 - e^{-\frac{\hbar \omega}{k_B T}} \right]$$  \hspace{1cm} (3.41)
This is an important difference with respect to other scattering experiments (like neutron scattering from helium) where, by detecting the scattered probe, one measures directly $S(q, \omega)$.

### 3.8.1 Measuring the dynamic structure factor

The principle of Bragg scattering was described in section 3.2.1. The evolution of the system is governed by the time dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \phi (r, t) = H_{\text{tot}} \phi (r, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}} (r) + \Theta (t) H_{\text{int}} \right] \phi (r, t). \quad (3.42)$$

The unperturbed system has the kinetic term and the harmonic confinement $V_{\text{trap}} (r)$ being produced by the trap potential. $\Theta (t)$ is the Heaviside step function to switch on the perturbation $H_{\text{int}}$ given by equation 3.3. Using first order perturbation theory, one can calculate the centre of mass displacement in the direction of the Bragg pulse $z$, as

$$i\hbar \frac{dP_z}{dt} = \langle [P_z, H_{\text{Br}}] \rangle. \quad (3.43)$$

The overall trap frequency $\bar{\nu}$ and width $d\langle \sigma^2 \rangle$ enter the expression for the energy $dE = (1/2) m \bar{\nu}^2 d\langle \sigma^2 \rangle$, which can be obtained from

$$i\hbar \frac{dE}{dt} = \langle [H, H_{\text{Br}}] \rangle. \quad (3.44)$$

The centre of mass displacement and the width of the atomic distribution are linked to the response by

$$\frac{1}{q} \frac{dP_z}{dt} = \frac{1}{\omega} \frac{dE}{dt} = 2 \left( \frac{V_q}{2} \right)^2 S(q, \omega) \left( 1 - e^{-\hbar \omega/(k_B T)} \right). \quad (3.45)$$

Note that $V_q \equiv 2\hbar \Omega_R$.

### 3.8.2 Dynamic structure factor from the centre of mass displacement

The net momentum imparted to the cloud can be observed through the centre of mass displacement after the cloud is released from the trap, independent of the cloud shape. The time derivative of the momentum is given by the Heisenberg picture, see equation 3.43. This calculation is reported elsewhere [80, 197]. One can rewrite the momentum as velocity of the centre of mass displacement $P_z (t) = m (dX (q, \omega) / dt)$. 

3.8 Dynamic Structure Factor from Bragg Spectra

For a given Bragg pulse, \( \tau_{Br} \), and time of flight \( \tau_{TOF} \), the centre of mass displacement travels \( \Delta X(q, \omega) = X_{fin}(q, \omega) - X_0 \), where \( X_0 \) denotes the cloud position at rest and \( X_{fin}(q, \omega) \) the final centre of mass of the cloud after the Bragg pulse and time-of-flight. Including detailed balancing, see equation (3.34), an integration shows

\[
\Delta X(q, \omega) = \frac{\tau_{TOF}}{m} \frac{2q}{h} \left( \frac{V_q}{2} \right)^2 \int d\omega' S(q, \omega') \left( 1 - e^{-\omega'/(k_B T)} \right) \frac{1 - \cos [(\omega - \omega') \tau_{Br}]}{(\omega - \omega')^2}.
\]

The fraction indicates the signal is convoluted with the spectral components of the Bragg pulse. For all permissible excitation frequencies \( \omega' \), the integration over the fluctuation frequency is constant. It follows with the definition of the static structure factor, equation (3.11),

\[
\int d\omega \frac{\Delta X(q, \omega)}{1 - e^{-\omega/(k_B T)}} \propto \int d\omega S(q, \omega) = N S(q).
\]

The centre of mass displacement leads via the static structure factor to the pair correlation function, see equation (3.14). The transferred momentum reflects in the number of scattered particles (atoms or pairs), \( N_{sc} \), such that

\[
\Delta P(q, \omega) = m \frac{d\Delta X(q, \omega)}{dt} = N_{sc} \cdot q = N_{sc} \cdot \hbar k.
\]

According to equation (3.47), the transferred momentum is therefore proportional to the dynamic structure factor, \( \Delta P(q, \omega) \propto N_{sc} \hbar k \propto S(q, \omega) \).

3.8.3 Dynamic structure factor from the width

Starting from equation (3.44), the Bragg Hamiltonian depends on the local density and only the kinetic energy term in \( H \) contributes to the above commutator. The calculation is similar to the derivation of the f-sum rule [197]. One finds

\[
\Delta E(q, \omega') = \frac{\tau_{TOF}}{\pi} \frac{2q}{h} \left( \frac{V_q}{2} \right)^2 \int d\omega' \omega' S(q, \omega') \left( 1 - e^{-\omega'/(k_B T)} \right) \frac{1 - \cos [(\omega - \omega') \tau_{Br}]}{(\omega - \omega')^2}.
\]

which holds for \( t > 0 \). The transferred energy from Bragg pulse is accessible via the width of the cloud distribution, \( \Delta E = (1/2) m \tilde{\nu}^2 \Delta \langle \sigma^2 \rangle \). As the trap frequency, \( \tilde{\nu} \), is fixed, one needs to measure only the increase in width, \( \Delta \langle \sigma^2 \rangle = \langle \sigma_{fin}^2 \rangle - \langle \sigma_{0}^2 \rangle \), where \( \langle \sigma_{fin}^2 \rangle \) is the final width after the Bragg pulse and \( \langle \sigma_{0}^2 \rangle \) the width of the unperturbed
cloud. The static structure factor follows again from equation (3.11)

\[ \int d\omega \frac{\Delta \sigma^2(q, \omega)}{1 - e^{-\hbar \omega/(k_B T)}} \propto \int d\omega \omega S(q, \omega). \] (3.50)

The energy transfer, \( \Delta \langle \sigma^2(q, \omega) \rangle \), depends on the product of the Bragg frequency (energy) and the number of scattered particles \( \omega \cdot N_{sc} \), such that

\[ \Delta E(q, \omega) = \frac{1}{2} m \bar{v}^2 \Delta \langle \sigma^2(q, \omega) \rangle = \hbar \omega \cdot N_{sc} \] (3.51)

With equation (3.50), one can see that the transferred energy in terms of the width is proportional to first moment of the dynamic structure factor, \( \Delta E(q, \omega) = \hbar \omega \cdot N_{sc} \propto \Delta \langle \sigma^2(q, \omega) \rangle \propto \omega S(q, \omega) \).

### 3.8.4 Application of sum-rules

Sum rules provide a model-independent tool to determine the moments of the dynamic structure factor avoiding the explicit determination of the response function and the requirement of the full solution of the Schrödinger equation. In general, the moments of order \( p \) are calculated as

\[ m_p = \hbar^{p+1} \int_{-\infty}^{+\infty} d\omega \omega^p S(k, \omega) \] (3.52)

Equation (3.11) states that the static structure factor is the zero order moment

\[ NS(k) = \hbar \int_{-\infty}^{+\infty} S(k, \omega) d\omega \] (3.53)

and thus proportional to the atom number \( N_{sc} \). The dynamic structure factor in first moment is also called the f-sum rule

\[ NE_R = \hbar^2 \int_{-\infty}^{+\infty} \omega S(k, \omega) d\omega \] (3.54)

for the known recoil energy \( E_R = \hbar k^2/2m \). As both of the equations involve \( N_{sc} \), the normalisation of the static structure factor yields

\[ S(k) = \frac{E_R}{\hbar} \frac{\int_{-\infty}^{+\infty} S(k, \omega) d\omega}{\int_{-\infty}^{+\infty} \omega S(k, \omega) d\omega}. \] (3.55)
The proportionality constants in equations 3.47 and 3.50 depend on experimental parameters and spectral information of the Bragg pulse such as the Rabi-cycle (Bragg laser detuning, pulse duration, Bragg laser power), time-of-flight, laser line widths, scattering length at different interaction strength $1/(k_F a)$ etc. Equation 3.55 plays the central role of extracting information from the spectra and allows one to obtain an absolute number for $S(k)$ without any free scaling parameter since both integrals have the same proportionality constant, which therefore cancel. The method of centre of mass displacement, equation 3.47, was used in the very first spectra to demonstrate the decrease of the static structure factor from $2 \rightarrow 1$ as the relative momentum, $k/k_F = 5$, was transferred at different interaction strengths across the Feshbach resonance ranging from the BEC limit to the BCS limit, see figure 6.7a. Equations 3.54 to 3.55 can be applied to compare with a now available theoretical prediction. Compared to the previously reported result, the accuracy of the data points is much better than the earlier results, which relied on an experimental determination of the two-photon Rabi cycling period $\Omega_R$.

3.9 Summary

Inelastic two-photon Bragg scattering with photons of large momenta can be used to probe the momentum distribution of strongly interacting Fermi gases. Linear response theory provides a model-independent way to describe the spectral functions in many-body systems obtained from Bragg spectroscopy. The Bragg photons couple weakly to the fermionic cloud and quantities are derived within first order perturbation theory. The spectral function is stored in the dynamic structure factor, $S(q, \omega)$, which only depends on the momentum and energy transfer of the photon. The net momentum transfer is given by the static structure factor, $S(q)$, after energy integration of the dynamic structure factor. The static structure factor measures instantaneous density fluctuations and is related to the two-body correlation function. Within linear response theory, sum rules are found in several limits, for instance the f-sum rule. The fluctuation-dissipation theorem and detailed balancing are equivalent formulations to include finite temperature in the dynamic and static structure factors. This theoretical background is applied to the measurement of pair-correlations in Fermi gases. The interaction potential in the Hamiltonian is given by the periodic potential of the Bragg beams. Measurements of the dynamic structure factor can be extracted from the centre of mass displacement or energy of atomic distributions perturbed by the Bragg pulse. The degree of two-body correlations in the Fermi gas is reflected in the static structure factor which can be
normalised with the f-sum thus rule avoiding a dependence on the atom number and other experimental parameters. Details on the acquisition of Bragg spectra are presented in chapters 6 and 7 together with image evaluation techniques.
Chapter 4

Degenerate quantum gas machine

Since the first production of bosonic [9,11], ultracold degenerate gases the experimental setups have undergone vast technical developments to cover the possibilities for investigating cold atoms. Our apparatus is designed to trap and evaporatively cool fermionic $^6$Li atoms and study them in a wide range of magnetic fields.

4.1 Introduction

The experiments in this thesis have been carried out in an ultra high vacuum glass cell. The original setup was designed and built by Fuchs [198] with the main goal to produce molecular BECs [199]. All the details concerning the chamber design, vacuum system and pumping can be found in that thesis. Major changes in the laser system for cooling and repumping as well as the installation of the offset locking for imaging were made before the first Bragg spectroscopy experiments [198]. The most recent detailed description of the apparatus, especially details on the Feshbach coils and the computer control facilities, is given in [200]. A brief outline of the principal stages of the experimental procedure before evaporation to a quantum superfluid is outlined in the following. Details on the principles can be found in textbooks such as [114,201,202]. The Feshbach coils are essential for these experiments and therefore recalled in section 4.2. The setup for the two optical dipole traps is explained in section 4.3 with regard to the characteristic parameters for chapters 6 and 7. The Bragg beams represent the spectroscopic tools for probing the cloud and are the subject of section 4.4. Detection with absorption imaging is an important requirement to obtain qualitative information on the atomic distributions. The central goals of the imaging setup are to minimise noise, obtain the correct atom numbers and correct cloud shape, which is of special interest for the determination of the temperature, as described in chapter 5.
CHAPTER 4. DEGENERATE QUANTUM GAS MACHINE

Figure 4.1: Schematic setup of the apparatus in top and side view. The main parts are the lithium oven, Zeeman slower and glass cell with surrounding coils. The pressure changes between the left and right pumping chamber.

Precooling atoms

To generate an ultracold Fermi gas the atoms have to undergo several stages of cooling. As the experiments take place in a thermally isolated high vacuum environment, cooling means extracting kinetic energy. The source of $^6$Li atoms is stored in solid form in an oven that heats the lithium above the sublimation temperature to a vapour with a thermal Boltzmann distribution released from an effusive source. The vacuum system without the laser system is sketched in figure 4.1. The pressure changes from $1.2 \times 10^{-4}$ mbar in the lithium oven ($T = 450 \degree C$) to $\sim 1.0 \cdot 10^{-11}$ mbar in the glass cell. The water-cooled Zeeman slower coil is wound on a 30 cm-long stainless steel tube with increasing inner diameter from one end to the other. It is directly connected to a custom-made glass cell made from Vycor quartz. The cell dimensions are $12 \times 3 \times 3$ cm$^3$. On the outside surface an antireflection coating is chosen for 1030 nm as well as 670 nm light to optimise the transmission for the cooling, imaging as well as trapping light. The magnetic trapping potential is generated by a set of water-cooled coils in anti-Helmhotz configuration. The symmetry

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1^Hellma

2^Base Vycor 7913
axis of the magnetic trap is in the vertical direction and defines the z-axis of the experimental setup. Three extra sets of compensation coils provide separate offset fields to shift the MOT into the optimum transfer position.

Atoms below a certain cut-off velocity are captured by the Zeeman laser beam and the magnetic field of the Zeeman coils. While the atoms travel against the Zeeman beam in the coil, they are slowed down due to a directional process of multiple photon absorption and emission. At the end of the tube, their final velocity is small enough that they do not overshoot the potential created by the magneto-optical trap (MOT). There, the atoms are pushed to the trap centre by the cooling and confining MOT forces. The MOT is produced by a combination of six counter-propagating circularly polarised laser beams (MOT beams) that intersect in the zero magnetic field of two magnetic coils in an anti-Helmholtz configuration. Basically, the MOT beams maintain the cooling process in momentum space by photon absorption-emission cycles while the magnetic field gradient provides a spatial dependence on the force which pushes the scattering atoms back to the trap centre. The atomic temperature is limited to about 200 μK as the fluorescent scattering mechanism imparts a recoil momentum to the atoms. To overcome three orders of magnitude in temperature to enter the degeneracy regime, the MOT light is switched off and further cooling is performed after compression and transfer into a far-detuned single optical dipole trap. Here, evaporative cooling is performed and the lowest temperatures are achieved down to 0.1 $T/T_F$, where $T_F$ is the Fermi temperature. Once an ultracold gas in the superfluid regime is created the experiments can start. The detection is performed with destructive absorption imaging, where the shadow picture is taken on a CCD chip for further evaluation processes.

The delicate technique of loading and evaporating atoms demands a precise control of the timing and triggers of the voltage-regulated experimental control parameters, such as used for the laser powers and frequencies, magnetic fields and camera trigger. Three National Instruments PCI output boards\(^3\) provide 24 analog output channels with output voltages ranging from $-10$ V to $+10$ V. The control program and graphical user interface is written in LabView\(^4\).

The laser system with 671 nm light incorporates the locking of lasers to the lithium absorption lines, the cooling system for the atoms, the Bragg lasers as an independent manipulation tool and the imaging laser for detection. The frequency control in the laser setup is referenced to a $^6\text{Li} \, D_2$ sub-Doppler resonance obtained from lithium vapour in saturation spectroscopy ($2^2S_{1/2} \rightarrow 2^2P_{3/2}$ transition). Once

\(^3\)National Instruments: PCI 6733 and PCI 6713
\(^4\)National Instruments: LabView 6
**Figure 4.2:** Laser locking frequencies in the $^6$Li energy level diagram.
the reference frequency is locked all other frequencies, for example for the slowing, cooling and imaging, can be achieved with acousto-optic modulators (AOMs). The relevant energy levels and the locking scheme are summarised in figure 4.2.

Figure 4.3 shows the optical setup for cooling. An external cavity diode laser (ECDL) with an output power of 15 mW provides the light for the spectroscopy. The pump beam is frequency-shifted with an AOM by 208 MHz before entering the spectroscopy loop. While the crossover peak is pumped with a 44 MHz detuning (velocity selective pumping), the probe beam monitors the transmitted intensity on a photo diode (PD). On this absorption dip the lock-in amplifier technique with a 250 kHz external modulation can be used to obtain an error signal which in turn provides the zero-crossing slope for the electronic lock. Though using a Toptica ECDL, the laser-head board is replaced to be compatible with the controller from MOG Laboratories Pty Ltd. The line width in this configuration can be as low as 400 kHz measured by beating two independent lasers and observing the width of the beat note on a spectrum analyser. The optimum (minimum) width is obtained when the grating of the ECDL has been aligned precisely. This also gives a large mode-hop-free frequency tuning range. All slave laser diode mounts, temperature controllers and laser diode current drivers are commercial products. The laser diodes used for the Zeeman slower laser and absorption imaging slave laser are 30 mW laser diodes with a centre wavelength of 675 nm available from Toptica. The other diodes are manufactured by Hitachi and have a specified maximum output power of 80 mW at 658 nm. Some lasers require two optical isolators to eliminate optical feedback. Figure 4.4 shows the optical setup for imaging and Bragg experiments. The laser light for Bragg spectroscopy and imaging is offset-locked, which is explained in appendix A.

4.2 Feshbach coils

In order to investigate strongly interacting Fermi gases, it is necessary to tune the atoms to the broad Feshbach resonance of $^6$Li where the scattering length is strongly enhanced and universal properties can be investigated. Because this Feshbach resonance is at 834 G, the magnetic coils, providing the high magnetic offset field, are

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5Toptica: DL 100
6MOGlabs, model DLC-202
7Thorlabs: TCLDM9
8Thorlabs: TED200
9Thorlabs: LDC202 and LDC205
10Hitachi: HL6526FM
Figure 4.3: Optical setup for cooling. For more details see text.
Figure 4.4: Optical setup for imaging. To generate the light frequencies for imaging and Bragg experiments, the light is offset-locked to the reference light. ECDL 2: imaging master laser.
labelled as the Feshbach coils. The set of two coils in Helmholtz configuration is designed to generate magnetic fields of up to 1.5 kG. They are made of square hollow copper tubing through which pressurised water is pumped for cooling. Both coils have 51 turns each and are wound on a mount made from hard plastic. The inner (outer) radius is 3.5 (5.5) cm with a thickness of 3 cm. The separation of both coils is 3.5 cm to fit the science glass cell in between. This design requires high currents of up to 200 A. The magnetic field has its axis along the direction of gravity. The original inductance was measured to be $433(10) \mu H$ which limits the switching times to 100 ms. The coils are slightly further apart than a perfect Helmholtz configuration, consequently causing a finite second derivative of the magnetic field. This curvature was measured and calculated to $0.033(2) \text{ G/cm}^2$. In this experiment, $^6\text{Li}$ atoms are trapped in the two lowest high-field seeking states $|1/2, -1/2\rangle$ and $|1/2, 1/2\rangle$, where the curvature provides a (anti-) trapping potential in the (vertical $y$-) horizontal $x, z$-plane. With parametric oscillation measurements at 834 G the trapping and anti-trapping frequencies at 834 G were determined to be, respectively,

$$\omega_{\text{mag}} = \omega_x = \omega_z = 2\pi \cdot 24.5 \text{s}^{-1} \quad \text{and} \quad \omega_y = 2\pi i \cdot 35 \text{s}^{-1}$$  \hspace{1cm} (4.1)

The magnetic field stabilisation is better than 20 mG over the course of a few days. The potential bowl of the magnetic trap with frequency, $\omega_{\text{mag}}$, is harmonic

$$U_{\text{mag}} = \frac{1}{2} m \omega_{\text{mag}}^2 z^2$$  \hspace{1cm} (4.2)

and usually dominates the axial confinement of the trap laser beam.

### 4.3 Dipole traps for evaporation and experiments

In the science glass cell, atoms are evaporatively cooled to create ultracold degenerate Fermi gases. Evaporative cooling has been performed elsewhere in high power optical dipole traps ($\sim 140$ W) [48], resonant build-up cavities [33], with two different hyperfine states [32] or with sympathetic cooling, i.e. using a refrigerant which can be another isotope [35, 36] or another species [21, 41, 213]. In this experiment, a single focused gaussian beam from a 100 W fibre laser at 1075 nm is optimised for evaporation of a single species gas. The power in this primary laser is precisely controllable through active stabilisation. A secondary 10 W fibre laser at 1064 nm is used to provide flexible confinements when needed for a particular experiment.
4.3 DIPOLE TRAPS FOR EVAPORATION AND EXPERIMENTS

4.3.1 Principle of dipole traps

Since the first realisation of detuned dipole traps for cold atoms \[204\], they have become a highly used device for studies on ultracold atoms. A detailed review on dipole traps can be found in \[205\]. While cooling in magneto-optical traps is limited by heating by fluorescent light produced by spontaneous scattering (radiation pressure, recoil energy), dipole traps are detuned from the atomic transition (far-off resonant scattering) but still provide a potential in which the atoms can be trapped. The electric field of the laser light \(E\) induces a dipole moment \(p\) in the atom depending on its polarisability \(\alpha\) \((p = \alpha E)\). The interaction energy is then \(U_{dip} = -\frac{1}{2} \langle p \cdot E \rangle\) and forms the trapping potential which depends on the spatial profile of the laser intensity \(I(r)\)

\[
U_{dip}(r) = \frac{3\pi c^2}{2\omega_0^3} \left( \frac{\Gamma}{\omega_0 - \omega} + \frac{\Gamma}{\omega_0 + \omega} \right) I(r),
\]

for a given driving laser frequency \(\omega\) and atomic transition frequency \(\omega_0\). \(c\) is the speed of light and \(\Gamma\) the natural line width, \(\Gamma = 2\pi 5.9 \cdot 10^6\) s\(^{-1}\) for the D\(_2\) transition in lithium. Red-detuned laser fields have an attractive dipole force which can confine atoms at an intensity maximum. Spontaneous photon scattering from the dipole trap is still possible, thus causing heating. The scattering rate is given by

\[
\Gamma_{dip}(r) = \frac{3\pi c^2}{2\omega_0^3} \left( \frac{\omega}{\omega_0} \right)^3 \left( \frac{\Gamma}{\omega_0 - \omega} + \frac{\Gamma}{\omega_0 + \omega} \right)^2 I(r)
\]

and decreases with the square of the detuning while the potential depth scales only linearly. To minimise heating due to spontaneous scattering, far-detuned dipole traps are used for trapping atoms.

4.3.2 Single focused dipole trap

The evaporation process is performed in a single focused red-detuned dipole trap. The atoms accumulate in the vicinity of the focus of the beam. The characterisation of this trap is approximated by ideal gaussian beam optics. The relevant parameters are the power \(P\), waist \(w_0\) at the \(1/e^2\) minimum radius and the Rayleigh length

\[
z_R = \frac{\pi w_0^2}{\lambda_{1075}}.
\]
Figure 4.5: Schematic of the primary optical dipole laser for evaporation and trapping (1075 nm) and of the second trap laser (1064 nm). Also shown is the imaging light (red lines).
The intensity distribution for a gaussian beam follows as

\[ I(r, z; P) = -\frac{2P}{\pi w^2(z)} \exp\left(-\frac{2r^2}{w^2(z)}\right), \]  

(4.6)

where \( r^2 = x^2 + y^2 \) and

\[ w = w_0 \sqrt{1 + \left(\frac{z}{z_R}\right)^2} \]  

(4.7)

is the beam waist along the beam axis. The trap depth \( U_0 \) can easily be calculated from equations (4.3) and (4.6) by setting \( r = z = 0 \) and depends on the final laser power \( P \), so \( U_0 \rightarrow U_0(P) \). Trapping of ultracold atoms implies that the thermal energy of the cold atoms is much smaller than the trap depth. When this condition is satisfied a harmonic approximation of the optical potential, given by equation (4.3), can be used which is simply obtained by a Taylor expansion

\[ U_{\text{dip}}(r) \simeq -U_0(P) \left[ 1 - 2 \left(\frac{r}{w_0}\right)^2 - \left(\frac{z}{z_R}\right)^2 \right]. \]  

(4.8)

The radial and axial trapping frequencies read at high field

\[ \omega_r = \sqrt{\frac{4U_0(P)}{mw_0^2}} \quad \text{and} \quad \omega_z = \sqrt{\frac{2U_0(P)}{mz_R^2}}. \]  

(4.9)

The mean trapping frequency is \( \bar{\omega} = (\omega_z \omega_r^2)^{1/3} \).

The light for the dipole trap laser is provided by a high power multimode fibre laser from IPG\(^{11}\). The output power reaches 100 W at a centre wavelength of 1075 nm with linear polarisation, a beam quality factor of \( M^2 < 1.05 \) and a line width of 3 nm. The beam waist used in our experiments is roughly 42 \( \mu \)m at the centre of the glass cell, limited by the high laser power used in the experiment. Smaller waists may result in damage to the glass cell surface as found in a test setup \(^{12}\).

Evaporation of atoms requires tuning the laser power in a well controlled way, eventually over three orders of magnitude. The high power range from 100 W down to 12 W is simply voltage-controlled through an external voltage control of the laser. Below 12 W, intensity fluctuations may lead to heating of the atoms. Therefore, the laser power is actively stabilised. A small fraction of the dipole trap light leaking through a mirror is measured on a photo detector\(^{12}\) after attenuation with a neutral

\(^{11}\)IPG: YLR-100-1075-LP

\(^{12}\)Newfocus: Model 1623
density filter. The measured voltage is compared to a setpoint signal from the computer control system and is used to derive an error signal which determines the amount of radio-frequency power sent by a PID controller to an AOM, see figure 4.5. The computer control regulates the laser intensities through this AOM reliably to \( \sim 17\) mW. More about the trap frequencies of single optical dipole traps can be found in [189, 198].

4.3.3 Crossed dipole trap

While the primary laser is optimised for evaporation, the experiments may need modified trap frequencies or a different Fermi energy. A versatile tool to manipulate the trapping potential is formed with a second far-detuned optical dipole trap laser. The laser with a centre wave length at 1064 nm has a maximum output power of 10 W and is not actively stabilised. In chapter 6, the secondary laser is overlapped with the shallow primary trap laser after evaporation. Different ramps down to the final power of the primary laser, \( U_0(P) \), allow one to change the trapping frequencies of the combined trap, which in fact varies the Fermi momentum reliably in the range of interest.

In chapter 7, the ultracold cloud is transferred after evaporation into the second trap while the primary trap is ramped off. The new trap is deep enough to trap atoms and heat them to a certain level. In a crossed optical dipole trap, the trap depth is

\[
U_{\text{dip}} = \left( \frac{2e^2 P}{w^2} \left( \frac{\Gamma_1}{2\omega_1^2} \left( \frac{1}{\omega_1 - \omega} + \frac{1}{\omega_1 + \omega} \right) \right) + \frac{\Gamma_2}{\omega_2^2} \left( \frac{1}{\omega_2 - \omega} + \frac{1}{\omega_2 + \omega} \right) \right) \quad (4.10)
\]

The harmonic approximation is valid again, and one recovers equation 4.8 for the axial optical confinement and equations 4.9 for the general trap frequencies.

In order to determine the trap frequencies for the combined trap, the trap frequencies are measured for 6.8 W at the position of the atoms without the primary trap. The technique to measure the frequencies is a standard procedure, which is the observation of the position of an oscillating cloud. In this thesis, trapping and evaporation is performed at 834 G. The values for the frequencies are \( \omega_{1064,y} = 2\pi \times 248\) s\(^{-1}\), \( \omega_{1064,x} = 2\pi \times 41\) s\(^{-1}\) and \( \omega_{1064,z} = 2\pi \times 24.7\) s\(^{-1}\). The last frequency includes the magnetic confinement. The waists of the secondary trap are 94.5 \( \mu m \) in the tight direction and 698 \( \mu m \) in the weak direction.

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\(^{13}\)SRS: SIM 960
\(^{14}\)Crystal Tech
\(^{15}\)IPG: YLR-10-1064-LP-SF
Because of the dependence of potential depth of the primary laser on the power $U_0(P)$, for a fixed power of the second trap laser, a combination of both traps leads to the overall mean trapping frequency

$$\bar{\omega} = \left(\sqrt{\omega_r^2 + \omega_{1064,y}^2} \sqrt{\omega_r^2 + \omega_{1064,x}^2} \sqrt{\omega_{1064,z}^2}\right)^{1/3}. \quad (4.11)$$

The mean trapping frequency yields the Fermi energy $\epsilon_F = (6N)^{1/3}\hbar\bar{\omega}$ and the Fermi momentum $k_F = \sqrt{2m\epsilon_F/\hbar^2}$.

### 4.4 Setup for Bragg spectroscopy

The principle of Bragg spectroscopy is described in section 3.2.1. The generation of the Bragg beams is explained in the following and a drawing is given in figure 4.6. The light is fed from the imaging slave and then passed through an AOM, which shifts the frequency. After retro-reflection the total frequency shift is $2 \times 126$ MHz for the experiments presented in chapter 6 and $2 \times 240$ MHz in chapter 7. This AOM is used to trigger the Bragg pulse, which is set to a duration of either 50 $\mu$s or 200 $\mu$s. A shutter is necessary to block residual light leaking through the AOM. The detuning is 2 GHz from the upper excited level, $|J = 3/2, m_J = -1/2\rangle$. This is large compared to the 80 MHz splitting of the two lowest hyperfine states, $|1/2, 1/2\rangle$ and $|1/2, -1/2\rangle$, and the beams couple to each state with a difference of 4%. Beam shaping results from coupling into a fibre. The gaussian output is then split into two paths: one path passes an AOM with a fixed frequency of 80 MHz while the second path goes through a variable frequency AOM. The difference with respect to the other beam is set between 0 and 600 kHz, which is called the Bragg frequency. The setup of the electronic circuit is reported in [189]. A small fraction of each beam is overlapped on a photo diode. This beat signal is read into a digital oscilloscope to record the Bragg frequency. The main part of the beams is shone into the cell where the two beams cross each other at a certain angle $\theta$. The intensity of each beam is tracked again by photo diodes. The angle determines the imparted Bragg momentum $k = 2k_L \sin(\theta/2)$, where $k_L$ is the laser wave vector at the wave length $\lambda_L = 671$ nm. The Bragg frequency corresponds to the energy of the probe particle in a two-photon process. The ratio of imparted momentum to Fermi momentum is $k/k_F$. This ratio is tunable either by changing $k$ or $k_F$. Changing $k$ requires an external re-setup of the Bragg beams to vary the angle $\theta$. For convenience $k_F$ is tuned with the power of the primary laser as will be explained in more detail in section 6.3.
Figure 4.6: Optical setup for the Bragg frequency generation. Bragg beams 1 and 2 have a small frequency difference of 0–600 kHz, which is electronically regulated with the LabView voltage via a voltage controlled oscillator.
4.5 Detection with absorption imaging

In order to match the state-of-the-art experimental setups in atom optics research, advanced imaging is necessary. The improvement of the imaging systems is often adapted to the specific goals of these experiments, for example imaging in experiments with atom chips, number squeezing, low dimensions, optical lattices etc., only to name a few. All the relevant measurements in this thesis are taken with destructive absorption imaging \[206\]. Other successful techniques are fluorescent imaging \[207\], which requires very high imaging power, or non-destructive phase contrast imaging \[208, 209\], where the translation from phase to real intensity can be rather difficult. A growing number of experimental setups use imaging along the axial trap direction to obtain images with cylindrically symmetric clouds and apply a textbook Abel transform to these images, e.g. \[210\]. Sophisticated setups accomplish single-atom and single-site resolution with optical molasses induced fluorescence imaging via a high-resolution microscope objective \[211–214\].

For the images here, it is important to obtain true atom numbers and cloud shapes; for instance in the Bragg experiment, the signal is given by small changes in the centre of mass of the cloud, and for the temperature calibration the spatial density distribution must reflect the true shape in the images. The imaging beam path is in-plane with the dipole trap lasers, and is therefore indicated as side imaging. In this beam path, there are minimal optical elements between the fibre output and the CCD camera\[16\]. The smaller the number of optical elements, the less likely are sources of unwanted spatial variations in the beam intensity, which could appear in images due to interference resulting from multiple reflections from optical surfaces, or diffraction from aperturing of the beam or from small imperfections in the optics (dust etc.). The size scale is often near the scale of the imaged object. Previous imaging was performed from the top where the beam path shared optical access to the glass cell with the vertical MOT beams. This requires somewhat more optics in the imaging beam path which degrades the quality of the images noticeably. For this work, the camera\[17\] for top imaging has been used only to measure trap frequencies in the weak optical and magnetically confined direction, where one is only interested in centre of mass motion and not absolute atom numbers.

\[16\]Prosilica: GC1380H
\[17\]Q Imaging: Retiga-Exi-F-M-12-IR
4.5.1 Imaging hardware

The imaging light is outcoupled from the offset locked imaging slave diode laser and is shifted by 91 MHz to be resonant with the transition $|1/2, 1/2\rangle \rightarrow |3/2, -3/2\rangle$. The AOM is amplitude controlled to switch the imaging light on and off. A shutter is necessary to prevent resonant first-order light leaking through the AOM to the chamber. The light is sent to the experiment via an optical fibre, see figure 4.5, which also cleans the spatial mode of the beam. After the cell, magnification is performed using two 2-inch achromats with focal lengths of 150 mm and 200 mm, respectively. The 12 bit CCD camera has a chip with $1392 \times 1040$ pixels, each with a side length of 6.45 $\mu$m. One pixel corresponds to $D = 4.85 \mu m$ or a resolution of $\Delta r \geq 4.85 \mu m$ on the camera. Note in this system the diffraction limited resolution is $\sim 2.5 \mu m$. Absorption imaging requires two pictures, as discussed below. The shortest possible time interval between the atom and reference picture is desirable to avoid timescales of mechanical movements or other fluctuations, which can lead to fringes in the processed pictures. For the images used here, this interval is 60 ms. Some imaging problems can be solved with post-evaluation but ideally the noise sources should be minimised. This requires a good camera, e.g. with kinetics mode to minimise the time interval between two pictures, fast readout, etc., and carefully designed imaging beam paths. If a CCD camera has a limited dynamic range, clouds with optical depths of the order $> 2$ can become difficult to image accurately. Unfortunately, the camera used here is a low budget, non-cooled camera and has a low quantum efficiency ($\sim 0.3$). Thus, the imaging noise can only be reduced to a certain degree.

4.5.2 Image processing

Absorption imaging is based on two images of pixel-by-pixel arrays $(x, y)$, where one image contains the shadow cast by the atomic cloud $B_1(x, y)$ and the other serves as a reference picture $B_2(x, y)$. The shadow is highly sensitive to the density of the cloud. This in turn depends on the photon scattering through the medium. The standard transmission behaviour including saturation through a medium of thickness $z$ is described by the Lambert-Beer law:

$$\frac{\partial I(z)}{\partial z} = -n \frac{\sigma_0}{\alpha} \frac{1}{1 + I(z) / (\alpha I_{sat}^0)} I(z). \quad (4.12)$$

$I_{sat}^0$ is the saturation intensity and $\sigma_0$ is the absorption cross section. For the D$_2$ two-level system in $^6$Li, the resonant cross section is given by $\sigma_0 = 3\lambda^2/2\pi = 2.14 \times 10^{-9}$.
cm$^2$, which leads to a saturation intensity of $I_{sat}^0 = 2.55 \text{ mW/cm}^2$. The absorption cross section is reduced by another factor of two, because the imaging laser light propagates horizontally and thus perpendicular to the quantisation axis of the magnetic field provided by the Feshbach coils. In that case, only the $\sigma^-$-projection of the linearly polarised imaging light interacts with the atoms. A third dark-image, $B_{dark}(x, y)$, obtained when all beams are off, can be taken as a background reference, to subtract any stray light and CCD dark counts. This is the same for each experimental run and is subtracted from all the atom and reference pictures, $I_A(x,y) = B_1(x,y) - B_{dark}(x,y)$ and $I_R(x,y) = B_2(x,y) - B_{dark}(x,y)$, respectively.

In the simplest analysis the shadow image on the CCD chip with respect to the reference image represents the integrated column atomic density $n(x, y) = \int n(x, y, z)dz$. In earlier experiments, the natural logarithm of the ratio of the atom and reference images led to $n(x, y)$. This assumption is valid for large and dilute samples when the optical depth, $od(x, y) = \sigma_0 \int n(x, y, z)dz$, is much smaller than unity.

In the following, the optical depth is assumed to take on any values and can only be found by including the effects of saturation [213]; hence one needs information on the incident and final intensities as well as $\alpha$ and $I_{sat}$, reason being that imaging a range of clouds from low to high optical densities can hide subtleties, such as the nonlinear response of the atoms to the probe beam and a reduction of the effective cross section. However, this change can be corrected by a dimensionless parameter $\alpha$, which has to be determined from the experiment. By using strong saturation imaging, the effective cross section is intensity dependent, $\sigma(I)$, when $I \gg \alpha I_{sat}^0$. So, the response of the atoms depends on the effective saturation intensity $I_{sat} = \alpha I_{sat}^0$.

The optical depth is $od(x, y) = \sigma_0 \int n(x, y, z)dz$ with the atomic density $n$ given by equation 4.12. The optical density represents the information measured in the absorption image in terms of the density $\delta_0(x, y) = -\ln(I_A(x, y)/I_R(x, y))$. In order to obtain the proper atom number from $N = \sum_{x,y} od(x, y)D/\sigma_0$, the correct value of $\alpha$ has to be extracted from

$$od(x, y) = \alpha \delta_0(x,y) + \frac{I_R(x,y) - I_A(x,y)}{I_{sat}}. \quad (4.13)$$

where $\alpha$ plays the role of the number correction to the saturation intensity due to the polarisation of the imaging beam, the structure of the excited state, and the different Zeeman sublevel populations of the degenerate ground state of the optical transition. It should be noted that for this thesis large samples of up to 200 000 atoms in one spin state are imaged and small structures of the clouds are irrelevant. Therefore, a
large optical depth can be an advantage. Due to the evaluation technique with the f-sum rule, see chapter 3.8.4, even optical errors such as astigmatism of a tilted lens can be compensated.

The imaging calibration here is performed according to (215). To determine $I_{sat}$, the imaging power after the fibre is set to a power of $P_{set} = 2.3$ mW. The power of $I_{pin} = 313 \mu$W is measured through a pinhole of 2 mm$^2$ diameter to obtain an intensity of 9.87 mW/cm$^2$. Dividing this intensity by $I_{sat}^0 = 2.55$ mW/cm$^2$ gives a ratio $r = I_{pin}/I_{sat}^0$. After taking five reference images at 10 µs at that set power, $P_{set}$, the average pixel count, $R_{set}$, is divided by $r$ to yield $I_{sat} = 2R_{set}/r$. The factor of 2 is due to side imaging; as mentioned before the absorption cross section of the atoms is effectively halved because only the $\sigma^-$-polarisation of the linearly polarised imaging beam can drive the atomic transition. Once $I_{sat}$ is fixed, $\alpha$ is varied in equation (4.13) until the measured atom number is constant over the full range of intensities used in the calibration procedure. As the imaging beam power was tuned, the duration of the pulse was varied from 0.96 µs ($I \sim 2.70$ mW) to 14.5 µs ($I \sim 0.15$ mW) while keeping the number of counts per pixel smaller than a tenth of the maximum count, i.e. < 400. We find $\alpha = 2.2$ and $I_{sat} = 1510$ (counts), respectively, referenced to a pulse length of $\Delta t = 10$ µs.

This pulse length is a compromise between a maximum possible photon scattering number and minimal smearing effects. Ideally, one would image with an ultra short pulse and high intensities. This is not practical, and therefore imaging is performed here with $\Delta t = 10$ µs and $\approx 2$ mW to minimize recoil blurring and Doppler shifts: The blurring is introduced by a random walk of the atom after gaining too much recoil momentum from scattered photons. For our pixel resolution of $\Delta r = 4.85$ µm, a critical number of scattered photons, $N_{p,crit} = 3(\Delta r/\Delta t)(m\lambda/(2\pi\hbar)) \approx 12$, can be found before recoil blurring starts to play a role (206). Doppler effects result from a Doppler shift, where during a given time $\Delta t$ an atom has gained a velocity after absorbing photons from the imaging beam. This new velocity leads to an effective change in the imaging frequency. When the photon scattering pushes the atom to a velocity that corresponds to a detuning of $\Delta = \Gamma/2$, i.e. is half the line width, the atom is not really being imaged with resonant light anymore. To calculate the critical number of scattered photons one can use the expression for the scattering rate on resonance

$$N_p = \frac{\Gamma}{2} \cdot \frac{I/I_{sat}}{1 + 2\Delta/\Gamma + (I/I_{sat}) \cdot \Delta t}, \quad (4.14)$$

For the experimental parameters this leads to $N_p \approx 15$ at the effective saturation
$I/I_{\text{sat}} = I_R/\alpha I_{0_{\text{sat}}} \approx 2$. The imaging power applied for data acquisition is higher than the saturation intensity but still much less than needed for high-intensity fluorescence imaging.

In absorption images, the detection sensitivity is limited by intrinsic photon shot noise and technical noise. The pictures do not suffer from fringes in general, but for the discussion of the temperature, see chapter\textsuperscript{[6]} and some measurements of the temperature dependent contact, see chapter\textsuperscript{[8]}, where the result is mainly based on pixel counts, a fringe removal programme is applied to help reduce photon shot noise. This shot noise follows a Poisson distribution, where the variance of the pixel counts is equal to the mean counts per pixel. The noise $\sigma_N$ in the real optical depth in the region of the atoms (ROI) is the square root of the variance of the noise, $\sigma_R^2 = \sigma_A^2$, in picture $A$ and $R$, which are assumed to have the same noise. Thus, $\sigma_N = (D/\sigma_0)\sqrt{\text{ROI}} \sqrt{2\sigma_R^2}$, measured in counts. The noise on the dark frame and the camera readout noise $\sigma_{rd}^2$ are ignored in this analysis. This shot noise can be reduced with an image algorithm which is discussed in the following section.

Fringe removal algorithm

The basic idea in the fringe removal algorithm is the reconstruction of an optimum reference image, $I_Q$, from a set of reference and absorption images. The idea is based on a Gram-Schmidt decomposition and MATLAB\textsuperscript{[18]} offers a sophisticated algorithm for the decomposition [216–218]. In contrast, filtering techniques such as Fourier filtering use the divided picture and thus can require assumptions about the atomic distribution. Filtering such as medians also reduces the signal sharpness, which is important to maintain for Fermi gases where the information is often stored in the wings.

The following procedure is reported in [219], where here the algorithm is outlined. A number $k$ of atom and reference $R_k$ images are taken. MATLAB treats these as a set of linear vectors and solves them to obtain an orthonormal basis set of images, where the optimum image $I_Q = \sum_k c_k I_{R,k}$ is the diagonalised version, i.e. the linear combination of their basis with coefficients $c_k$. The algorithm uses $\delta = \sum_x m_x (I_{A,x} - I_{Q,x})^2$, where $m_x$ is a mask free of signal and $\delta$ is the least square difference which has to be minimised; explicitly

$$\frac{\partial \delta}{\partial c_j} = 2 \sum_x m_x I_{R,x,j} \left( I_{A,x} - \sum_k c_k I_{R,x,k} \right) = 0. \quad (4.15)$$
This reduces to
\[ \sum_k c_k B_{j,k} = \sum_z m_z I_{R,z,j} I_{A,z} \]  
(4.16)

with the matrix elements \( B_{j,k} = \sum_z m_z I_{R,z,j} I_{R,z,k} \). This has to be solved for \( c_k \) with the solver type ‘LU decomposition’ from MATLAB, where the linear equations are sorted into lower and upper triangular matrices.

This algorithm is primarily aiming to filter fringes. But in the end, the shot noise in the optimum image \( I_Q \) is also reduced compared to a single reference image \( I_R \), the reason being that more than one image is used to construct the reference picture. The improvement goes with the square root of the number of images and results in an improvement in the optical density, which for a large number of reference pictures, \( \sigma_N = (D/\sigma_0)\sqrt{OPT\sqrt{\sigma_R^2}} \) or equivalently by a factor of \( \sqrt{2} \) smaller than the standard absorption image. In other words, the noise of the reference image has been decomposed in the optimum reference picture and the noise only comes from the atomic picture.

Other noise sources can also play a role. The atomic cloud may act as a geometric lens or gradient index lens with an index of refraction. This could lead to systematics in measurements of the temperature and density. For imaging with resonant light, lensing effects can be avoided as the refractive part becomes zero.

In most cameras a glass window protects the CCD chip from eventual external damage. Due to the finite thickness of this glass, the imaging light can undergo multiple reflections leading to interference fringes in the processed picture (etaloning). For this reason we remove the glass plate.

Due to the geometry of the imaging beam to trap laser, the cloud is imaged at a certain angle. For very large clouds, e.g. when the cloud is heated and imaged after a release time, the cloud has expanded in all directions. But in the horizontal direction, the cloud size is so big (> \( z_R \approx 50 \mu m \)) that some atoms will lie outside the depth of focus (±20 µm). When heating atoms, the temperature, a global parameter, can appear different in the horizontal and vertical directions due to this focussing. In fact, the temperature seems warmer in the horizontal direction, and the deviation from the vertical direction becomes worse, proportional to the heating rate. Therefore, when heating clouds, we rely on the vertical cloud size, so that we use only the information from the atoms that are in focus.
4.6 Summary

The production of degenerate quantum gases does not come in commercially available machines but requires highly customised setups. In order to investigate strongly interacting Fermi gases, the isotope $^6\text{Li}$ is laser-cooled and condensed below the degeneracy temperature with optical devices in a ultra-high vacuum cell. The optical potentials from a high-power laser set the energy scale of the system, that is the Fermi energy and momentum for Fermi gases. These quantities characterise the basic parameters of the experiments explained chapter 6 and 7. The technical requirements for Bragg spectroscopy are provided by low power and frequency controlled lasers. Opposed to previous theses about this setup, imaging techniques are considered more carefully. This allows a good quality of pictures free of fringes and mostly dominated by photon shot noise, camera dark counts and read-out noise.
Chapter 5

Temperature of unitary Fermi gases

The determination of the temperature in strongly interacting Fermi gases is delicate, from a theoretical as well as an experimental point of view. It is difficult to find accurate models for the strongly interacting fermionic density profiles at finite temperature. This chapter discusses the aspects of thermometry of Fermi gases and how they are achieved with regard to the results presented in chapter 7.

5.1 Introduction

The study of the thermodynamics of universal properties provides valuable insights into strongly interacting Fermi gases, see e.g. [153, 220–224]. The BEC-BCS crossover with its naturally strong correlations poses theoretical challenges as most perturbation theories break down and new are necessary. Determining a universal temperature scale is problematic since it is difficult to construct a quantitative theory in terms of a well-defined small parameter and the equation of state is only known with approximations. The temperature is ideally described by a model-independent as well as a temperature sensitive quantity. Early theoretical models to explain temperature related data were obtained from the BCS mean field picture [48, 225, 226]. In general, numerical models need a good comparison with the experiment to find the appropriate coefficients. The universal relations with the contact parameter may offer a theory in terms of a well defined small parameter, but these relations are not easily accessible and do not seem to show a sensitivity to temperature in the interesting low temperature regime, where the contact changes marginally with temperature. Appropriate boundary conditions are crucial in the solution of the problem.
At unitarity, the energy of a strongly interacting Fermi gas deviates from the ideal gas case over a wide temperature range. Figure 5.4 depicts the energy per particle of an ideal (green line) and strongly interacting (red solid line) Fermi gas in the trap, respectively. The energy per particle is calibrated with respect to the Fermi energy of the non-interacting gas, $\epsilon_F$. In the unitary case, at temperatures $T > 0.5\ T_F$ the curve is nearly a straight line. Below a certain temperature, $T^\ast$, pairing effects exist but a clear onset of pairing is not visible in the energy of a trapped gas. Just below $T = 0.3\ T_F$, the unitarity energy seems to have a plateau. At the critical temperature of superfluidity, $T_C \approx 0.2\ T_F$, the ideal and unitary gas saturate due to Pauli blocking. One observes that the unitary energy has here the biggest deviation from the energy of an ideal gas. The strong interactions lead to pairing of fermions, and thus bosonic structure, which is most pronounced at low temperatures.

The experimental determination of the temperature in spin-balanced Fermi gases at unitarity is of critical importance. The gases are stored in a high vacuum and cannot equilibrate with an external reservoir of known temperature. Exceptions are sympathetically cooled Fermi gases, where a bosonic gas acts as an refrigerator for the spin-balanced Fermi gas, given both are in constant equilibrium. The temperature for bosonic clouds is usually easy to measure. Another exception are Fermi gases with an imbalanced spin population, where the density of the majority spins, which do not pair up, behave like an ideal Fermi gas and an accurate fitting model is applicable.

The most common tool to experimentally access information from fermionic spin balanced, single species clouds are density profiles obtained from absorption images. Different models have been developed to determine the temperature of a Fermi gas though there is no common agreement of a valid analytic model for these profiles. Lacking an analytic model for the density profiles, fitting of Fermi statistical distributions lags behind the related fitting of bosonic distributions where analytic bimodal functions are readily available. When images of clouds are taken, one observes that attractive interactions lead to a shrinking of the cloud. But at unitarity the difference in the shape of a balanced interacting and a non-interacting Fermi gas appears minuscule\cite{112}. The interactions, parameterised by the local $1/(k_Fa)$, vary across the cloud and the temperature varies over different cloud shells. Bosonic clouds below the critical temperature may be accompanied by vortices as a signature of superfluidity. Signatures of superfluidity in strongly interacting Fermi gases have been observed\cite{12} but not linked to the temperature, stimulating the study of the temperatures in strongly interacting Fermi gases.
In the following different evaluation procedures for the temperature are compared. First, the processing of the images of heated clouds at unitarity is described in section 5.2. Then, the determination of the temperature by fitting an empirical temperature to unitary cloud profiles \([48]\) is explained in section 5.3. The temperatures for the results in chapter 6 are obtained in this way, despite the model dependent technique. Next, section 5.4 presents a comparison with the NSR theory by taking the energy per particle from the mean square size of the profiles \([50]\) (and not from the equation of state as originally proposed). Any deviation is included as an uncertainty in the temperature acquisition. Another commonly used technique is described in section 5.5 based on isentropic sweeps of the magnetic field to the weakly interacting regime, i.e. the unitary gas is mapped onto the BCS regime \([30]\). In this limit the entropy is conserved and can be made very close to that of an ideal Fermi gas. Therefore, one data set is taken with adiabatic ramps to \(1/(k_Fa) = -1.5\) and the data is compared to the respective NSR prediction. All results are summarised in a final plot, figure 5.4 and compared in section 5.6. Other methods are also briefly discussed in section 5.7.

### 5.2 Images for the temperature calibration

In order to heat the clouds, first they are fully evaporatively cooled at 834 G to create the same conditions and to set the Fermi energy. The mean trap frequency for this trap is \(\bar{\omega} = 2\pi \times 66\, \text{s}^{-1}\) leading to a Fermi energy of \(\epsilon_F/\hbar = \bar{\omega}(6N^\uparrow)^{1/3} = 2\pi \times 6.8 \times 10^3\, \text{s}^{-1}\) for \(N^\uparrow = 190\,000\) atoms in one spin state. The optical potential depth is \(\sim 90 \times 10^3\, \text{s}^{-1}\), which is a little more than \(13 \times \epsilon_F\). Experimentally, this trap allows for the heating and storage of clouds at unitarity up to \(1.1 T/T_F\) without any detectable atom loss.

After evaporation the confining trap is non-adiabatically switched off and the cloud is allowed to expand for a variable amount of time. The trap is non-adiabatically ramped up and left on for rethermalisation of the cloud for 400 ms, which is larger than \(\bar{\omega}^{-1}\) and about 10 times greater than the inverse of the weak confinement frequency. Five pictures for each release time are taken. In chapter 6 the density distributions of a Fermi gas are derived and the image process is explained in section 4.5. Images imply already one integration along the line of sight.

The cloud has an oblate shape and is imaged from the side, i.e. in plane with the cloud, see figure 5.1. One-dimensional profiles in the horizontal and vertical direction can be taken from the images. They are normalised before a fitting. In the vertical direction of the cloud, in-situ images may suffer from optical astigmatism.
Figure 5.1: Image and integrated profiles in the $x$- and $y$-direction for a cold cloud at 834 G after $\tau_{TOF} = 1.3$ ms. The units are given in pixels.

(tilted camera lenses) as less than 10 pixels are provided for the profile. Released clouds are problematic for the $x$-direction as the camera has a relative angle to the dipole trap beam of 30.2°. Due to the projection on the camera, the cloud is in reality 2 times larger along the weaker confinement direction than seen on the camera. After heating, the horizontal direction is easily out of the depth of focus and the edges of the cloud might be falsely blurred, as discussed in section 4.5. As a consequence, the temperatures are taken from normalised profiles in the tight direction (vertical direction, $y$-direction), which is dominated by the in-focus path of the cloud. Although, the expansion behaviour, taken from hydrodynamic expansion equations, can be used to calculate back to the trapped case, adiabaticity in the switch-off of the trap beam may alter the cloud expansion rate.

For the temperature discussion in this chapter, four data sets are taken: Set I is imaged at 834 G with a release time of $\tau_{TOF} = 1.3$ ms. After this time-of-flight the optical density dropped to 5.3 (about 580 counts per pixel on the CCD camera).
### 5.3 Empirical temperature

One method to determine the temperature at unitarity is based on an empirical temperature \( \tilde{T} \) \[15\]. The assumption is made that the density distribution of a unitary gas behaves like an ideal Thomas-Fermi function, which is scaled by an interaction parameter \( \xi(0) = 1 + \beta = 0.43 \) with \( \beta \approx -0.57 \) in the zero temperature limit \[37, 50, 62, 58, 116, 117, 118, 131, 143, 152, 227, 231\]. A consequence of universality on resonance is that the chemical potential of the gas must scale with a universal function \( \xi(T/T_F) \) which only depends on the reduced temperature \( T/T_F \) \[63\], such that \( \mu(r) = \xi(T/T_F) \epsilon_F(r) \). In the case of \( T = 0 \), the chemical potential and density for a trapped gas are related by

\[
\mu(r) = \mu_0 - V(r) = \xi_0 \epsilon_F(r) \propto n^{2/3}(r) .
\]

The exponent 2/3 is exact, and hence the density profile involves the same scaling with the density as a non-interacting Fermi gas, with a renormalized Fermi tempera-

<table>
<thead>
<tr>
<th>label</th>
<th>( 1/k_F a )</th>
<th>add</th>
<th>TOF</th>
<th>techniques</th>
</tr>
</thead>
<tbody>
<tr>
<td>set I</td>
<td>0</td>
<td>-</td>
<td>1.3 ms</td>
<td>( \tilde{T}, \langle \sigma^2 \rangle )</td>
</tr>
<tr>
<td>set II</td>
<td>0</td>
<td>-</td>
<td>0.2 ms</td>
<td>( \tilde{T}, \langle \sigma^2 \rangle )</td>
</tr>
<tr>
<td>set III</td>
<td>0</td>
<td>500 ms hold</td>
<td>1.3 ms</td>
<td>( \tilde{T}, \langle \sigma^2 \rangle )</td>
</tr>
<tr>
<td>set IV</td>
<td>-1.5</td>
<td>500 ms ramp</td>
<td>1.3 ms</td>
<td>( \langle \sigma^2 \rangle )</td>
</tr>
</tbody>
</table>

**Table 5.1:** Summary of data taken for the temperature calibration. Five images are taken for each heating. The evaluation techniques with the empirical temperature \( \tilde{T} \) and mean square size \( \langle \sigma^2 \rangle \) are described in the text.

This setting gives reliable counts per pixel but still provides a good signal-to-noise and enough pixels in the profile for fitting. Images for set II are taken almost in-situ at 834 G, \( \tau_{TOF} = 0.2 \) ms. For the coldest temperature in this set, the optical density is about 8.5, including the correction of the saturation intensity, and about 200 counts are left at the peak optical density, which is still much higher than the background noise of about 16 counts per pixel. In set III the clouds are given an additional hold time of 500 ms on top of the rethermalisation time and then imaged after a release time of \( \tau_{TOF} = 1.3 \) ms at 834 G. The 500 ms hold time is necessary because in a further set IV the cloud is ramped within this time up to 992 G and imaged at that field after \( \tau_{TOF} = 1.3 \) ms. Then, set III and IV are comparable. Table 5.1 summarises briefly the different conditions.
CHAPTER 5. TEMPERATURE OF UNITARY FERMI GASES

However, for finite temperature, \( \xi(T/T_F) \) may vary from the temperature dependence of a non-interacting gas \([229]\). From fits of these functions to integrated one-dimensional atomic density distributions, the empirical temperature emerges from one of the fitting parameters \([37,48]\). This model-dependent but relatively temperature-insensitive method has been used to determine the heat capacity of a strongly interacting \(^6\)Li Fermi gas \([48]\) and found to be in accordance with a pseudogap theory.

Fitting one-dimensional profiles

In the non-interacting case the cloud size has a different characteristic length at different temperatures. In general, at high temperatures \( T \gg T_F \) the gaussian width \( \sigma_x = \sqrt{2k_B T/m\omega_x^2} \) is correct, but at lower temperatures \( T \ll T_F \) the cloud cannot be smaller than the Thomas-Fermi radius \( R_{TF,x} = \sqrt{2\epsilon_F/m\omega_x^2} \). These quantities affect not only the temperature range but also the size range. The density distribution shows a different behaviour inside and outside the Fermi radius

\[
n_{1D}(x) \propto \begin{cases} 
(1-x^2/R_{TF}^2)^{5/2} & , \ x \ll R_{Fx} \\
\exp(x^2/\sigma_x^2) & , \ x \gg R_{Fx}
\end{cases}
\]  

(5.2)

where \( \sigma_x^2 \propto T \) but \( R_{TF}^2 \propto \epsilon_F(r) \). Thermometry for very cold Fermi clouds is somewhat difficult to derive from the cloud shape as the signature of the temperature relies on the outer rims of the cloud where the signal-to-noise usually drops.

The three-dimensional momentum distribution at finite temperature follows from equation \([1.37]\), where the Fermi-Dirac integral is expressed in terms of the polylogarithmic function, \( \text{Li}_n(z) = \sum_{k=1}^{\infty} z^k/k^n \), where \( z \rightarrow z(q,x) \) is complex. In particular, it follows \( \text{Li}_n(z) \rightarrow -\text{Li}_{3/2}[\exp\left([\mu - V(r)]/(k_B T)\right)] \) for the three-dimensional case and

\[
\text{Li}_n(z) \rightarrow -\text{Li}_{5/2}\left[-e^{-\mu/k_B T}\right]
\]  

(5.3)

for the one-dimensional case, respectively. From the fugacity, \( \exp(\mu/(k_B T)) \), one can define the parameter \( q = \mu/(k_B T) \), which determines the cloud shape. A small fugacity (large and negative \( q \)) yields the gaussian distribution of thermal clouds. For a high fugacity (positive \( q \)), the clouds approach the zero-temperature distribution in one direction \( n_{1D,0} \left(1-x^2/R_{TF}^2\right)^{5/2} \). In the trapped case, where a local density approximation can be used, the spatial degrees of freedom are integrated out and the temperature, \( T \), is a global parameter, but the ratio \( T/T_F(r) \) changes across the
shells as the chemical potential, $\mu(r)$, changes. Imaging errors, such as out of focus imaging, saturation etc., can lead to errors in the measurements of $T/T_F$. Signal-to-noise in the low-density wings of the distribution is a very important factor to obtain reliable information. In the discussion so far, only one dimensional profiles were considered which can be used for in-trap pictures or released clouds. The profiles of released clouds are independent of the trap shape but information about regions with different local $T/T_F(r)$ is integrated out. Two dimensional fits are possible too, but not used here, for instance, integration over elliptical equipotentials (azimuthal averaging, Abel transform). This technique has the advantage that the number of points included in the average grows with the distance from the cloud centre. Hence, the signal-to-noise is best in the wings. However, these procedures require large clouds and are very sensitive to the determination of the cloud’s centre position as well as symmetry.

![Figure 5.2: Extracting $c_x$ from fitting to a one-dimensional profile in the vertical direction of a unitary cold cloud after a release time of $\tau = 1.3$ ms. A Thomas-Fermi profile at zero temperature is used to fit the circles representing the parabolic inner part of the cloud. The gaussian fit is for comparison.](image)

The fitting model for the normalised, integrated image profiles is based on an analytic function for weakly interacting Fermi gases that can be scaled for strongly interacting Fermi gases as discussed in many textbooks, e.g. [202]. This technique is applied to sets I, II and III. With the universal constant $\beta = -0.57$, the Fermi
CHAPTER 5. TEMPERATURE OF UNITARY FERMI GASES

temperature becomes \( T' = \sqrt{1 + \beta T} \), i.e. the temperature is understood in terms of the empirical reduced temperature \( \sqrt{1 + \beta T} = T/T_F(r) \). The density profile reads then for atoms in one spin state \( N_\uparrow \)

\[
n(x, T) = -\frac{6N_\uparrow}{\sqrt{\pi} R_{TF,x}} (\hat{T})^{5/2} \text{Li}_{5/2} \left[ -\exp \left( \frac{\mu}{\epsilon_F} - \frac{x^2}{R_{TF,x}^2} \right) \right], \tag{5.4}
\]

which includes the polylogarithmic function \( \text{Li}_{5/2} \) and the chemical potential \( \mu \). The first part is left as a fit parameter \( a \) and \( \mu/(\epsilon_F\hat{T}) \) is represented as \( q \) where \( q \geq 0 \) for \( T \leq T_C \), otherwise \( q = 0 \). (The influence of \( \hat{T} \) on \( q \) is small since for high temperatures the chemical potential is a large negative number.) The atom number can be determined from the profiles. The Thomas-Fermi radius can be calculated from fixed trapping frequencies:

\[
R_{TF,x} = \sqrt{\frac{2\epsilon_F}{m\omega_x^2}} = \sqrt{\frac{2(6)^{1/3}}{m\omega_x^2}} N_\uparrow^{1/6} = c_x N_\uparrow^{1/6} \tag{5.5}
\]

Alternatively, the Thomas-Fermi radius is obtained from the zero temperature profile

\[
n_{1D}(x) = \frac{16N_\uparrow}{5\pi R_{TF,x}} \left( 1 - \frac{x^2}{R_{TF,x}^2} \right)^{5/2} \tag{5.6}
\]

and we again obtain \( R_{TF,x} = c_x N_\uparrow^{1/6} \). In practice, this expression is fitted to the centre of the coldest experimentally achievable cloud, under the assumption that finite temperature effects in a Fermi gas mostly affect its wings \[232, 233\]. Both approaches are consistent in the resulting \( c_x \) value but as mentioned above, to account for pixel imperfections, the equation \ref{5.6} is used to provide the Thomas-Fermi radius, see figure 5.2. With \( c_x \) fixed, the fit function for the one-dimensional profile becomes

\[
n(x, \hat{T}) = a\text{Li}_{5/2} \left[ -\exp \left( q - \frac{x^2}{c_x^2 N_\uparrow^{1/3}} \right) \right]. \tag{5.7}
\]

Temperatures obtained in this way are used later in the presentation of the temperature dependent contact. Figure 5.3 shows two typical profiles which yield temperatures of 0.07 \( T/T_F \) and 0.52 \( T/T_F \). In this representation the uncertainty in the fitted temperature is given by the standard deviation of five images, which is in average 0.02 \( T/T_F \).
5.4 Comparison with NSR theory

In the low temperature limit $T/T_F < 1$, strong coupling theories are required to accurately describe the thermodynamics of unitary Fermi gases with strong interactions. In general, any theoretical model to characterise a two-component Fermi gas at unitarity assumes the s-wave scattering problem and the short range model, as introduced in chapter 2. A theoretical model must produce a uniform universal function from which a complete set of universal thermodynamic functions can be derived. Furthermore, it is more convincing if no fitting functions or adjustable parameters are required. Strong coupling theories are based on approximate many-body $t$-matrix theories, i.e. the ladder structure of Green’s functions with interaction need to be determined. Nozière and Schmitt-Rink (NSR) described in this way a normal interacting Fermi gas [162]. In order to include strong pair fluctuations in the strongly interacting regime, it is necessary to include the ladder sum. The NSR idea could be fully extended to the below-threshold ($< T_C$) regime, which is referred to as the GPF (gaussian pair fluctuation) approach [83], to provide a quantitatively reliable description of the low-temperature thermodynamics of a strongly interacting Fermi superfluid. The NSR theory uses different assumptions below and above the critical temperature. Below $T_C$ quasi particles are assumed while above $T_C$ fermions are the basic particles. This difference causes discrepancies at $T_C$ which can be interpolated across for trapped clouds. Even though there is a discontinuity in the

![Figure 5.3: Single shot temperature profiles in the tight direction after 1.3 ms time of flight at 0.07 $T/T_F$ and 0.52 $T/T_F$.](image-url)
theoretical universal function of the GPF theory, the result for the trapped equation is much smoother. The NSR theory breaks down at the critical temperature because so far only two-particle scattering is used. Improvements at the critical temperature may be achieved with the inclusion of 3, 4 or many-body scattering mechanisms. Compared to other theories, the NSR predictions show very good agreement with the experimental data over a wide range of temperatures and different setups [117] (JILA, ENS, Duke, Rice). The predictions of the NSR theory deviate from those of mean-field crossover theories [167]. The NSR result for the equation of state is very accurate at low and high temperatures. At first, the thermodynamic potential, \( \Omega(\mu, T) \), is defined with respect to the ideal case, \( \Omega^{(1)}(\mu, T) \). According to basic thermodynamics, their derivatives provide, for instance, the energy \( E(T) \) and entropy \( S(T) \). These potentials can form a set of universal thermodynamic functions of a trapped Fermi gas at unitarity. The question is how the thermodynamic potentials scale with the temperature at unitarity. The large scattering length in the unitarity limit leaves the interatomic distance as the only relevant length scale. This rescaling influences the energy and entropy, and leads to the equation of state for an ideal noninteracting Fermi gas. In the trapped case, one has to make use of the local density approximation. The atom number is set by \( N = \int d\mathbf{r} n(\mathbf{r}) \) with the pressure dependent particle density \( n(\mathbf{r}) = \partial P(\mathbf{r})/\partial \mu(\mathbf{r}) \) and \( \partial \mu(\mathbf{r})/\partial r = -m\omega^2 r \) where \( \omega \) is the mean trap frequency. The rather complicated calculation is performed in terms of the inverse fugacity [82].

Comparison of the data with NSR theory

The temperatures obtained from the empirical temperature in all sets I-IV can be compared with the NSR theory if the energy per particle is determined. Five integrated profiles are averaged before the mean square size \( \langle \sigma^2 \rangle \equiv \langle r^2 \rangle \) is recorded. In order to reduce noise, \( \langle r^2 \rangle \) is actually extracted from the polylogarithmic density distributional fit to the averaged profile. Then, the energy per particle follows from [50]

\[
\frac{E}{N_i} = 3m\omega_i^2 \langle r_i^2 \rangle
\]  \hspace{1cm} (5.8)

where \( i \) indicates the respective integration direction. At \( T = 0 \), the Fermi energy \( ((6N_i)^{1/3}\hbar\bar{\omega}) \) sets the Fermi radius and its re-expression as the mean square size
Now, the energy per particle with respect to the global Fermi energy for the non-interacting case is given by

$$\frac{E}{N_i \epsilon_F} = \frac{3}{4} \frac{\langle r_i \rangle}{\langle r_{TF,i} \rangle} \times b_i.$$  \hfill (5.10)

Since the images are for expanded clouds, the factor $b_i$ contains the re-scaling back to the trapped case ($b_i = \frac{\langle r_i,1.3\text{ms} \rangle}{\langle r_i,0.2\text{ms} \rangle}$) as well as to the same units as of $\langle r_{TF,i} \rangle$. Plotting $E/N_i \epsilon_F$ against the temperatures obtained with equation 5.7 allows a comparison with the NSR theory based on the calculation of the energy of state. The energy per particle taken in the vertical direction is depicted in figure 5.4 over a range of temperatures. The data agrees well within the error based on atom number fluctuations in five shots which is reflected in the calculated in-trap Fermi radius.

### 5.5 Weakly interacting limit

Another method considers the entropy as a more readily measurable quantity than the temperature. The entropy, energy, and critical temperature of a strongly interacting degenerate Fermi gas have been derived from the fundamental relation $T = \partial E/\partial S$ of the thermodynamic potentials, i.e. the total energy $E$ and entropy $S$ \cite{50}. However, the strongly interacting regime has to be mapped adiabatically onto the weakly interacting BCS limit \cite{51,225}, using the knowledge that the mean square size of the cloud is directly proportional to the entropy for weak interactions. This method is model-independent due to the fundamental thermodynamic relation but complicated power-law fitting is necessary to connect the temperature range above and below the critical temperature continuously \cite{231}. Systematic errors can occur for non-adiabatic ramping of the magnetic field.

The non-interacting temperature, $T_i$, of an ideal Fermi gas is accessible from the density profile. The entropy of a non-interacting Fermi gas is known and is unchanged in an adiabatic sweep. The isentropic sweep away from resonance tends to decrease the temperature so that $T_i$ is always somewhat below the temperature $T$ at unitarity \cite{165,231,235}. The remaining question of mapping the temperature for a trapped Fermi gas at unitarity to $T_i$ is addressed with the NSR theory and the universal thermodynamic function $S(T)$. By equating $S(T)$ and $S_i(T)$, where

$$\epsilon_F = \frac{1}{2} m \Omega_i^2 R_{TF,i}^2 = 4 m \Omega_i^2 \langle r_{TF,i}^2 \rangle$$

according to $R_{TF,i}^2 = 8 \langle r_{TF,i}^2 \rangle$; thus

$$\epsilon_F = \frac{1}{2} m \Omega_i^2 R_{TF,i}^2 = 4 m \Omega_i^2 \langle r_{TF,i}^2 \rangle$$

(5.9)
$S_i$ is the entropy of an ideal Fermi gas, the temperature $T$ of strongly interacting Fermi gases is expressed as a function of the non-interacting temperature $T_i$. $S(T)$ and $S_i(T)$ must be congruent in the BCS limit. Due to the accuracy with which the entropy function is ascertained from the equation of state in the NSR theory, the mapping of the temperatures in the different regimes is well defined [82].

### Imaging in the BCS limit

A set of clouds, set IV, is produced by evaporating and heating at unitarity and then ramping in 500 ms to 992 G ($1/(k_F a) = -1.5$). Imaging is performed at that magnetic field after 1.3 ms time of flight. Here, some steps of the programme for the empirical temperature are used. The Thomas-Fermi density profiles from the fits are used to obtain the mean square size of the cloud but the fitting parameters are ignored. Instead, the mean square size is plotted against the temperature obtained at 834 G (set III), where an additional hold time compensates the ramp time to reach 992 G. The data agrees well with the NSR prediction at $1/(k_F a) = -1.5$.

The ratio of the mean square size at 992 G and 834 G, $\langle \sigma^2_{992} \rangle / \langle \sigma^2_{834} \rangle$, is plotted against the temperature expressed as $E_{834}/N\epsilon_F$ in figure 5.5. The error bars are the standard deviation of five images. By independently measuring the ratio of the mean square size, $\langle \sigma^2_{992} \rangle / \langle \sigma^2_{834} \rangle$, and the ratio of the (total) energy at 992 G and 834 G, $E_{992}/E_{834}$, it can be shown that $\langle \sigma^2_{992} \rangle / \langle \sigma^2_{834} \rangle \approx 1 E_{992}/E_{834}$, i.e. the energy scales with the width not only linearly but with a slope of unity [236].

### 5.6 Comparison of the methods

The method of fitting Thomas-Fermi profiles to one-dimensional profiles to obtain the empirical temperature is a relatively quick method and only requires one absorption image, if $c_z$ is given, for instance through a calibration. The standard deviation of five images is better than 0.02 $T/T_F$. Nevertheless, the model-dependence remains disputable.

One can also take the mean square size of the cloud and use the calibration curve at $1/(k_F a) = 0$ provided by the NSR theory. To find the total uncertainty from both techniques, we include the standard deviation of five images, $\delta_{\text{fit}}$, and the deviation of the empirical temperature from the NSR calibration, $\delta_{\text{NSR}}$, and add these in quadrature as $\delta_{\text{tot}}^2 = \delta_{\text{fit}}^2 + \delta_{\text{NSR}}^2$. The temperature deviates on average by $\pm 0.03 T/T_F$ and the total error, $\delta_{\text{tot}}$, is in agreement with the NSR calibration curve over the applied temperature range, as shown by the error bars in figure 5.8. The
5.6 COMPARISON OF THE METHODS

Figure 5.4: Presentation of the temperature calibration. Black dots are data points from unitarity fits and are to be compared with the NSR curve for 1/(k_F a) = 0 (red line). Adiabatic sweeps to 1/(k_F a) = −1.5 yield the blue dots and are to be compared with the NSR curve for 1/(k_F a) = −1.5 (blue line). Also plotted are the ideal gas case (green line) and the power law obtained by the Duke group [231] (red dashed line). Note that all error bars on the data points are only the standard deviations from the empirical temperature.

temperature measurement performed by the ENS group [130,173] agrees with the NSR curve within 1% [167].

For comparison the clouds are imaged at 1/(k_F a) = −1.5 after they are heated at unitarity, to see if the temperature obtained at unitarity can be reproduced after an adiabatic sweep to the weakly interacting regime, see blue data points in figure 5.4. The temperature obtained from set III is compared to the temperature read off the NSR calibration curve at 1/(k_F a) = −1.5 using again δ_{tot}^2 = δ_{fit}^2 + δ_{NSR}^2. In the tight direction of the cloud the relative error is better than 5% or 0.03 T/T_F on average. The lowest two energy data points are excluded since they may have been underestimated due to a high optical density.
Figure 5.5: Ratio in the $y$-direction of the mean square size in the weakly interacting regime, $\sigma_{992}^2 \equiv \langle \sigma_{992}^2 \rangle$, to the mean square size at unitarity, $\sigma_{834}^2 \equiv \langle \sigma_{834}^2 \rangle$, plotted against the temperature expressed in terms of the ratio of unitarity energy, $E_{834}/N$, per particle to the Fermi energy, $\epsilon_F$. The data is in qualitative agreement with [10].

5.7 Alternative approaches

It has also been suggested to adiabatically convert the unitary gas to the deep BEC limit (isentropic thermometry), where a subsequent measurement of the BEC temperature $T'$ of a resulting Bose gas can be taken [234]. Such techniques have been used [11], but the conversion between $T'$ and the unitary temperature $T$ remains model dependent. Moreover, a side effect of sweeping to the deep BEC side is heating due to the adiabatic formation of molecules and a subsequent molecular decay.

An alternative may be to use the information about the temperature from the equation of state, $P(\mu, T)$. The experimentally derived energy per particle [173] and theoretically predicted values [235] are found to be in good agreement over the range $0 - 0.8 T/T_F$. The theoretical model uses the NSR scheme to calculate the equation of state to obtain measurable quantities such as the entropy and chemical potential. For the experimental data, sympathetic cooling of $^6$Li by $^7$Li was used. In-situ images of doubly integrated density profiles lead, as proposed [237], to the equation of state of a homogeneous Fermi gas of $^6$Li atoms. This requires the measurement of the local pressure $P(\mu(z), T)$ or the local thermodynamic potential $\Omega(\mu(z), T) = -P(\mu(z), T)\delta V$ in a small volume $\delta V$ at position $z$, where the chemical potential follows from the local density approximation $\mu(z) = \mu_0 - V(z)$ and the
central chemical potential $\mu_0$. Independently, the temperature in those experiments by the ENS group was determined from bosonic $^7$Li which played the role of a refrigerant in the cooling cycle \[173\].

At high temperatures $T/T_F \geq 1$, gaussian fitting is accurate to within 1 %. The fugacity, $z = \exp (\mu/k_B T)$, is much smaller than unity as the chemical potential $\mu$ converges to $-\infty$. Thus, the fugacity is a small parameter and the virial expansion is an appropriate model, where the thermodynamic potential of the interacting Fermi gas can be calculated with a cluster expansion in powers of the fugacity \[116, 169\]. The temperature independent virial coefficients $\Delta b_n = b_n - b_n^{(1)}$ appear as the $n$th prefactors of the polynomial function of the fugacity:

$$\frac{\Omega - \Omega^{(1)}}{V} = -\frac{2k_B T}{\lambda^3} \left[ \Delta b_2 z^2 + \ldots + \Delta b_n z^n + \ldots \right].$$

The thermal deBroglie wave length is given by $\lambda \equiv [2\pi \hbar^2/(mk_B T)]^{1/2}$ and the volume as $V$. Note that the difference $\Omega - \Omega^{(1)}$ is quantum cluster expanded. At unitarity, the virial coefficients are known up to fourth order. The virial expansion can bridge many-body and few-body systems in the high temperature limit. In a trapped gas the virial expansion can work well down to $T \approx 0.5 T_F$ \[169\].

When the fugacity and the virial expansion coefficients are known, then it should be possible to find the energy and the density profile for the trapped case. One has to make use of the local density approximation to calculate the quantities in the trapped cloud. A series of fugacities would then enter the polylogarithmic function. With knowledge of the virial expansion coefficients, this would provide a straight forward method to obtain analytic density profiles for temperatures down to $T \leq 0.5 T_F$.

### 5.8 Summary

Strongly interacting Fermi gases with a balanced spin mixture are prepared in an ultra-high vacuum chamber, and conventional thermometry via an externally equilibrated refrigerant is not possible. Absorption images yield the spatial density distribution, from which the temperature is extracted. Accurate expressions for the density profiles are difficult to define for unitary Fermi gases. So far, the solution is a shape comparison with the noninteracting Fermi gas together with a rescaling, since the interactions shrink the cloud. In order to determine the temperature, these modified Thomas-Fermi profiles are applied. For comparison, the mean square size as a model-independent quantity is related to the energy per particle. The NSR
theory provides a calibration curve that relates the energy to the temperature and therefore the temperatures can be read off if the mean square size is given. Therefore, the two methods determine the temperature from the density distribution of a strongly interacting Fermi gas. The empirical temperatures agree with the NSR calibration within 5%.
Chapter 6

Universal behaviour of pair correlations

Universality in ultracold strongly interacting Fermi gases is studied by stimulated, two-photon inelastic Bragg scattering for a range of energy and momentum transfer. The high momentum transfer allows a spectroscopic measurement of pair correlations and the high momentum distribution of the gas. At unitarity, the short-range physics is governed by contact interactions. The relevant universal parameter is the contact, $I$, which connects microscopic and macroscopic properties as discussed in chapter 2. The contact depends on the dimensionless interaction strength $1/k_F a$ and the relative temperature $T/T_F$; the latter is discussed in chapter 7. This chapter provides the basic understanding for the static structure factor from which the contact can be determined. The static structure factor and its universal behaviour is measured in the unitarity regime.

6.1 Introduction

Strongly interacting Fermi gases provide a paradigm to study properties such as superfluidity or universality [35, 44, 48–51, 117], as described in chapter 1. The quantity considered here to investigate universality is the static structure factor. The static structure factor quantifies macroscopically short-range pair correlations, which are difficult to measure directly. With the help of Tan’s universal relations it can be shown that the static structure factor follows a simple universal law. Universality, the contact, $I$, and the Tan relations have been introduced in chapter 2. Recall that the physical background, on which the universal relations are built, assumes that the zero range scattering length $a$ exceeds the interparticle separation $r$ which greatly exceeds the short range of the interaction potential $r_0$. Starting with the universality
of the static structure factor in section 6.2 its applicability to Bragg spectroscopy is described. Experimental verification in section 6.3 contains the details on how the Bragg spectra are obtained. With the basic theory of linear response theory from chapter 3, the sum rules can now be applied. In this context, section 6.4 presents how the interaction dependence of the contact across the crossover is extracted from previous work of this group [80].

6.2 Universality of the static structure factor

In a quantum fluid, short-range structure depends upon the relative wave function of the interacting particles, \( \psi^{\uparrow\downarrow} \propto 1/r - 1/a \). Tan showed that the pair correlation function, \( g^{(2)}_{\uparrow\downarrow} \), diverges as \( I/r^2 \) at short relative distance between two particles, \( r < 1/k_F \), and may be written as

\[
g^{(2)}_{\uparrow\downarrow}(r) = \frac{I}{16\pi^2} \left( \frac{1}{r^2} - \frac{1}{ar} \right),
\]

This universal law is related to the (microscopic) correlation function, as discussed in equation 2.9. According to Tan, the contact \( I \) quantifies the likelihood of finding two fermions with opposite spin close enough to interact with each other. \( I \) embodies all of the information necessary to determine the many-body properties, i.e. it depends on the density \( n \propto k_F^3 \), the interaction strength \( 1/k_F a \) and temperature \( T/T_F \) of the system. The two-body correlation function \( g^{(2)}_{\uparrow\downarrow} \) is usually not easy to access experimentally. Hence it is necessary to measure macroscopic quantities with a well defined dependence on the correlation function.

The static structure factor, \( S(k) \), for example, is a macroscopic quantity and depends on the two-body correlation function through its Fourier transform, see equation 3.14.

\[
S(k \gg k_F) = 1 + n \int dr \left[ g^{(2)}(r) - 1 \right] e^{ikk\cdot r}.
\]

In general, two particles can have parallel or antiparallel spin, so the total static structure factor is

\[
S = \frac{S_{\uparrow\uparrow} + S_{\downarrow\downarrow}}{2} + \frac{S_{\uparrow\downarrow} + S_{\downarrow\uparrow}}{2}.
\]

For a spin balanced gas, the number of spin-up and spin-down atoms is equal, and thus \( S_{\uparrow\uparrow} = S_{\downarrow\downarrow} \) and \( S_{\uparrow\downarrow} = S_{\downarrow\uparrow} \) lead to \( S = S_{\uparrow\uparrow} + S_{\uparrow\downarrow} \). Furthermore, for large
momentum transfer, \( q = \hbar k \gg \hbar k_F \), e.g. a spin-up particle only scatters into states with a preoccupied spin-down particle or an empty state due to the Pauli exclusion principle. Hence, the autocorrelation of parallel spins goes to unity, \( g^{(2)}_{\uparrow\uparrow} (r) \rightarrow 1 \), and consequently in equation the static structure factor approaches unity, \( S_{\uparrow\uparrow} \rightarrow 1 \). This means that for a spin balanced Fermi gas only the correlation between particles with composite spins contribute to the two-body correlation function \[ \text{[6.3, 82]} \].

\[
S(k \gg k_F) = 1 + S_{\uparrow\downarrow}. \quad (6.4)
\]

The Fourier transform of equation [6.1] is explicitly \[ \text{[83]} \]

\[
S_{\uparrow\downarrow}(k \gg k_F) = \frac{I}{4Nk_F} \frac{k_F}{k} \left[ 1 - \frac{4}{\pi k_F a} \left( \frac{k_F}{k} \right) \right]. \quad (6.5)
\]

The total static structure \( S(k \gg k_F) = 1 + S_{\uparrow\downarrow} \) can be measured with Bragg spectroscopy, from which \( S_{\uparrow\downarrow} \) is extracted. In Bragg spectroscopy one probes the linear response of instantaneous fluctuations in the gas. Signatures of correlated pairs and free particles are represented in the dynamic structure factor, \( S(k, \omega) \) \[ \text{[75]} \]. In fact, the response can be quantified by measuring either the momentum \[ \text{[83]} \] or energy transferred by a Bragg pulse. Integration over the \( S(k, \omega) \) gives \( S(k) \) which represents in turn the two-body correlation function through the Fourier transform, see equation [6.5]. The static structure factor \( S(k) \) derived in chapter follows a universal law (to first order). Equation [6.5] shows that the ratio \( I/Nk_F \) follows a universal scaling, that is, the universal character is understood as a dependence solely on the dimensionless interaction strength via the inverse scattering length \( a \), the relative probe momentum according to the short-range interparticle distance \( 1/r << 1/r_0 \propto k/k_F \), and the dimensionless universal contact parameter \( I/Nk_F \).

In theory this expression is universally applicable to any dilute strongly interacting Fermi system with contact interactions after a rescaling. The expression is also model independent which opens the possibility to compare the observed mechanisms with other areas in physics, e.g. crystallography or solid state physics.

**6.3 Experimental verification**

Bragg spectra reflect the composition of the gas, being dominated by bosonic molecules below the Feshbach resonance, pairs and free fermionic atoms near unitarity, and free fermions above resonance. The Bragg spectra are reconstructed in the inset of figure [6.7a]. After the Bragg pulse, the distorted cloud shows the effects of the...
underlying correlations. The revealing of these correlations can be complicated by elastic collisions between scattered and unscattered particles [238], which are hard to separate in the BEC-BCS crossover. Nonetheless, elastic collisions do not present a major problem as they preserve centre of mass motion.

In this section it is shown how the universal behaviour of the static structure factor is verified over a wide range of probe momenta $k/k_F$ as well as at different interaction strengths $1/k_Fa$. The measurements are compared to new calculations for the contact based on a below-threshold Gaussian pair fluctuation theory [82]. The general trend of $S(k)$, and therefore the two-body correlation function, is a smooth increase with both lower probe momenta and higher $1/k_Fa$ on passing from the BCS to the BEC side. Equation 6.5 forms the heart of this chapter and describes the short-range pairing on both sides of the Feshbach resonance. An equivalent interpretation identifies this result as a measurement of the interaction dependence of the contact for a spin balanced gas in the zero temperature limit, as previous theoretical [70, 83, 84] and experimental [36, 133] works have studied.

The experimental proof of the universal character of equation 6.5 up to first order requires an independent variation of the probe momenta $k/k_F$ over a wide range at different values of the interaction parameter $1/(k_Fa)$. For different combinations of these parameters, Bragg spectra of ultracold Fermi gases are taken with the momentum transfer method as described in chapter 4 to relate the centre of mass displacement, $\Delta X$, to $S(k, \omega)$ and $S(k)$. These investigations take place in strongly interacting Fermi gases, so there are inevitable collisions between scattered and unscattered particles after the Bragg pulse which alter the atomic distribution. But these collisions preserve the centre of mass momentum and therefore measuring $\Delta X$ still provides an accurate measure of the momentum transferred regardless of the spatial details of the cloud. This technique was found to be adequate over the whole BEC-BCS crossover regime where the collisional details change [80]. The shape of the spectra is non-trivial. For that work, $k/k_F = 5$ and $T/T_F \approx 0.1$, and spectra have been calculated with a method based on a random phase approximation [192]. In this chapter, the data evaluation relies completely on the experimental data and no fitting is applied.

6.3.1 Procedure

The experimental sequence starts with the preparation of an ultracold sample of $^6$Li atoms which is loaded from a magneto-optical trap into a single optical dipole trap ($\lambda = 1075$ nm). Evaporative cooling at a magnetic field of 834 G leads to a
resonance superfluid containing $N \approx 3 \times 10^5$ atoms in an equal mixture of the two lowest lying ground states $|F = 1/2, m_F = \pm 1/2\rangle$ at $T \leq 0.1 T_F$.

To gain more control over the trapping frequencies of the cloud, a second far detuned laser ($\lambda = 1064$ nm) is ramped up adiabatically to intersect with the first trapping beam at an angle of $74^\circ$. The configuration of the trap and Bragg beams is depicted in fig. 6.1. In this crossed beam configuration both laser intensities are controlled individually such that the mean harmonic confinement frequency of the crossed trap $\bar{\omega}$ can be tuned over the range $\bar{\omega} = 2\pi \times (38 \rightarrow 252) \text{ s}^{-1}$. At the same time the aspect ratio $\omega_{x,y}/\omega_z$ varies from 3.4 to 16, so the cloud is always in the three-dimensional regime. Consequently, the control over the trap frequencies determines the Fermi wave vector $k_F$ according to $k_F = (48N)^{1/6} \sqrt{m\bar{\omega}/\hbar}$, which is explicitly $k_F = 2.1 \mu m^{-1} \rightarrow 5.3 \mu m^{-1}$. As the length scale is related to the atomic density $n(r)^2 = 6\pi k_F^3$, the change in trapping frequencies translates to a change in the relative momentum $k/k_F = 3.5 \rightarrow 9.1$. Figure 6.2 shows graphically the range over which the ratio $k/k_F$ can be varied with the laser powers of the primary trap.

Next, the scattering length $a$ is addressed with an adiabatic ramp to the final magnetic field allowing the dimensionless interaction strength, $1/(k_F a)$, to be tuned in such a way as to keep the product $k_F a$ constant. Note that the parameters $k_F$
and $a$ are independent ‘control knobs’ whereas $1/(k_F a)$ is only constant for a chosen $k_F$ if the respective scattering length $a$ is fine-tuned with the magnetic field, $B$. Assuming 140 000 particles in one spin state, for $1/k_F a = +0.3$, the magnetic field is changed from $B = 802.8$ G at $2\pi 250$ s$^{-1}$ and $k_F/k = 0.284$ to $B = 820.0$ G at $2\pi 44$ s$^{-1}$ and $k_F/k = 0.119$. For $1/k_F a = -0.2$, the magnetic field is changed from $B = 860.2$ G at $2\pi 252$ s$^{-1}$ and $k_F/k = 0.285$ to $B = 844.5$ G at $2\pi 45$ s$^{-1}$ and $k_F/k = 0.120$. After equilibration at the final magnetic field for $\tau \gg 10 \bar{\omega}^{-1}$, the Bragg pulse ($P_{Br} = 40 \, \mu W$) is applied onto the trapped cloud for 50 $\mu$s, which is short compared to the two-photon Rabi cycling period, ensuring that spectra are obtained in the linear response regime. The imparted momentum is $k/k_F$ with fixed $k = k_L \sin(\theta/2)$, that is, with a constant angle between the two Bragg beams, and the Fermi momentum $k_F$ is tunable. The recoil energy $\omega_R = 2\hbar k_F^2/m$ for one atom with mass $m$ is defined by the angle of the Bragg beams. For this setup $\omega_R = 2\pi 300 \cdot 10^3$ s$^{-1}$. To enhance centre of mass signal the cloud travels for $\tau_{\text{trap}} = 1$ ms in the trap and expands further for $\tau_{\text{TOF}} = 2$ ms after turning off the trap. The imaging frequency is tuned to be resonant with the final magnetic field. The trapping frequency along the direction of the Bragg beam is $2\pi 24.5$ s$^{-1}$, which is the weakest confinement. Therefore, one has a quarter of the corresponding oscillation time, $\leq 10$ ms, before the cloud turns around. This procedure is carried out for every Bragg frequency $\omega = 0 - 2\pi 430 \cdot 10^3$ s$^{-1}$. The process from single pictures to $S(k, \omega)$ is described in the following.
6.3 EXPERIMENTAL VERIFICATION

6.3.2 Creating Bragg spectra

From the images, line profiles and their first moment are extracted using the fact that the transferred momentum is directly proportional to the resultant $\Delta X(k, \omega)$, see chapter 3. A graphic guide to the procedure is depicted in figure 6.3. The vertical axis is labelled as $x$, and represents the direction of the applied Bragg pulse. The horizontal, non-Bragg direction in the image is labelled as $y$. Each image $i$ yields a two-dimensional atomic distribution, $n_i(x, y)$, and is taken for a different Bragg frequency $\omega$.

For every image $i$ where the Bragg frequency is varied, a one-dimensional sum is taken over the $y$-direction to obtain a line profile in the $x$-direction, $n_i(x)$. The region of interest in the $x$-direction is chosen to be as small as possible to include all atoms but exclude unnecessary background that only adds noise. After summation the area under each line profile $n_i(x)$ is normalised to unity. From the line profiles $n_i(x)$ the first moment, labelled '(1)', is evaluated from

$$X^{(1)}_i = \frac{\sum_x n_i(x) \cdot x}{\sum_x n_i(x)}.$$  \hfill (6.6)

Hence, $X^{(1)}_i$ denotes the centre of mass taken from the line profile of each image $i$. $X^{(1)}(\omega) \equiv X^{(1)}_i$ represents a spectrum where the centre of mass changes with the applied Bragg frequency, $\omega$.

Since the interest lies in the centre of mass displacement, it is necessary to determine a reference position of an unperturbed cloud, denoted as $X^{(1)}_{\text{off}}$. This is the equivalent of taking the centre of mass position following an off-resonant Bragg pulse. The offset $X^{(1)}_{\text{off}}$ is subtracted from all the $X^{(1)}(\omega)$. Now the quantity of interest is

$$\Delta X^{(1)} = X^{(1)}(\omega) - X^{(1)}_{\text{off}}.$$  \hfill (6.7)

Derivation of the dynamic structure factor

To compare Bragg spectra, the dynamic structure factor is normalised to the atom number $N$ with the definition for the f-sum rule, described in equation 3.54. The f-sum rule states that the integration over the energy times the dynamic structure factor is proportional to the atom number. Hence, the normalised dynamic structure factor is obtained from the centre of mass displacement using

$$P_{\Delta X}(\omega) = \frac{\Delta X^{(1)}(\omega)}{\sum_\omega \Delta X^{(1)}(\omega) \cdot \omega}.$$  \hfill (6.8)
Figure 6.3: From images to line profiles to spectrum: (a,d) unperturbed cloud. (b,e) Scattered cloud at the recoil frequency. (c) Integrated line profiles for all images. (f) Centre of mass displacement (points) spectrum obtained from line profiles. The line is a guide to the eye.
Finally, the real dynamic structure factor is for any momentum $k$

$$S_{\Delta X}(k, \omega) = \frac{P_{\Delta X}(\omega)}{1 - e^{-\omega/k_B T}}, \quad (6.9)$$

which takes into account finite temperature through detailed balancing. For the measurements that follow in this chapter, the temperature at unitarity is $\sim 0.1 T/T_F$ and the denominator approaches unity in the relevant frequency range.

### 6.3.3 Dynamic response

Being now able to control the relative probe momentum $k/k_F$ and the interaction strength $1/(k_F a)$, a sequence of energy resolved Bragg spectra can be taken for any parameter set. Figure 6.4 shows Bragg spectra for various probe momenta sorted by $1/(k_F a) = 0.0, + 0.3, - 0.2$. At high momenta, the pair and free-atom excitations are clearly distinguished at frequencies of $\omega_R/2 \sim 2\pi \cdot 150 \cdot 10^3 \text{ s}^{-1}$ and $\omega_R \sim 2\pi \cdot 300 \cdot 10^3 \text{ s}^{-1}$, respectively. With decreasing probe momenta, the signal strength at the pair frequency ($\omega_R/2$) increases. The signal at pair frequencies is generally increasing from $1/(k_F a) = - 0.2$ to $+ 0.3$ until the bound state is reached on the BEC side (bound molecule regime).

These spectra represent the dynamic structure factor of the strongly interacting Fermi gas. Probed with Bragg spectroscopy, they respond to single atom and pair excitations. The height and sharpness of the pair peak is commensurate with the condensate fraction. At unitarity, it indicates a substantial fraction of correlated pairs. At $1/(k_F a) = - 0.2$ (BCS side), the pair size is larger than on the BEC side [56]. The spectra, and therefore $S(k, \omega)$, are continuous and more dominated by incoherent response to the density fluctuation $\rho_{kk}$, see chapter 3. The pair peak at $\omega_R/2$ is considered as a direct scattering of pairs and not as a collective mode that responds coherently and resonantly to that same excitation. As a result, one does not expect a discrete spectrum.

In this experiment, single pair excitations in $S^{(1)}(k, \omega)$ are most likely as they are obtained by exciting from a momentum state $p \leq \hbar k_F$ to a state $(p + \hbar k)$. Because of the exclusion principle, $|p + \hbar k|$ must be larger than $\hbar k_F$. The available values of $p$ are exactly the same as for a noninteracting Fermi gas (chapter 3.3), i.e. the values of $p$ are situated between the Fermi sphere $S_F$ and the sphere $S_F$ shifted by $-q$. The excitation energy of the particle-hole pair is $\epsilon_{p+q} - \epsilon_p$. In the case of $q > 2\hbar k_F$ and as seen in these spectra, the single pair spectrum does not start from $\omega = 0$, but from some finite value of $\omega$. For $q < 2\hbar k_F$, the spectrum of collective excitations would have covered a finite range of energy, starting linearly with $\omega$ from
Figure 6.4: Spectra from the centre of mass displacement for different $k_F/k$ and different interaction strengths, $1/(k_Fa) = 0.0, -0.2$ and $+0.3$. Clear signals of atomic response are seen at the recoil frequency $\omega_R$ and of pair response at $\omega_R/2$. The higher $k_F/k$ the more pair signal emerges. From the BCS to BEC side, a) to c), the pair signal becomes stronger until on the BEC side bound molecules dominate over the atomic response.
zero to some maximum value plus a sharp cut-off \[71\].

The spectra shown in figure 6.4 are selected spectra for better visibility. The whole set of spectra for all interaction strengths, \(1/(k_Fa) = +0.3\) (BEC), 0.0 (unitarity), \(-0.2\) (BCS), can be plotted in a two-dimensional false colour representation. The vertical axis represents the energy in terms of the frequency \(\omega/\omega_R\) and the horizontal axis denotes the inverse of the relative probe momentum, \(k_F/k\). The more signal of either pairs or atoms the higher is the intensity (bright yellow). Black areas correspond to off-resonant response. In the very high momentum limit, i.e. \(k_F/k \to 0\), response of single atoms is expected at \(\omega/\omega_R = 1\), while at lower momenta, \(k_F/k \to +0.5\), which is equivalent to \(k/k_F = 2\), the pair response becomes more significant \[75\]. On the BEC side, response at the pair frequency is visible for all momenta. At unitarity, the single-particle response is stronger at a high momentum transfer, but there is significant weight at the pairing frequency at low momenta. On the BCS side, the atomic signal is most pronounced but still shows some tendency to \(\omega/\omega_R = 0.5\). The blue dots depict the frequency referring to the centre of mass of the spectrum. In first approximation a linear slope can be fitted through the blue dots. The value of the slope depends on the interaction strength, \(1/(k_Fa)\). The slope is a fit of the type \(1 + s \cdot k_F/k\), giving \(s = -1.82\) (BEC), \(-1.43\) (unitarity) and \(-1.13\) (BCS), respectively. This plot is reminiscent of the calculation of the effective mass of the band structure in solid state physics, where the effective mass, \(m^*\), follows from \(m^* = h^2 (d^2E/dk^2)^{-1}\) and the energy \(E\). Despite the resemblance, clear parallels cannot be made. For a start, a parabolic fit shows difficulties. Nevertheless, the frequency according to which the centre of mass of the whole atomic distribution occurs can be related to an energy of the effective mass, which changes with the excitation momentum. This leads to the well-known assumption that for infinitely low excitation momenta, \(k/k_F \ll 1\), collective modes can be excited. The effective mass, \(m^*\), is related to the heat capacity and the spin susceptibility.

### 6.3.4 Static response

At the beginning of this chapter, equation 6.5 was introduced stating that with knowledge of the contact \(I/Nk_F\) it is theoretically possible to measure an exact quantity in a unitary Fermi gas. One only needs to measure the static structure factor accurately. A powerful tool to unambiguously determine \(S(k)\) on the experimental side is given by sum rules as explained in section 3.8.4. \(S(k)\) follows from the zero moment weighted \(S(k,\omega)\), while the normalisation to the atom number is
Figure 6.5: Illustration of $S(k, \omega)$ as a false colour representation of the signal strength for different probe momenta and different interaction strengths, $1/(k_F a) = +0.3$ (BEC), 0.0 (unitarity), $-0.2$ (BCS). The frequency according to the centre of mass of the spectrum is given by the blue points. The slope is a fit of the type $1 + s \cdot k_F/k$, giving $s = -1.82$, $-1.44$ and $-1.13$, respectively. For infinitely high probe momenta $\omega/\omega_R = 1$, i.e. excitation occurs only into free atomic states. $S_{\uparrow\downarrow}(k)$ measures the pairing strength and approaches $0.5 \omega/\omega_R$ for lower momenta. An open question is if this is the limit of measuring the effective mass of collective excitations in the low momentum regime with $k_F/k \geq 1$. White dashed lines are a guide to the eye.
obtained from the first moment weighted $S(k, \omega)$ (f-sum rule). This procedure is model-independent and does not require any details of the experimental parameters. The total static structure factor therefore reads according to equation 3.54

$$S_{\Delta X}(k) = \frac{\sum_\omega S_{\Delta X}(k, \omega) \cdot \omega_R}{\sum_\omega S_{\Delta X}(k, \omega) \cdot \omega_R} \propto \frac{\sum_\omega \Delta X(k, \omega) \cdot \omega}{\sum_\omega \Delta X(k, \omega) \cdot \omega}$$  \hspace{1cm} (6.10)$$

where $\hbar \omega_R$ is the recoil energy. One simply integrates over the zeroth and first moment of the energy resolved Bragg spectra to obtain the total static structure factor. In order to extract $S_{\uparrow \downarrow}(k)$, one can use equation 6.4.

For every interaction strength $1/(k_F a) = -0.2, 0.0, +0.3$ the static structure factor $S_{\uparrow \downarrow}(k)$ can be represented as a function of $k/k_F$ according to equation 6.5. Figure 6.6 summarises without any free parameters how the experimental data obtained from the Bragg spectra compare to the theoretical prediction of equation 6.5, where $I/(N k_F)$ is obtained from calculations [82] in the zero temperature limit.

From equation 6.5 it is clear that at unitarity ($a \rightarrow \infty$) $S_{\uparrow \downarrow}(k)$ is expected to vary linearly with $k_F/k$. The first order corrections with decreasing probe momenta cause a downwards correction for positive $1/(k_F a)$ and an upwards correction for negative $1/(k_F a)$. Within the experimental uncertainties the experimental data agree well with the theory displaying a downward curvature for $1/(k_F a) = +0.3$ and upward curvature for $1/(k_F a) = -0.2$ due to the first order term. The fitted slope of $0.77 \pm 0.07$ for $1/(k_F a) = 0$ is slightly below the zero temperature prediction of 0.81 which is most likely due to reduced pairing at the finite temperature ($T/T_F = 0.10 \pm 0.02$ at unitarity). The next chapter confirms this reduced pairing. This temperature effect is less pronounced for the other two sets. At $1/(k_F a) = -0.2$ the temperature will be lower following the adiabatic magnetic field sweep [234] while on the BEC side at $1/(k_F a) = +0.3$ the temperature will be higher but pairing persists at much higher temperatures.

### 6.4 Interaction dependence of the contact

In this section, the interaction dependence of the contact across the Bose-Einstein condensate (BEC) to Bardeen-Cooper-Schrieffer (BCS) crossover is discussed for a single momentum transfer and low temperatures. The contact characterises in an elegant way the smooth decrease of pair correlations when a Fermi quantum fluid crosses over from BEC to BCS superfluids. There have been a number of experiments that measured the interaction dependence of the contact. The contact $C$ was first extracted [71] from the number of closed-channel molecules determined through
Figure 6.6: Verification of equation 6.5 as measured and calculated static structure factor versus $k_F/k$ for $1/(k_F a) + 0.3, 0.0, -0.2$. The relative probe momentum $k/k_F$ is varied by changing the mean trapping frequency $\bar{\omega}$. Vertical error bars are due to atom number fluctuations and uncertainties in measuring the centre of mass and horizontal error bars are due to atom number fluctuations and uncertainties in $\bar{\omega}$. Solid lines are the zero temperature theory and the dashed line is a straight line fit to the $1/(k_F a) + 0$ data yielding a slope of $0.77 \pm 0.07$. For better visibility of the downwards and upwards curvature the straight dash-dotted lines indicate the case without the first order correction of the theoretical prediction.

photo-association [36]. Also, in agreement with [70], the contact was measured by comparing the momentum distribution of a ballistically expanded cloud, the high-frequency tail of a radio-frequency spectrum, and the momentum distribution from photo-emission spectroscopy [133]. The same work verified experimentally the adiabatic and virial Tan relations which are interpreted with regard to thermodynamic relations. The contact density was determined from the equation of state for a homogeneous gas [130].

The interaction dependence of $S(k)$ across the Feshbach resonance has been measured with Bragg spectroscopy at a single momentum transfer $k/k_F = 4.8$ in our group and has been published in previous work [80,139]. However, the normalisation technique relied on experimental parameters and not the f-sum rule, and hence $S(k)$
was less accurate. Both the f-sum rule and the analytic expression, equation 6.5, provide a precise prescription to determine the contact for various $1/(k_F a)$. The transformation to values of the contact is as follows

$$\frac{I}{Nk_F} = S_{\uparrow \downarrow}(k) \cdot 4 \cdot \left( \frac{k_F}{k} \right)^{-1} \left[ 1 - \frac{4}{\pi} \frac{1}{k_F a} \left( \frac{k_F}{k} \right) \right]^{-1},$$  \hspace{1cm} (6.11)

where $k/k_F = 4.8$. The experimental sequence is similar to the description in section 6.3.2. After evaporation in a single optical dipole trap the magnetic field is ramped to different values near the Feshbach resonance. The subsequent Bragg pulse applied to the trapped gas was 50 $\mu$s long. The Bragg beams have been set up in such a way that the momentum transfer results in a recoil frequency of $\omega_R = 2\pi \cdot 300 \cdot 10^3$ $s^{-1}$. The release time after the trap is switched off is 3 ms, and hence the centre of mass displacement of the atomic distribution is chosen to yield the Bragg spectra. The evaluation of the first moment of the line profiles follows from section 6.3.2. Processing the Bragg spectra with equation 6.11 leads to a plot of the interaction dependent contact, as shown in figure 6.7a. The transition from molecular excitations below the Feshbach resonance to atomic excitations above resonance is smooth. As Tan predicted, the contact accurately connects the BEC and BCS limit smoothly. As mentioned before, the theoretical challenges in describing the BEC-BCS crossover arise from its strongly correlated nature and there is no small parameter to set the accuracy of the theories. Techniques such as Monte-Carlo or strong coupling theories lead to a number of quantitative properties, such as the equation of state, frequency of collective oscillations, pairing gap, or the superfluid transition temperature. However, other fundamental properties such as the single-particle spectral function measured by rf-spectroscopy and the dynamic structure factor probed by Bragg spectroscopy are not as well understood. The dynamic structure factors from Bragg spectra like those shown in figure 6.7a have been compared to calculations based on a random-phase approximation and good agreement has been found [192].

### 6.5 Summary

The structure factor of a strongly interacting ultracold Fermi gas follows a universal law which is a direct consequence of Tan’s relation for the pair correlation functions. The Bragg spectra for this experimental proof result from the centre of mass displacement a cloud experiences following a Bragg pulse. The pair response and single atom response are clearly distinguishable. Integration and the application of the f-
sum rule lead to the static structure factor which represents a macroscopic measure of the pair correlations. The contact in the BEC-BCS crossover is extracted from the static structure factor using the universal law. These measurements provide one of the first demonstrations of a broadly applicable exact result for strongly interacting Fermi gases in the BEC-BCS crossover.
Chapter 7

Temperature dependence of the contact

The strong interactions in the unitarity regime set the intrinsic properties of the Fermi gas. Pair correlations persist up to temperatures higher than the critical temperature, approaching $T_F$, and hence raising the question of preformed pairs. Chapter 6 highlighted the connection between the static structure factor and the contact. In this chapter, measurements of the static structure factor are restricted to the unitarity limit, where the contact is linearly proportional to the static structure factor. Therefore, a measurement of the static structure factor at different temperatures gives direct information on the temperature dependence of the contact.

7.1 Introduction

The contact depends on the interaction strength $1/k_F a$ and the temperature $T/T_F$ of the Fermi gas. The concept of the contact was introduced in chapter 2. In this chapter, the goal is to measure the contact in a unitary Fermi gas for increasing temperatures. At unitarity, $a \to \infty$, the second term in brackets in equation 6.5 vanishes and the spin anti-parallel static structure factor reduces to

$$S_{\uparrow \downarrow}(k \gg k_F) = \frac{T}{N k_F} \frac{k_F}{4k}.$$  \hspace{1cm} (7.1)

The static structure factor now becomes directly proportional to the contact. If the temperature is increased, the two-body correlation function should decrease, as more single particle states become occupied. Hence the contact is predicted to decrease with increasing temperature.
Different theoretical models have been developed to calculate the temperature dependent contact, in the homogeneous as well as the trapped case. In the high temperature limit for a trapped gas, $T > 0.5 T_F$, the fugacity is small and the virial quantum cluster expansion is accurate [84]. In the low temperature regime around and lower than the critical temperature $T_C$, various many-body $t$-matrix approximation based models are used [84, 139, 165]. Also, quantum Monte-Carlo calculations have been performed [75, 131, 132]. All the predictions differ slightly near the critical temperature as the low and high temperature regimes have been connected differently. The contact at $T = 0$ seems to lie in the range $3 - 3.4 I/(Nk_F)$. A precise measurement of the contact therefore would resolve the discrepancy between the different approaches and help to decide which underlying model is the most descriptive for the unitarity regime.

At unitarity, one can distinguish two temperature thresholds, the onset of pairing at $T^*$ and superfluidity at $T_C$. The question arises, how the contact is linked to the pairing temperature [230], as pair-correlations persist up to temperatures higher than $T_C$. While this thesis was being written, a debate about the nature of a strongly interacting Fermi gas above $T_C$ has been going on, i.e. whether it is a Fermi liquid [173] or a state with an excitation gap/pseudogap [86, 240, 241]. Pair-correlations above $T_C$ have been seen in imbalanced Fermi gases with radio-frequency spectroscopy [111, 61, 220] and pairing without superfluidity has been observed.

In solid state physics, evidence of pairing above $T_C$ has been demonstrated for cuprate superconductors through dispersion measurements close to the Fermi surface [242]. These type of experiments lack the possibility to directly measure the (momentum) pair correlation functions. However, they can search for features unique to Cooper pairing, e.g. features which are present in the electronic excitation spectrum above $T_C$.

In this chapter, two experiments are presented to obtain Bragg spectra and dynamic structure factors, either with distributions imaged immediately after the Bragg pulse, $S_{\Delta P}(k, \omega)$, or after equilibration, $S_{\Delta E}(k, \omega)$. The outline of the experimental sequence is the subject of section 7.2. The principal ideas and differences of the experiments is discussed in section 7.3. Bragg spectra that yield $S_{\Delta P}(k, \omega)$ from the centre of mass displacement as well as from the width of the atomic distribution are explained in detail in section 7.4. The acquisition of $S_{\Delta E}(k, \omega)$ follows in section 7.5. From the dynamic structure factors the values of the static structure factor and contact are determined. The results are discussed in section 7.6 together with theoretical predictions. Note that for the remainder of this thesis the momentum is labelled in terms of the wave vector, i.e. $\mathbf{q}/\hbar = \mathbf{k}$, where $|\mathbf{k}| = k$, which is different.
7.2 EXPERIMENTAL VERIFICATION

The experimental verification of the temperature dependence of the contact is performed in a different setup from subsection 6.2 and is sketched in figure 7.1. After evaporation the atoms are adiabatically transferred in 600 ms into the second single far-detuned dipole trap where $N_\uparrow = 180\,000$ particles are measured in one spin state at $(0.09 \pm 0.05)\,T/T_F$. The combination of the residual magnetic field curvature and optical trap yield homogeneous trap frequencies of $\omega_z = 2\pi \, 210 \, s^{-1}$, $\omega_x = 2\pi \, 56 \, s^{-1}$, $\omega_y = 2\pi \, 24.5 \, s^{-1}$, or $\bar{\omega} = 2\pi \, 66 \, s^{-1}$; hence, the Fermi energy defined by $\epsilon_F = h\bar{\omega} (6N_\uparrow)^{1/3}$ is $\epsilon_F = 2\pi \, 7.2 \cdot 10^3 \, s^{-1}$ and the Fermi wave vector is $k_F = \sqrt{2m\epsilon_F}/\hbar = 2.9 \, \mu\text{m}^{-1}$.

This is the starting point for every heating sequence as it is intended to maintain the same Fermi energy for all experiments. The confining trap is switched off for a variable time before non-adiabatically ramping it back on. Rethermalisation is allowed for $\tau_{\text{therm}} = 400 \, \text{ms}$ which is larger than $10 \, \omega_y^{-1}$. The trap allows heating
to a maximum temperature of 1.0 $T/T_F$ without a significant loss of atoms. The determination of the temperature is described in chapter $\textit{[3]}$. The temperatures are obtained for each Bragg spectrum individually and the release time for absorption imaging is usually $\tau_{TOF} = 2$ ms. The relative uncertainty in temperature is about 7%.

The Bragg setup is designed so that two low-power laser beams of $P_{Br} = 40$ $\mu W$ intersect at an angle $\theta_{Br} = 49.5^\circ$ to form a moving lattice potential at the position of the atoms. The velocity of the potential is determined by a small tunable frequency difference $\omega$. In this configuration, the Bragg resonance condition leads to a recoil energy $\omega_R = 2\hbar k^2/m = 2\pi \cdot 51.6 \cdot 10^3$ s$^{-1}$ and a pair frequency $\omega_{pair} = \omega_R/2 - 2\pi \cdot 25.8 \cdot 10^3$ s$^{-1}$. The momentum transfer to the atoms is given by the ratio $k/k_F = 2.7$ and is characterised by the recoil momentum of $\hbar k = 2\hbar k_L \sin(\theta/2)$, $k_L$ being the laser wave vector. The Bragg pulse is applied for $\tau_{Br} = 200$ $\mu s$ on the trapped atoms to obtain a Bragg spectrum. The resulting Fourier width is $\leq 2\pi \cdot 800$ s$^{-1}$, which is small compared to $\omega_R$ and therefore is ignored from now on.

### 7.3 Momentum and energy interrelation

Bragg spectra so far are based on the traditional centre of mass displacement, $\Delta X(k, \omega)$, associated with the relative momentum transfer, $\Delta P(k, \omega)$, for a particle or pair with mass $m$ after a time $\Delta t$, i.e. $\Delta P(k, \omega) = m \Delta X(k, \omega)/\Delta t$. To measure the transferred momentum the trap is switched off shortly after the Bragg pulse and after a short release time the cloud distribution is imaged. Therefore, the dynamic structure factor is linked to the momentum such that $\Delta P(k, \omega) = N_{sc} \hbar k \propto S(k, \omega)$ for $N_{sc}$ scattered particles, and hence linked to $\Delta X(k, \omega)$. The notation, $\Delta P$, refers to the way the Bragg spectrum is obtained, i.e. after a short release time. Note that the Bragg pulse transfers always momentum $\hbar k$ and energy $\hbar \omega$.

However, the dynamic structure factor can also be extracted from the relative energy transfer, $\Delta E(k, \omega)$. The energy of the transferred momentum is manifested by an increase of the width, $\langle \sigma^2(k, \omega) \rangle$, such that $\Delta E(k, \omega) = \hbar \omega \cdot N_{sc} = (m/2) \bar{v}^2 \Delta \langle \sigma^2(k, \omega) \rangle \propto \omega S(k, \omega)$. The last step shows that the energy is proportional to the first moment of the dynamic structure factor with respect to energy.

Both $\Delta P(k, \omega)$ and $\Delta E(k, \omega)$ are proportional to the number of scattered photons, $N_{sc}$. The momentum depends on the zeroth moment of $S(k, \omega)$ while the energy represents the first moment of $S(k, \omega)$ [197]. The momentum and energy are
7.3 MOMENTUM AND ENERGY INTERRELATION

<table>
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<th>Profile</th>
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<td>$\Delta X$</td>
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<td>$\Delta \sigma^2_x, \Delta \sigma^2_y$</td>
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<tr>
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<td>symmetric</td>
<td>$\Delta \sigma^2_x, \Delta \sigma^2_y$</td>
<td>$\omega S(k, \omega)$</td>
</tr>
</tbody>
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Table 7.1: Summary of the evaluation procedures. Images taken shortly after the Bragg pulse are indicated by ‘0’. $\Delta X$ denotes the centre of mass and $\Delta \sigma^2_x, \Delta \sigma^2_y$ the width in the $x$- or $y$-direction, respectively.

related to the $S(k, \omega)$ according to equation 3.45 by

$$ S(k, \omega) \propto \frac{\Delta P(k, \omega)}{k} = \frac{\Delta E(k, \omega)}{\omega}. $$

(7.2)

Two different experiments are performed in the following. On the one hand, the clouds are imaged immediately after the Bragg pulse and the respective spectra carry the index ‘im’. On the other, the cloud is held in the trap to equilibrate and any centre of mass movement is damped out. These Bragg spectra are indexed with ‘eq’. First, the conventional method is applied which leads to asymmetric atomic distributions. In section 7.4.1 it is explained how the centre of mass displacement, $\Delta X(k, \omega)$, along the Bragg scattering direction is evaluated from the images. Normalised Bragg spectra are labelled as $\Delta P_{im}(k, \omega)$.

Second, the same experimental data set is used in section 7.4.2 to extract the width, $\Delta \sigma^2_x$. Normalised Bragg spectra are denoted by $\Delta E_{im}(k, \omega)$. Note that the evaluation of the second moment of a line profile coincides with the expression of the energy transfer, despite the distribution not being in thermal equilibrium. Third, in section 7.5, another experiment is performed with equilibrated, and hence symmetric, atomic distributions. The evaluation of the widths provide Bragg spectra labelled as $\Delta E_{eq}(k, \omega)$. The method of equilibrated atoms in the trap should examine if an alternative approach to the evaluation of the centre of mass displacement provides more accurate results. This might be important when other experiments are performed, for instance, at low momentum transfer ($k < k_F$). The momentum transfer with a short release time and the energy transfer with an equilibration time have previously been used in optical lattice experiments with bosons [185–187]. Table 7.1 summarises briefly the strategies for the upcoming sections.
7.4 Bragg spectra after immediate release

The momentum transfer method has been applied in previous work [80]. A graphic outline is shown figure 6.3. The slight modifications in the process from single pictures to the final dynamic structure factor is described in the following. After the cloud is heated a Bragg pulse is applied while the dipole trap is on and the total time between the Bragg and imaging pulse is always 3 ms. For temperatures below $0.4 T/T_F$, the cloud travels after the Bragg pulse further in the trap for 1 ms. Then the trap is switched off and the atoms are released for 2 ms before an absorption image is taken. When the temperature is above $0.4 T/T_F$, the atoms are held after the Bragg pulse another 2.95 ms in the trap and the time-of-flight before imaging is reduced to 0.05 ms. The reason for this separation is to aim for a good signal-to-noise in the images. The hold time in the trap is always short compared to the inverse trap frequencies. So the hold time does not influence the measured displacements. As seen later, the results are well maintained by the f-sum rule in the normalisation, which bypasses technical details such as release times.

From previous measurements in this group, the centre of mass displacement turned out to be a robust method [80], as elastic collisions after the applied Bragg pulse preserve the centre of mass motion, $\Delta X$, throughout the crossover regime. Furthermore, $\Delta X$ is less sensitive to atom number fluctuations. Particle conservation requires a summation over all involved scattered atoms, and therefore it is important to count all atoms but to avoid the noise of pixel counts. In the former experiments [80], a momentum transfer of $k = 5 k_F$ was used. For that momentum, scattered atoms eventually separate from the parent cloud leaving a gap in-between. In a summation over the region of interest, this gap may added noise. In the present work, the momentum transfer is reduced to $k = 2.7 k_F$ and thus the centre of mass displacement is less enhanced for the same time-of-flight after the Bragg pulse. Instead of a separate cloud, the distribution becomes very distorted but contiguous and the region of interest includes less noise from pixels without signal.

Another advantage of a lower momentum is an increase of the contribution of the spin anti-parallel structure factor, according to equation 7.1, since the relative momentum determines the probed pair size. The lower $k/k_F$, the larger the probed pairs can be. In general, the signal of atoms at the edges of the distorted cloud might become as small as the noise of the pixel counts. The region of interest has to be selected carefully which means that in the direction of integration it has to be as small as possible to include all of the atoms but to exclude background that only adds noise.
For the evaluation of a single image it is assumed that the pictures have a horizontal axis labelled as $x$ which is also the direction of the applied Bragg momentum. The vertical, perpendicular direction to the Bragg scattering in the image is labelled with $y$. Each image $i$ is taken for a different Bragg frequency $\omega$. Compared with results in the previous chapter, an additional fringe removal procedure, see section 4.5, is applied with respect to the reference pictures to reduce uncorrelated noise.

### 7.4.1 Bragg spectra from the first moment

#### Building Bragg spectra

For every image $i$, a one-dimensional sum is taken in $y$-direction to obtain a line profile in the $x$-direction, $n_i(x)$. Each line profile $n_i(x)$ is normalised to unity. The first moment of $n_i(x)$ is equivalent to the centre of mass and labelled ‘$(1)$’. Hence, the centre of mass follows as

$$X_i^{(1)} = \frac{\sum_x n_i(x) \cdot x}{\sum_x n_i(x)}.$$  \hfill (7.3)

As mentioned above, the cloud distribution is asymmetric after a short release time and a gaussian fit to approximate the line profile in order to gain a better signal-to-noise cannot be applied as this could omit part of the signal.

To quantify the centre of mass displacement, $\Delta X_i^{(1)}$, for each $n_i(x)$, the position of the unperturbed cloud, $X_{\text{off}}^{(1)}$, needs to be known. It is convenient to use values from off-resonant Bragg frequencies and subtract $X_{\text{off}}^{(1)}$ from $\Delta X_i^{(1)}$. Error may occur when the trap centre drifts during one sequence, e.g. due to thermal lensing at the spot where the laser enters the glass cell or other optical elements. The picture number is related to the Bragg frequency, so therefore $i$ is now replaced by the Bragg frequency $\omega$, and so $X_i^{(1)} \equiv X^{(1)}(\omega)$. Thus a Bragg spectrum, where the centre of mass of $n_i(x)$ has been evaluated, may be written as

$$\Delta X^{(1)}(\omega) = X^{(1)}(\omega) - X_{\text{off}}^{(1)}.$$  \hfill (7.4)

#### Derivation of the dynamic structure factor

As shown in section 3.8, the centre of mass displacement spectrum, $\Delta X(\omega)$, is proportional to the dynamic structure factor. In order to calculate the static structure factor, the Bragg spectra need to be normalised and the f-sum rule has to be applied, see section 3.8.4. In the previous experiments, the signal of the centre of mass was
Figure 7.2: Bragg spectra from the centre of mass displacement, $\Delta P_{im}(k, \omega)$, after momentum transfer for different temperatures $T/T_F$. At high temperatures the spectrum is dominated by uncorrelated atoms gaussian-distributed around the recoil frequency $\omega_R$. The pair signal evolves at the pair frequency ($0.5 \omega_R$) for decreasing temperatures.

easily distinguishable due to higher momenta and low temperatures, and therefore a model independent summation over the pixel was sufficient. The recoil energy was higher ($\omega_R = 2\pi \cdot 295 \cdot 10^3 \text{ s}^{-1}$) and the onset of the spectrum was clearly around $2\pi \cdot 10^3 \text{ s}^{-1}$. Now, the probe momentum is lower ($k = 2.7 k_F$) and the resonance frequency is 6 times lower ($\omega_R = 2\pi \cdot 51 \cdot 10^3 \text{ s}^{-1}$), which means that a spectrum has significantly non-zero values at very low frequencies. These values are even more pronounced for increasing temperatures. When the f-sum rule is applied, small fluctuations of $S(k, \omega)$ in the low frequency range will cause large errors. Moreover, the Bragg spectra are weighted for increasing temperatures by the Boltzmann factor and the denominator in equation (3.47) deviates from unity. The dynamic structure factor for higher temperatures contains then a significant weight at negative frequencies where it is impossible to obtain data. This necessitates fitting to the Bragg spectra, which are to a first approximation two gaussians.

First, the Bragg spectra need to normalised to the atom number, which is governed by the f-sum rule, $N\omega_R = h \sum \omega S(\omega)$. So the normalised spectrum $\Delta P_{im}(\omega)$ follows as

$$
\Delta P_{im}(\omega) = \frac{\Delta X^{(1)}(\omega)}{\sum \omega \Delta X^{(1)}(\omega) \cdot \omega}.
$$

(7.5)
The fit function consists of two gaussians multiplied by the detailed balancing term; hence
\[
\Delta P_{im,fit}(\omega) = \left[ a_1 e^{-\frac{(x-c_1)^2}{2b_1^2}} + a_2 e^{-\frac{(x-c_2)^2}{2b_2^2}} \right] \cdot \left(1 - e^{-\frac{\hbar \omega}{k_B T}}\right).
\]
(7.6)

The centre positions of the gaussians are fixed to the excitation frequencies \(c_1 = \omega_R/2, c_2 = \omega_R\) but the amplitudes \(a_1, a_2\) and widths \(b_1, b_2\) are free. The parameter \(T/T_F\) is known and \(\hbar \omega/k_B T = (\omega/\omega_r) (T/T_F)\) is defined in terms of the recoil frequency \(\omega_R\). A gaussian may not describe the coldest spectra well. The estimated error of \(\Delta P_{im,fit}(\omega)\) to the data is about 4% for the coldest cloud, 1% at 0.5 \(T/T_F\) and decreasing for even higher temperatures. For this estimation, a calculated zero temperature spectrum at 3 \(k/k_F\) is taken \cite{235} and the same fit routine is applied as for the spectra.

The real dynamic structure factor, \(S_{im,\Delta P}(k,\omega)\), after the immediate release time is for any momentum \(k\)
\[
S_{im,\Delta P}(k,\omega) = \frac{\Delta P_{im,fit}(k,\omega)}{1 - e^{-\frac{\hbar \omega}{k_B T}}}.
\]
(7.7)

These Bragg spectra are shown in figure 7.2. The solid lines connect the data points and the dashed line represents the fits from which \(S(k,\omega)\) is extracted. At low temperatures the pair peak near \(\omega = 0.5 \omega_R\) in the spectrum is well pronounced. For increasing temperatures \(T/T_F\), the pair peak smoothly vanishes and the spectrum is more and more dominated by response at the atomic resonance.

### 7.4.2 Bragg spectra from the second moment

#### Building Bragg spectra

The same line profiles \(n_i(x)\) as used in the previous section can also provide the second moment, which is equivalent to the mean square size and thus the energy of the cloud distribution. The second moment, labelled ‘(2)’, of the asymmetric line profiles may be written as
\[
X_i^{(2)} = \frac{\sum_x n_i(x) \cdot (x - X_{0,COM})^2}{\sum_x n_i(x)}
\]
(7.8)
where \(X_{0,COM}\) is the centre of mass of an unperturbed cloud and is the same for every image \(i\). When looking at the second moment, there is also information stored in the direction perpendicular to the Bragg pulse, \(n_i(y)\), where the cloud is symmetric.
For every image $i$, a sum can be taken in the $x$-direction to obtain a line profile in the $y$-direction, $n_i(y)$. After summation the area under each line profile $n_i(y)$ is normalised to unity. While the $n_i(x)$ are asymmetric, the $n_i(y)$ are symmetric. A priori there is no reason to fit a function to $n_i(y)$, or especially to expect a gaussian to work. However, a gaussian fit to the symmetric line profile in the $y$-direction seems to be reliable compared to an evaluation of the second moment from the raw data due to a gain of better signal-to-noise. One may use a gaussian function, such as

$$ g(x) = a \cdot e^{-\frac{(x-c)^2}{2b^2}}, \quad (7.9) $$

where $a$ is the amplitude, $c$ the centre position and $b$ the width. During the processing it has been easier to look at the second moment to check the sensitivity of the fit; thus second moment of the fit function is $g(x) \cdot (x-c)^2$. Equation 7.8 has been used to calculate the second moment in the $y$-direction and similarly one obtains $Y_i^{(2)}$. At the end, two spectra are obtained from the second moment of the line profiles: $X_i^{(2)}$ based on the raw data and no fit and $Y_i^{(2)}$ based on a fit to the second moment of each line profile. The spectra $X_i^{(2)}$ and $Y_i^{(2)}$ are equal to the mean square size, and thus $X_i^{(2)} \equiv \sigma_x^2(\omega)$ and $Y_i^{(2)} \equiv \sigma_y^2(\omega)$. The interest lies in the relative increase in width with the applied Bragg frequencies. Therefore, the widths of the unperturbed cloud, $X_{off}^{(2)}$ and $Y_{off}^{(2)}$, have to be determined. Conveniently, one can use the width values where an off-resonant Bragg pulse was applied. Then, the Bragg spectra following from the mean square sizes of the line profiles are

$$ \Delta X^{(2)}(\omega) = X^{(2)}(\omega) - X_{off}^{(2)} \equiv \Delta \sigma_x^2(\omega), \quad (7.10) $$
$$ \Delta Y^{(2)}(\omega) = Y^{(2)}(\omega) - Y_{off}^{(2)} \equiv \Delta \sigma_y^2(\omega). \quad (7.11) $$

These Bragg spectra are plotted in figure 7.3.

**Derivation of the dynamic structure factor**

The normalisation of the Bragg spectra from the widths is set to unity, because the second moment is proportional to the term which appears in the f-sum rule integral. Thus

$$ \Delta E_{im,x}(\omega) = \frac{\Delta \sigma_x^2(\omega)}{\sum_\omega \Delta \sigma_x^2(\omega)}. \quad (7.12) $$
Figure 7.3: Bragg spectra from the mean square size, $\Delta E_{im}(k, \omega)$, after immediate release for different temperatures $T/T_F$. At high temperatures the spectrum is dominated by uncorrelated atoms gaussian-distributed around the recoil frequency $\omega_R$, which is weighted by $\omega$ as the energy depends on the first moment of $S_{im}(k, \omega)$. The pair signal evolves at the pair frequency ($0.5\,\omega_R$) multiplied by the weighting $\omega$ for decreasing temperatures.

The same expression yields $\Delta E_{im,y}(\omega)$. Both can be averaged to

$$\Delta E_{im}(\omega) = \frac{\Delta E_{im,x}(\omega) + \Delta E_{im,y}(\omega)}{2}. \quad (7.13)$$

A function with two gaussians times the detailed balancing term and frequency is fit to $\Delta E_{im}(\omega)$, where the fit function is similar to equation (7.6) multiplied by the frequency $\omega$; hence

$$\Delta E_{im,\text{fit}}(\omega) = \omega \cdot \left[ a_1 e^{-\frac{(\omega-c_1)^2}{2b_1^2}} + a_2 e^{-\frac{(\omega-c_2)^2}{2b_2^2}} \right] \cdot \left( 1 - e^{-\hbar \omega/k_B T} \right). \quad (7.14)$$

Again, the centre positions of the gaussians are fixed to $c_1 = \omega_R/2$ and $c_2 = \omega_R$, respectively, but the amplitudes $a_1, a_2$ and widths $b_1, b_2$ are free. The real dynamic structure factor $S_{im,\Delta E}(k, \omega)$ is calculated using equation (7.7), but with a weighting of $\omega$

$$S_{im,\Delta E}(\omega) = \frac{\Delta E_{im,\text{fit}}(\omega)}{\omega \left( 1 - e^{-\hbar \omega/k_B T} \right)}. \quad (7.15)$$
The two results from the first and second moment, \( S_{im,\Delta P}(k,\omega) \) and \( S_{im,\Delta E}(k,\omega) \), lead to the same \( S(k,\omega) \) and can be averaged. However, the noise in \( S(k,\omega) \) obtained from the second moment is large at low frequencies. The reason is the division by the frequency in equation (7.15) and for low frequencies the noise becomes large. To compensate for this artefact a weighting of \( S_{im,\Delta P}(k,\omega) \) and \( S_{im,\Delta E}(k,\omega) \) is considered. The weighing is chosen such that the contributions from \( S_{im,\Delta P}(k,\omega) \) and \( S_{im,\Delta E}(k,\omega) \) are equal at high frequencies (\( \omega_{max} \)) but at low frequencies the contribution of \( S_{im,\Delta E}(k,\omega) \) is small

\[
S_{im}(k,\omega) = S_{im,\Delta P}(k,\omega) \left( 1 - \frac{\omega}{2\omega_{max}} \right) + S_{im,\Delta E}(k,\omega) \left( \frac{\omega}{2\omega_{max}} \right). \tag{7.16}
\]

The equal weighting at high frequencies is possible due to equation 3.45 which states that the momentum transfer and energy transfer contribute by the same factor to \( S(k,\omega) \).

![Figure 7.4: Dynamic structure factor, \( S_{im}(k,\omega) \), after averaging the dynamic structure factors of the Bragg spectra from the first (centre of mass displacement) and second moment (width). Atoms respond at \( \omega = \omega_R \) while pairs contribute at 0.5 \( \omega_R \). Note that \( S_{im}(k,\omega) \) has non-zero values at negative frequencies.](image)

Figure 7.4 presents \( S_{im}(k) \) from the momentum and energy transfer of Bragg spectra with immediate imaging after the Bragg pulse. The static structure factor
$S_{im}(k)$ is determined from equation 7.55.

$$S_{im}(k) = \frac{\sum_\omega S_{im}(k,\omega) \cdot \omega}{\sum_\omega S_{im}(k,\omega) \cdot \omega R}.$$  \hspace{1cm} (7.17)

The result is discussed in section 7.6.

In section 3.7 the fluctuation dissipation theorem was considered. At the end, it was shown that instead of $S(k,\omega)$ at higher temperatures, the dissipative part of the correlation function, $\chi''$, can be used. The difference is a coth-function, which diverges at zero energy and shows an upward tail. When comparing $\chi''$ and $S$ over the applied temperature range, this signature is marginal. The noise in the spectra at these frequencies is larger and cannot be compared with the artefact of the coth-function.

### 7.5 Bragg spectra after equilibration

So far, it has been tested to see if the evaluation of the second moment of the line profiles for non-equilibrated atomic distributions gives the same result as the traditional evaluation of the centre of mass. Another approach to measure the energy transferred is to allow the cloud time in the trap to equilibrate after the Bragg pulse again. The atoms are held after the Bragg pulse in the trap which is designed to be deep and therefore holds atoms at higher temperatures. The question arises whether performing the evaluation on an equilibrated cloud provides better signal-to-noise and whether Bragg scattering experiments for $k < 2k_F$ (where the signal from the centre of mass is small) still shows well pronounced features of a Bragg spectrum.

In order to allow the atoms to equilibrate after the Bragg pulse, the trap is kept on for another 400 ms after the Bragg pulse. The deep trap allows no loss of atoms following the Bragg pulse up to temperatures of 1.0 $T/T_F$. The equilibration damps all centre of mass movement and the signal will be manifested as a pure increase in width of the cloud size. In-situ images are taken for temperatures $T/T_F \geq 0.4$ and, with a time of flight, when $T/T_F < 0.4$. Because the atomic distributions for each Bragg frequency are symmetric, the second moment can be extracted in both the directions parallel and perpendicular to the Bragg pulse direction, which are the $x$- and $y$-directions.

#### Building Bragg spectra

For every image $i$, a one-dimensional sum is taken in the $y$- $\{x\}$-direction to obtain symmetric line profiles in the $x$- $\{y\}$-direction, $n_i(x)$ $\{n_i(y)\}$. In both directions,
a gaussian function as in equation (7.9) can be fitted, where for evaluation purposes
the second moment, \( g(x) \cdot (x - c)^2 \), is monitored. Applying this expression reduces
the in-profile pixel noise and the spectra are only dominated by the shot-to-shot
uncertainty of the atom number. An example of the single gaussian fit to a line
profile is shown in figure 7.5. The area under each line profile \( n_i(x) \) \{n_i(y)\} is

![Graph showing single gaussian fit to a line profile](image)

**Figure 7.5:** Example of fitting a single line profile of an image. On the left is shown
the integrated line profile (top) and its second moment (bottom). The gaussian fit
(blue) to the data (black points) improves the signal-to-noise. On the right the total
spectrum is shown with (red) and without the improvement (black points) due to
the fit. Black points correspond to individual pictures \( i \).

normalised to unity. The second moment is labelled ‘(2)’, as before, and represents
again the mean square size. It may be written as

\[
X_i^{(2)} = \frac{\sum_x n_i(x) \cdot (x - X_0)^2}{\sum_x n_i(x)} \\
Y_i^{(2)} = \frac{\sum_y n_i(y) \cdot (y - Y_0)^2}{\sum_y n_i(y)}
\]

\[
(7.18) \quad (7.19)
\]
7.5 BRAGG SPECTRA AFTER EQUILIBRATION

where $X_0 \{Y_0\}$ is the centre of mass of an the cloud and is now calculated for every image $i$. This approach is insensitive to shot-to-shot drifts in the centre of mass position of the cloud. At the end, two spectra are obtained, $X^{(2)}_{i,fit}$ and $Y^{(2)}_{i,fit}$ for the mean square size in both the $x$- and $y$-directions. In order to work out the energy transferred to the cloud, one needs to compare the widths after a Bragg pulse with the widths of an unperturbed cloud, $X^{(2)}_{fit,off}$ and $Y^{(2)}_{fit,off}$. These can be taken from values where a Bragg pulse has a far off-resonant frequency was applied. Replacing the picture number with the Bragg frequency $i \rightarrow \omega$ relates the spectra to the mean square size $X^{(2)}_{i,fit} \equiv \sigma^2_x(\omega)$ and $Y^{(2)}_{i,fit} \equiv \sigma^2_y(\omega)$. The spectra are now

\[
\Delta X^{(2)}_{i,fit}(\omega) = X^{(2)}_{i,fit}(\omega) - X^{(2)}_{fit,off} \equiv \Delta \sigma^2_x(\omega) \tag{7.20}
\]

\[
\Delta Y^{(2)}_{i,fit}(\omega) = Y^{(2)}_{i,fit}(\omega) - Y^{(2)}_{fit,off} \equiv \Delta \sigma^2_y(\omega). \tag{7.21}
\]

These spectra from the equilibrated cloud are normalised for both directions according to equations (7.12)

\[
\Delta E_{eq,x}(\omega) = \frac{\sigma^2_x(\omega)}{\sum_\omega \sigma^2_x(\omega)} \tag{7.22}
\]

and averaged according to equation (7.13)

\[
\Delta E_{eq}(\omega) = \frac{\Delta E_{eq,x}(\omega) + \Delta E_{eq,y}(\omega)}{2}. \tag{7.23}
\]

These spectra from equilibrated clouds are depicted in figure (7.6) and resemble the spectra of figure (7.3) but with significantly less noise.

**Derivation of the dynamic structure factor**

The spectra are fitted again with a function of two gaussians, as in equation (7.14), to obtain the actual dynamic structure factor like equation (7.15)

\[
S_{eq}(k,\omega) = S_{eq,\Delta E}(k,\omega) = \frac{\Delta E_{eq,fit}(\omega)}{\omega (1 - e^{-\hbar\omega/k_B T})}. \tag{7.24}
\]

for any momentum $k$. $S_{eq}(k,\omega)$ is plotted for some different temperatures in figure (7.7). The static structure factor is calculated also from equation (7.16) thus

\[
S_{eq}(k) = \frac{\sum_\omega S_{eq}(k,\omega)}{\sum_\omega S_{eq}(k,\omega) \cdot \omega_R}. \tag{7.25}
\]
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Figure 7.6: Bragg spectra from the mean square size, $\Delta E_{eq}(k, \omega)$, after energy transfer for different temperatures $T/T_F$. At high temperatures the spectrum is dominated by uncorrelated atoms gaussian-distributed around the recoil frequency $\omega_R$. Again, the spectra a weighted by $\omega$ due to the evaluation of the relative energy transfer. The pair signal evolves at the weighted pair frequency ($0.5 \omega_R \cdot \omega$) for decreasing temperatures.

Figure 7.7: Dynamic structure factor, $S_{eq}(k, \omega)$, after energy transfer for different temperatures $T/T_F$. At high temperatures the spectrum is dominated by uncorrelated atoms gaussian-distributed around the recoil frequency $\omega_R$. The pair signal evolves at the pair frequency for decreasing temperatures. Due to the division by the frequency to obtain $S_{eq}(k, \omega)$ from the energy, the noise is pronounced at low frequencies.
Even though these dynamic structure factors appear slightly noisier than those in figure 7.4, these are much less noisy than what would be obtained from the data of figure 7.3 alone.

7.6 Temperature dependence of the contact

Once the static structure factors, \( S_{\text{im}}(k) \) and \( S_{\text{eq}}(k) \), are determined, they are translated into the contact \( I/(Nk_F) \) using equation 7.1. The contact for different temperatures is plotted in figure 7.8 for values from the momentum transfer spectra (triangles) and from the energy transfer spectra (circles). The contact decreases smoothly from \( \sim 3.0 \) to 0.5 for increasing temperatures \( T/T_F = 0.1 - 1.0 \) and a discontinuity in the critical temperature region is not visible. The data has vertical errors due to atom number fluctuations and statistical uncertainties resulting from the number of spectra used. A change in the Fermi energy, thus \( k/k_F \), due to atom number fluctuations is marginal (maximum 4%). An upper bound of the vertical error can be given by the experimental limit of extracting the static structure factor, i.e. the \( S(k) \) is taken from momentum transfer Bragg spectra of a spin polarised gas. The temperature measurement has been discussed in chapter 5.

The contact at the lowest temperature is \( I/(Nk_F) = 3.1 \pm 0.3 \), which is slightly lower but still in agreement with \( I/(Nk_F) = 3.4 \pm 0.2 \) taken from the equation of state [173]. Note that the contact values are clearly non-zero for \( T > T_C \) indicating a gradual build up of pair-correlations. This is not to be confused with pseudogap effects, as the probe momentum in this experiment is \( 2.7 k/k_F \), which probes the high momentum tail of the momentum distribution. Therefore, the signal seen here is dominated by the \( 1/k^4 \) tail and not a pseudogap pairing, which would occur near the Fermi surface \( k/k_F \approx 1 \) [240]. Note that the potential of the contact to explain the pairing gap is unclear due to the definition in the high momentum limit while the structure factor might still be suitable to explain the pairing gap due to the link to the pair-correlation function between opposite spins. Therefore, equation 7.1 has to be given careful consideration for transferred momenta of \( k/k_F \rightarrow 1 \).

The above experimental result is compared to the theoretical models for the trapped Fermi gas based on many-body \( t \)-matrix approximations, which are the gaussian pair fluctuation (GPF) [135], self-consistent approach (GG) [85] and non-self-consistent approach (\( G_0G_0 \)) [81]. The high temperature region uses the second \( (b_2) \) and third \( (b_3) \) order of the accurate quantum virial expansion method [135].

While all theories agree with a decay of the contact for temperatures larger than \( T_C \), they deviate in the low temperature regime around and below \( T_C \). The
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Figure 7.8: Temperature dependence of the contact. The contact at zero temperature lies between $I = 3$ and $3.4$ and decays monotonically to values $\leq 0.5$ for $T/T_F = 0.1 - 1.0$. The data points are obtained using equation (7.1) for the static structure factor of Bragg spectra after momentum transfer (triangles) and energy transfer (circles). Vertical error bars are due to statistical errors of eight spectra and atom number fluctuations. The horizontal errors reflect the uncertainties in the temperature determination. The solid lines are the theoretical predictions based on $t$-matrix approximations ($G_0^0$, GG, $G_0^0G_0$) and the dashed and dashed-dotted lines result from a virial expansion calculation.
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differences are even more visible in the calculation for the homogeneous case. Therefore, the homogeneous case is briefly revisited: The $G_0G_0$ theory predicts a maximum around the critical temperature $T_C$ due to a strengthening of local pairing correlations in the absence of long-range order. Then, quasi-particle (phonons etc.) correlations may contribute to the momentum distribution. The $G_0G_0$ theory also assumes that the phonon mode is dominant in the whole superfluid phase. The same assumption is in disagreement with the GPF model which states that the phonon mode is effective only in a very narrow window ($T \leq 0.07 T_F \ll T_C$) where the contribution from phonons is of relative order $10^{-3}$. Another calculation uses the assumption of a Fermi liquid behaviour for a weakly coupled Fermi gas [165] and suggests that phonon excitations will enhance the contact according to a temperature behaviour $\propto T^4$ and maximises at around $0.5 T/T_F$. However, the Fermi liquid theory actually strongly overestimates the contact at $T_C$ [135]. In contrast, the calculations with the GPF and GG approach find that the contact decreases monotonically as the temperature increases, except at $T \ll T_C$, where the contact plateaus. Near the critical point strong pair fluctuations occur. The strong coupling theories cannot handle these divergences properly. Therefore, it is not clear if the peak in the $G_0G_0$ theory is due to an increase of the contact or due to a breakdown of the approximations in this approach. So far, the literature has not reported on the temperature dependent contact calculated with the renormalisation group theory to account for the criticality. Note that in the weakly interacting limit already at $1/(k_Fa) = -1$ all strong coupling theories for the contact are in qualitative agreement [135]. Since the contact is predicted to decrease with temperature in the superfluid phase it is most likely to find the same decrease for a unitary Fermi superfluid.

The same theories predict concordantly for the homogeneous case that $\mathcal{C}$ decays slower at high temperatures than in the trapped case. This weak temperature dependence is because the contact is not defined for long-range order, see equation 2.7. However, quasi-particles are probed in the low-momentum limit, for which the contact is partly defined. A more precise measurement in the homogeneous case would be necessary to make a statement about the detailed predictions.

In the zero temperature limit, it is possible to calculate the contact density $\zeta$ analytically at unitarity from $\mathcal{C}/(nk_F) \equiv \mathcal{I}/(Nk_F) = 512\zeta/(175\xi^{1/4})$ where $\xi$ is given by the universal parameter $[65,135]$. According to this, the contact in the trapped case scales linearly with the contact density but the decay at higher temperatures is non-trivial. For the theoretical values $\mathcal{I}/(Nk_F) = 3.0 - 3.4, \zeta = 0.92 - 0.82$. From this experiment, the averaged contact is about $\mathcal{I}/(Nk_F) \approx 2.85$ for the coldest
sample at 0.1 $T/T_F$, which yields $\zeta = 0.79(7)$. The ENS result is $\zeta = 0.93(5)$ at 0.03(3) $T/T_F$ \cite{130}. Finite temperatures seem to have an immediate effect, which is consistent with the interaction dependent contact measurements \cite{133,234}, where the values at $1/(k_Fa) = 0$ seem to be systematically lower than expected.

Though the contact can be measured, more detailed theoretical as well experimental analysis is necessary as open questions remain. It is still not clear how the contact evolves from the well defined short-range structure $r \ll (k_F)^{-1}$ to the medium-range limit $r \approx (k_F)^{-1}$ \cite{84}, i.e. the details on the transition behaviour from single-particle to pseudogap pairing and collective excitations.

7.7 Summary

The temperature dependence of Tan’s contact $\mathcal{I}/(N k_F)$ has been measured at unitarity with inelastic two-photon Bragg spectroscopy. The evaluation is based on the dynamic structure factor from traditional centre of mass displacement and energy transfer measurement. Two sets of measurements have been performed to show that both the energy of an immediately released as well as equilibrated cloud leads to the dynamic structure factor. The resulting static structure factor yields the contact from a universal law, see equation\[7.1\]. The values for the contact, $\mathcal{I}/(N k_F)$, agree qualitatively with the theoretical predictions but the precision of the experimental values is not good enough to resolve the differences between the theoretical models. If the experimental accuracy can be improved, it would be interesting to focus on the contact in the region around the critical temperature. From the fact that the contact persists for temperatures higher than the critical temperature $T_C$, it can be concluded that the pair-correlations exist above the superfluid transition temperature. The dichotomy whether or not these relate to pairing near the Fermi surface where pseudogap effects are expected remains an open question. The energy transfer method of Bragg spectroscopy may give improved signal-to-noise in the phonon regime, i.e. with a relative momentum transfer $k/k_F \leq 1$, to investigate thermodynamics of quasi-particles. Access to pair-correlations at a macroscopic level may give insight to the pseudogap regime found in high-$T_C$ superconductors \cite{242}.
Conclusion and Outlook

In conclusion, aspects of a recently proposed quantity, the universal contact, have been investigated for dilute strongly interacting Fermi fluids with customised techniques. The contact parameter is measured with Bragg spectroscopy for different large momenta, \( k \gg k_F \), as well as for different temperatures, in line with theoretical predictions of several theory groups. This contact parameter will find application in future work as it can quantify the temperature-coupling phase diagram and may be used to help understand the nature of unitary Fermi gases.

Summary

The apparatus produces ultracold Fermi gases of \( ^6\text{Li} \) by laser and evaporative cooling in an ultra-high vacuum glass cell. At high magnetic fields around 834 G, the interaction between different spin states can be varied from tightly bound molecules to weakly correlated pairs, using the broad Feshbach resonance.

Universal static structure factor

On resonance, when the s-wave scattering length exceeds the interparticle spacing, the gas is unitarity limited. Universal relations, first derived by Tan, accurately describe the unitarity regime. Particularly in chapter 6 of this work, the universal relation for the static structure factor, \( S(k) \), is verified above and below the Feshbach resonance over a wide range of momenta using Bragg spectroscopy. The measured Bragg spectra quantify the linear response to the density-density correlations and lead to the dynamic and, consequently, the static structure factor. Sum rules enable us to bypass details of some difficult experimental parameters and provide the correct normalisation of the spectra. Since only the relative momentum distribution is important to show the universal law, the Bragg momentum transfer is fixed by the geometry of the Bragg beams and the Fermi momentum is tuned by varying the geometric mean trapping frequencies of the crossed beam dipole trap. In contrast to
previous work, the Bragg beams are set up to transfer momentum along the direction where the trapped condensate is weakly confined. For relative probe momenta of $k/k_F = 3.5 - 9.1$, the universal behaviour is measured at the interaction strengths $1/k_F a = +0.3, 0, -0.2$. At unitarity, the static structure factor depends linearly on the momentum transfer. On the BEC side the predicted downwards curvature is visible while on the BCS side the slight upward bending is confirmed.

**Interaction dependent contact**

The central parameter for the universal relations is the contact parameter, which quantifies in the high-momentum tail of the momentum distribution and links the microscopic details of the atoms to the macroscopic properties of the whole system. The contact parameter measures the degree of correlations depending *inter alia* on the interaction strength. Our previous measurements [80] involved a comprehensive study of the static structure factor of the Bose-Einstein condensate (BEC) to Bardeen-Cooper-Schrieffer (BCS) crossover at low temperatures using Bragg spectroscopy. A smooth transition from molecular to atomic Bragg spectra is observed with a clear signature of pairing at and above unitarity. Pairing is seen to decay as the density is lowered, highlighting the many body nature of pair correlations. By applying sum rules and the universal behaviour of $S(k)$, the interaction dependent static structure factor is translated into the contact. The contact varies monotonically over the BEC-BCS crossover in good agreement with results and theoretical predictions of other groups.

**Temperature dependent contact**

At unitarity the temperature dependence of the contact is measured and described in chapter 7. The contact starts from the zero-temperature value of around 3.3 and decreases smoothly but is measurably greater than zero up to $T \approx T_F$ which is much higher than the critical temperature for superfluidity, $T_C \approx 0.2 T_F$. In principle, the monotonic decay of the contact data confirms the theoretical predictions. Unfortunately, the data is not precise enough to favour a certain theoretical model as different theories predict different values of the contact near $T_C$. The temperature is determined from the empirical fits and compared to the NSR theoretical calculations. Therefore, the measured temperature is model dependent, but in good agreement with the measured equation of state [173]. The measurements are restricted to the trapped case, for which the contact does not show a pronounced peak around the critical temperature region. The large momentum transfer used
here prevents us from observing the pairing gap.

**Outlook**

Universal relations open the way for new studies in strongly interacting Fermi gases. The contact as a new parameter allows pairing mechanisms to be investigated. Amongst all remaining open questions, the most compelling are probably the pairing gap and the contact at the critical temperature. The experimental setup is currently being changed to make contributions to these issues. Improvements of the experimental setup should lead to more accurate Bragg spectra. A new imaging system with a high quantum efficiency camera with kinetics mode and higher resolution have been constructed. The imaging beam is now along the axial direction of the cloud to get symmetric images and reconstructions of the equation of state [237]. Below are some of the directions that may be pursued in future studies. Note that the suggestions are only concerned with the contact and/or Bragg spectroscopy, although the general idea of strongly interacting Fermi gases forms a very rich testbed in general.

**Bragg spectroscopy above \( T_C \)**

In order to investigate the pseudogap pairing in the critical temperature region near \( T_C \), excitation momenta close to the Fermi wave vector are necessary. With momentum resolved Bragg spectroscopy, the momentum dependence of pair correlations can be studied. Therefore, the experiments using several lower probe momenta can search for pairing near the Fermi surface at and above \( T_C \). For a momentum transfer of \( k/k_F = 3 - 1 \), some pairing gap signatures might be apparent. For probe momenta \( k/k_F < 1 \), the compressibility sum rule might lead to a measurement of the speed of sound.

**Measurement of the homogeneous contact**

The theoretical predictions for the temperature dependent contact show different results around the critical temperature. It is not clear if the local maximum of the contact around \( T_C \) is due to a strengthening of fluctuations [31] or a breakdown of theoretical models [135]. The differences of the calculations are more pronounced in the homogeneous case. Spatially resolved Bragg spectroscopy might shed light on this controversy. Bragg scattering allows information to be extracted in the linear response regime, where structure factors are model-independent quantities.
and represent a measure of instantaneous fluctuations. Since these fluctuations are more enhanced in the critical region, the static structure factor should reflect these divergences in the contact values for the critical temperature region. These studies require Bragg spectra to be measured with a higher accuracy and precision.

Measurement of new universal quantities

It may be possible to extract new universal relations concerning the dynamic structure factor with Bragg spectroscopy, such as \( \Delta S_{\sigma\sigma'}(k,\omega,T) \cong \Delta W_{\sigma\sigma'}(k,\omega,T) I \), where the Wilson factor, \( W_{\sigma\sigma'}(k,\omega,T) \), captures the few-body physics in a system with two spin states, \( \sigma \) [132]. Another universal quantity is the contact for three identical bosons (trimer) [243]. Eventually, Bragg spectroscopy may have the potential to scatter trimers, if they are stable within an experimental cycle, as the trimer-frequency could be \( \omega_R/3 \).

Measurement of the contact in different dimensions

Meanwhile, a two-dimensional trap is currently being set up and the higher stability of pairs in this system will allow for highly interesting and frontier experiments on pair correlations and novel phenomena in lower dimensions, probed eventually with Bragg spectroscopy. One candidate would be the spectroscopy of p-wave pairs [244]. Another possibility is again the investigation of the contact in two-dimensional systems [245]. The dimensional confinement stabilises fluctuations but measurements of the contact around a critical temperature are speculative at this stage. The contact of one-dimensional systems is also of interest [246] but not specifically planned in our group.

Determination of the contact from the high-frequency tail

Similar to the rf-spectra one can estimate the contact from the dynamic structure factor since it is proposed that the high-frequency tail of \( S(k,\omega) \) has a universal decay proportional to \( \omega^{7/2} \). By multiplying the spectra at low temperatures with this factor, the high-frequency part approaches a constant value above \( \omega \approx 2 \omega_R \). This offset is then interpreted as the contact. At unitarity this value is about 5\% of the maximum of \( S(k,\omega) \) and therefore very difficult to detect experimentally. However, on the BEC side the contact is larger and it is estimated that around \( 1/k_F a = 1 \) the contact is about 25\% of the maximum of \( S(k,\omega) \).
Appendix A

Offset locking

For imaging at different high magnetic fields it is convenient to change the frequency via the LabView control program while the imaging laser stays locked to a reference laser, despite a large frequency offset. Offset-locking stabilises the beat signal between the imaging and reference laser and allows the imaging frequency to be changed over a wide range with a voltage controlled oscillator \[^{247}\]. The positive slope of the zero crossing provides the error signal for the laser controller \(^{1}\) of a second ECDL (ECDL 2). A schematic is given in figure A.1.

The reference frequency is provided by the cooling laser that beats with the ECDL 2. The grating of the ECDL 2 is pre-aligned to 670.977 nm (D$_2$ line) with a wavemeter or alternatively via fluorescence of a lithium hollow cathode lamp. The better the grating is aligned to a minimum lasing threshold, the narrower the beat signal, and external optical feedback must be well suppressed. The beat signal can be as narrow as 460 kHz (FWHM) and has a typical frequency in the range $f_{\text{beat}} = 700 - 1000$ MHz. The laser beams for the beat signal have a total power of 300 µW and are focused on a custom-made amplifying photodiode. After that the signal passes another electronic amplifier \(^{3}\). In order to observe the beat signal, a directional coupler\(^{3}\) sends a small amount to a spectrum analyser\(^{4}\) or frequency counter. The main signal is electronically mixed\(^{5}\) with a voltage controlled oscillator\(^{6}\), where $f_{\text{VCO}} = 612 - 1200$ MHz. The frequency difference $\Delta f = |f_{\text{beat}} - f_{\text{VCO}}|$ is amplified to a certain power level with an amplifier\(^{7}\) and attenuator\(^{8}\) before being split equally.

\[^{1}\]MOGlabs Pty Ltd, model DLC-202
\[^{2}\]\textit{Minicircuits: ZX60-3018G-S}
\[^{3}\]\textit{Minicircuits: ZX05-5-S}
\[^{4}\]\textit{Rohde & Schwarz}
\[^{5}\]\textit{Minicircuits: ZX30-17-5-S}
\[^{6}\]\textit{Minicircuits: ZX95-1200W-S}
\[^{7}\]\textit{Minicircuits: ZX60-3018G-S}
\[^{8}\]\textit{Minicircuits: ZX60-3018G-S}
OFFSET LOCKING

with a splitter\(^9\). Both signals travel along separate cables before being recombined with a phase detector\(^10\) where the delay line of 1.5 m introduces a delay time, \(\tau\), and phase shift \(\phi = 2\pi \Delta f \tau\). For the delay length of 1.5 m, \(\tau \approx 7.5\) ns. A low pass filter\(^11\) removes the sum frequency above 50 MHz. A load of 500 \(\Omega\) and 1 \(\mu\)F filters noise at \(\sim 2\) kHz. The error signal as a function of the beat frequencies is a series of cosine fringes, with a period that is set by the length of the delay line. The positive slope of the main zero crossing is used as an error signal which directly enters the laser controller box.

This locking can be made very stable if the gain is large enough to provide a minimum error signal amplitude of 250 mV. The beat lasers do not come out of lock unless the main ECDL unlocks. The only instabilities are seen when the VCO voltage is driven close to 1 GHz and the amplifying photodiode is bandwidth limited.

The voltage range is given by LabView, 0 – 10 V, which covers \(f_{\text{beat}} \approx 780 – 1100\) MHz. These frequencies provide resonant light for absorption imaging over the magnetic field range of 700 – 1000 G in the lowest spin state and 650 – 950 G in the second lowest spin state, respectively. The frequency can be shifted further with AOMs to be resonant with magnetic fields up to 1200 G.

Since the second ECDL 2 only provides 12 mW, injection seeding of another diode laser (imaging slave) is necessary. From there, light for the Bragg beams is provided as well as for both the top and side imaging. Originally, the possibility for zero-field imaging was included in the design by injecting the slave light into the imaging slave, see figure\(^4.3\).

\(^9\)Minicircuits: ZFRSC-2050
\(^10\)Minicircuits: ZRPD-1
\(^11\)Minicircuits: PLP-50
Figure A.1: Schematic of the components in the offset locking circuit.
Bibliography


List of publications

During my time as a PhD student, I was co-author in the following papers:

*Temperature Dependence of the Universal Contact Parameter in a Unitary Fermi Gas*
E.D. Kuhnle, S. Hoinka, P. Dyke, H. Hu and C.J. Vale

*Studies of the universal contact in a strongly interacting Fermi gas using Bragg spectroscopy*
E.D. Kuhnle, S. Hoinka, H. Hu, P. Dyke, P. Hannaford and C.J. Vale

*Universal behaviour of Pair Correlations in a Strongly Interacting Fermi Gas*
E.D. Kuhnle, H. Hu, X.-J. Liu, P. Dyke, M. Mark, P.D. Drummond, P. Hannaford and C.J. Vale

*Bragg Spectroscopy of a Strongly Interacting Fermi Gas*
G. Veeravalli, E.D. Kuhnle, P. Dyke and C.J. Vale

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